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MATHEMATICAL MODELS OF ECOLOGICAL POLLUTION PROCESSES

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Summary

In this work two mathematical models of sea pollution are described. The first model is deterministic and is characterized by ordinary linear differential equations. The second model is stochastic. Under various assumptions the formulas of distribution and density of pollution substance are given. Models are numerically realized by specific examples. The results of computations show that suggested methods are easy to implement.

Keywords*: Pollution, model, ordinary differential equation, stochastic process, distribution, concentration*

Introduction

The ocean and sea pollution by the substances of different kind, especially by oil products has reached a dangerous level. With the increasing number of oil shipping vessels, there is now a greater chance that oil spill accidents will occur during the transportation of crude oils and oil products, placing the marine environment at risk. Crude oils and refined oil products are highly complex mixtures, and the correlation of spilled oils and suspected sources is a difficult task due to the processes like weathering and oil refining. For example, weathering (the exposure of crude oils to physical, chemical, and biological processes in the environment) changes the composition and distribution of petroleum hydrocarbons which compose about 98% of crude oil. As is known, light fractions evaporate during a certain period of time. Most toxic part, at most 0.01% , dissolves in water. The remaining oil composes high-polymeric fraction (tar, pyrobitumen), of which some quantity sinks, some part floats on the surface and significant mass composes a swimming body in the depth of water (see [1], [2]).

First step to avoid ecological cataclysms is to take preventive measures. At the same time it is important to perform rehabilitation works after the accident in due time. In order to do this, it is necessary to make the description of the situations that could arise at the beginning and during the rehabilitation work. Our aim is to describe mathematically the process of spreading of pollution in different situations. Two methods of solving of this problem are offered and therefore two different models are created. Both models are dynamic. The first of them is a mathematical model of expansion of pollution in the depth of water. The appropriate method is based on the hydrodynamic laws and is given by the system of ordinary differential equations. The process of solution expansion, or the process of concentration equilibrium, is motivated by heat diffusion and molecular interaction. The impact of external factors such as water flow, winds etc. are ignored in the first model and are considered in the second one. The appropriate method is based on the theory of stochastic processes and gives the density of distribution of the pollution mass for arbitrary time according to random meteorological factors.

Both models are numerically realized in MATLAB system by specific examples.

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1. Dynamic deterministic model

The following model describes the process of pollution when the pollution substance is soluble and composes a swimming body. We assume that it's initial shape in the depths of water is a cylinder. Let the radius of the cylinder be R and the height be H. Around this cylinder consider concentric cylindrical shells by step r, numerated as $1,2,\ldots,N$. By the Fick's law (see [3]), mass M of the substance passing through the surrounding thickness Δr in a unit time is calculated as follows: $M = D\cdot\frac{\Delta c}{\Delta r}\cdot S,$ where D is the coefficient of diffusion of the substance; Δc is the difference of concentrations, S is the area of boundary between the shells. The quantity $\frac{\Delta c}{\Delta r}$ is called the gradient of concentration.

Let the amount of substance be $M_k(t)$ in the k-th shell at time t. During time dt, in k-th shell, the amount of substance will change as $dM_k(t)$:

$$dM_k(t) = \frac{M'_{k-1}(t) - M'_k(t)}{\Delta r} S_{k-1} D dt - \frac{M'_k(t) - M'_{k+1}(t)}{\Delta r} S_k D dt, \qquad (1.1)$$

where S_k is the area of the boundary between k-th and $k+1$-th shells; $M'_k(t) = \frac{M_k(t)}{V_k}$ is the concentration of the substance in the k-th shell .

Hereafter we shall write r instead of Δr. Formula (1.1) is suitable for shells $3,4,\ldots,N-1$. Passing from shell 1 to shell 2, we take $\frac{R}{2}+\frac{r}{2}$ instead of Δr. The shell $N+1$ (exterior area) is infinite, and the concentration is constant (is equal 0). So we have:

$$\begin{cases}
\frac{dM_1(t)}{dt} = -\frac{D}{R/2 + r/2}\cdot 2\pi RH\left(\frac{M_2(t)}{((R+r)^2 - R^2)H} - \frac{M_1(t)}{\pi R^2 H}\right) \\
\frac{dM_2(t)}{dt} = \frac{4DR}{(R+r)}\left(\frac{M_1(t)}{R^2} - \frac{M_2(t)}{r(2R+r)}\right) + \frac{2D(R+r)}{r^2}\left(\frac{M_3(t)}{2R+3r} - \frac{M_2(t)}{2R+r}\right) \\
\frac{dM_{k+1}(t)}{dt} = \frac{2D}{r^2}\left(\frac{M_{k+2}(t)(R+kr)}{2R+(2k+1)r} + \frac{M_k(t)(R+(k-1)r)}{2R+(2k-3)r} - M_{k+1}(t)\right), \qquad (k = 2,3,\ldots N-2) \\
\frac{dM_N(t)}{dt} = \frac{2D(R+(N-2)r)}{r^2}\left(\frac{M_{N-1}(t)}{2R+(2N-5)r} - \frac{M_N(t)}{2R+(2N-3)r}\right) - \frac{2D}{r^2}\cdot\frac{M_N(t)(R+(N-1)r)}{2R+(2N-3)r} \\
\frac{dM_{N+1}(t)}{dt} = \frac{2D}{r^2}\cdot\frac{M_N(t)(R+(N-1)r)}{2R+(2N-3)r}
\end{cases}$$

Finally we obtain the following system of ordinary differential equations:

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$$\begin{cases} \dfrac{dM_1(t)}{dt} = -\dfrac{4D}{(R+r)R} M_1(t) + \dfrac{4DR}{r(R+r)(2R+r)} M_2(t) \\ \dfrac{dM_2(t)}{dt} = \dfrac{4D}{(R+r)R} M_1(t) - \dfrac{2D(R^2+r^2+4Rr)}{r^2(R+r)(2R+r)} M_2(t) + \dfrac{2D(R+r)}{r^2(2R+3r)} M_3(t) \\ \dfrac{dM_{k+1}(t)}{dt} = \dfrac{2D(R+(k-1)\,r)}{r^2(2R+(2k-3)\,r)} M_k(t) - \dfrac{2D}{r^2} M_{k+1}(t) + \\ \qquad + \dfrac{2D(R+k\,r)}{r^2(2R+(2k+1)r)} M_{k+2}(t), \qquad (k = 2,3,\dots N-2), \\ \dfrac{dM_N(t)}{dt} = \dfrac{2D(R+(N-2)\,r)}{r^2(2R+(2N-5)\,r)} M_{N-1}(t) - \dfrac{2D}{r^2} M_N(t) \\ \dfrac{dM_{N+1}(t)}{dt} = \dfrac{2D(R+(N-1)\,r)}{r^2(2R+(2N-3)\,r)} M_N(t) \end{cases}$$

Naturally the initial conditions are the following: $M_1(0) = m, \quad M_k(0) = 0 \quad (k = 2,3,\dots,N+1)$.

Note. A similar system can be obtained for the pollution of some other kind, like the pollution with spherical or hemispherical shells. There are no principal obstacles in this respect. This method can be also applied in case of superficial pollution (pollution by oil for example). This is a problem on the plain, and it can be described even simpler, but the difficulty of determining of the coefficient of fluidity arises.

Example. Above model was numerically implemented by means of MATLAB (function **ode 45)** . Computations were performed in SI system for different values of parameters of the process. Table1.1 and Fig.1.1 indicate the distribution of mass in the shells ($M\times 10^{-4}$) at certain moments of time *t* (sec$\times 10^{-4}$), $D = 0.006$, $R = 10m$, $r = 5m$, $H = 5m$, $N = 7$, $M_1(0) = 10000kg$.

Table 1.1. The distribution of mass in the shells (M×10^{-4})

№	*t* (sec.) (×10^{-4})	$M_1(t)$	$M_2(t)$	$M_3(t)$	$M_4(t)$	$M_5(t)$	$M_6(t)$	$M_7(t)$	$M_8(t)$
1	0.0000	1.0000	0	0	0	0	0	0	0
2	0.0001	0.9998	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.0010	0.9984	0.0016	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.1221	0.8340	0.1405	0.0228	0.0024	0.0002	0.0000	0.0000	0.0000
5	0.5507	0.5123	0.2613	0.1438	0.0581	0.0184	0.0048	0.0009	0.0005
6	1.0472	0.3430	0.2428	0.1918	0.1194	0.0612	0.0259	0.0068	0.0091
7	2.0941	0.1938	0.1765	0.1808	0.1547	0.1130	0.0675	0.0224	0.0914
8	3.0525	0.1356	0.1354	0.1512	0.1433	0.1164	0.0761	0.0267	0.2154
9	4.0453	0.1017	0.1061	0.1233	0.1221	0.1035	0.0701	0.0250	0.3482
10	5.0000	0.0801	0.0852	0.1008	0.1017	0.0877	0.0602	0.0217	0.4626

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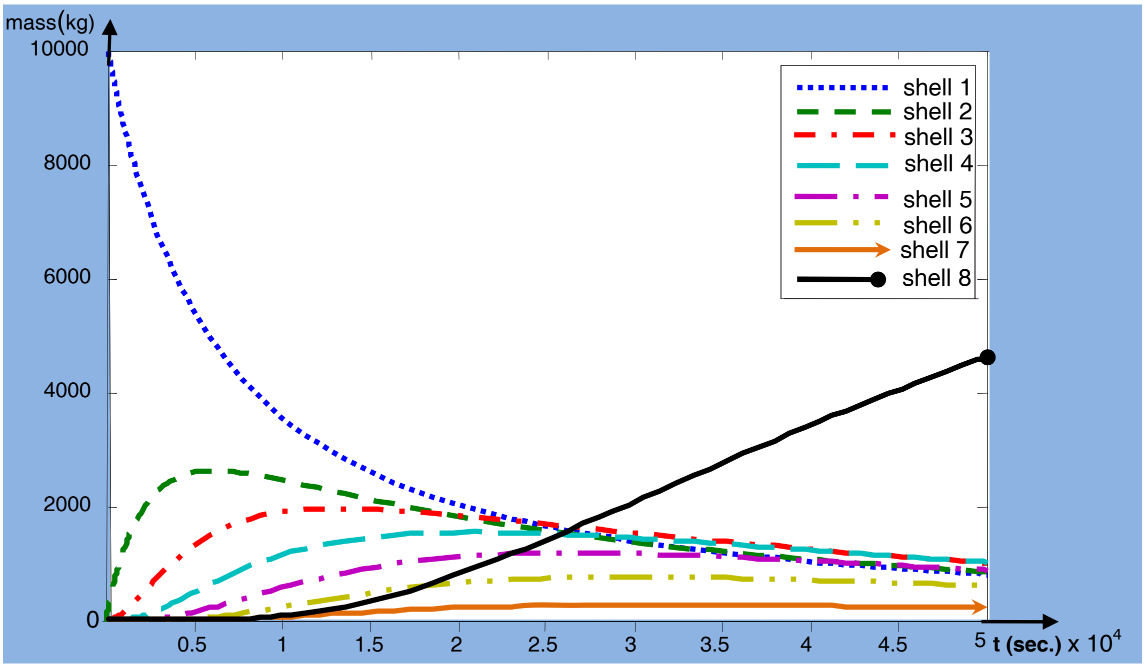

Fig. 1.1. The distribution of mass in the

The concentration of mass in the shells (kg/m^3) in the same time-intervals as above are given in Table 1.2 and Fig.1.2.

Table 1.2. The concentration of mass in the shells (kg/m^3)

№	*t* (sec.) ($\times 10^{-4}$)	shell 1	shell 2	shell 3	shell 4	shell 5	shell 6	shell 7
1	0.0000	1.5915	0	0	0	0	0	0
2	0.0001	1.5912	0.0003	0	0	0	0	0
3	0.0010	1.5891	0.0020	0	0	0	0	0
4	0.1221	1.3274	0.1789	0.0207	0.0017	0.0001	0	0
5	0.5507	0.8154	0.3327	0.1307	0.0411	0.0107	0.0023	0.0004
6	1.0472	0.5459	0.5459	0.1744	0.0845	0.0354	0.0127	0.0029
7	2.0941	0.3084	0.2249	0.1644	0.1094	0.0654	0.0330	0.0095
8	3.0525	0.2159	0.1723	0.1375	0.1014	0.0673	0.0373	0.0113
9	4.0453	0.1618	0.1350	0.1121	0.0864	0.0539	0.0343	0.0106
10	5.0000	0.1275	0.1085	0.0917	0.0719	0.0508	0.0295	0.0092

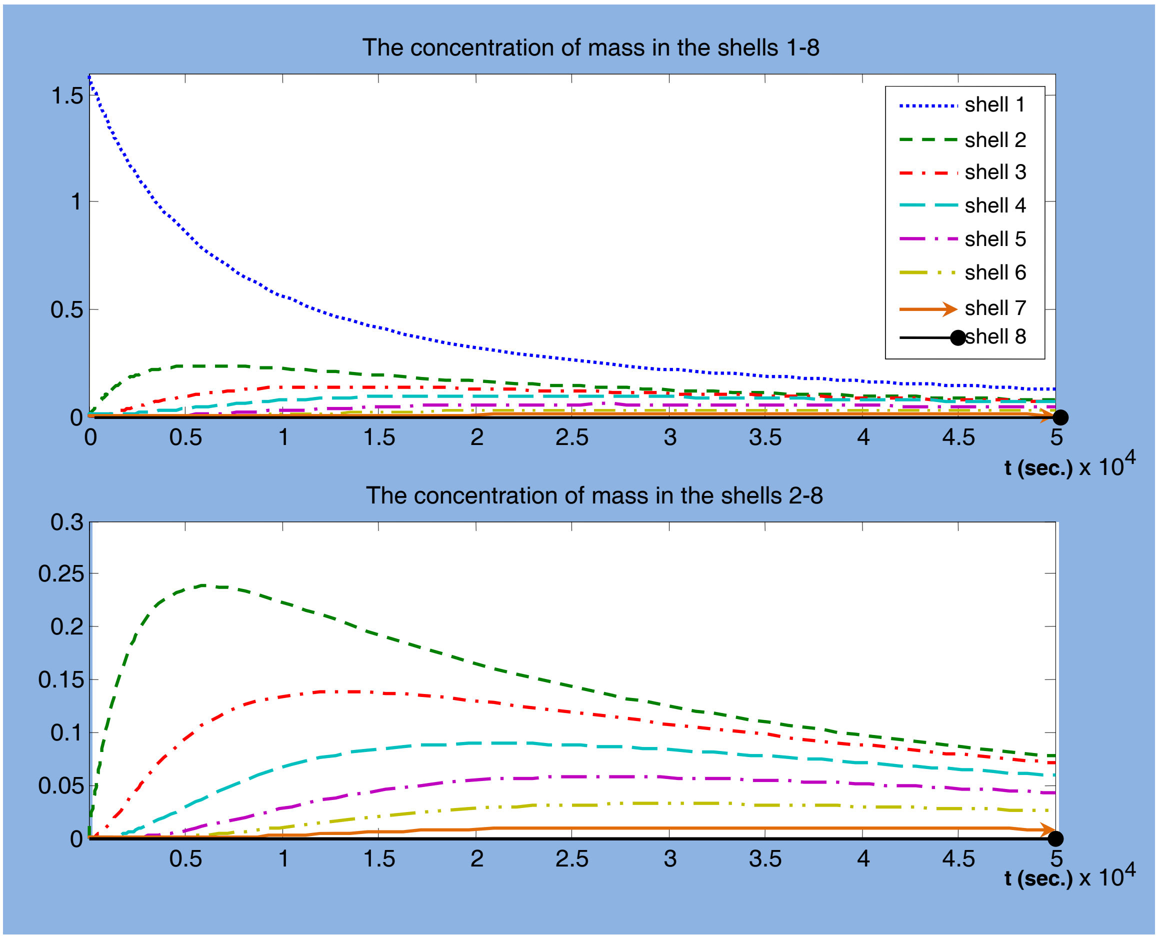

Fig. 1.2. The concentration of mass in the shells

2. Dynamic stochastic model

On the surface of water oil spread depends on diffusive and meteorological factors, where the later means wind with specified speed and direction. Both speed and direction vary through time intervals, thus they are stochastic values. Therefore process of pollution by oil is a stochastic process, namely, linear stochastic motion on the plane. In this model we ignore diffusive factor.

Let us state the problem as follows: let $\xi_0(x_0, y_0)$ be a random point on the plane (x, y) with the density $f_0(x, y)$ of a known distribution function. Without loss of generality we assume, that the amount of oil is equal to 1. Denote

$$\xi_0 = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}; \quad \xi_t = t\,v \begin{pmatrix} \cos\psi \\ \sin\psi \end{pmatrix}, \; t \ge 0, \psi \in [0, 2\pi], v \in [v_{1,} v_2],$$

where ψ and v are stochastic variables, direction and speed of the wind respectively. Linear motion of this point can be described by means of the vector

$$Z(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \xi_0 + \xi_t .$$

Let f_v and f_ψ be densities of stochastically independent variables v and ψ, and let φ denote characteristic function of a stochastic variable with appropriate index. Using standard method (see [4]), first we find the characteristic function of vector $Z(t)$ and then elaborate the density:

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$$\varphi(s_1,s_2)=Ee^{i(s_1x(t)+s_2y(t))}=Ee^{i(s_1x_0+s_2y_0)}\cdot Ee^{itv(s_1\cos\psi+s_2\sin\psi)}=$$

$$=\varphi_0(s_1,s_2)\int_{v_1}^{v_2}\int_0^{2\pi}e^{itv(s_1\cos\psi+s_2\sin\psi)}f_v(v)f_\psi(\psi)dvd\psi,$$

$$f_t(x,y)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(s_1x+s_2y)}\cdot\varphi(s_1,s_2)ds_1ds_2=$$

$$=\int_{v_1}^{v_2}\int_0^{2\pi}f_v(v)f_\psi(\psi)dvd\psi\cdot\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\varphi_0(s_1,s_2)\cdot e^{-i[s_1(x-tv\cos\psi)+s_2(y-tv\sin\psi)]}ds_1ds_2\ .$$

Hence

$$f_t(x,y)=\int_{v_1}^{v_2}\int_0^{2\pi}f_0(x-vt\cos\psi,y-vt\sin\psi)f_v(v)f_\psi(\psi)dvd\psi\ . \tag{2.1}$$

If $\psi=\psi_0$ is constant, then

$$f_t(x,y)=\int_{v_1}^{v_2}f_0(x-vt\cos\psi_0,y-vt\sin\psi_0)f_v(v)dv,$$

If besides $v=v_0$ is constant too, then

$$f_t(x,y)=f_0(x-v_0t\cos\psi_0,y-v_0t\sin\psi_0)\ .$$

Let's consider the case, when ψ is uniformly distributed in $[0,2\pi]$ and f_0 is a symmetric function. We have

$$\varphi_\xi(s_1,s_2)=Ee^{itv(s_1\cos\psi+s_2\sin\psi)}=\frac{1}{2\pi}\int_{v_1}^{v_2}\int_0^{2\pi}e^{itv(s_1\cos\psi+s_2\sin\psi)}f_v(v)dvd\psi=\int_{v_1}^{v_2}I_0\left(\sqrt{s_1^2+s_2^2}\cdot tv\right)\cdot f_v(v)dv,$$

where $I_0(u)=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{iu\sin\theta}d\theta$ is Bessel function of order 0 (see [5]).

$$f_t(x,y)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(xs_1+ys_2)}\varphi_0(s_1,s_2)\varphi_\xi(s_1,s_2)ds_1ds_2=$$

$$=\frac{1}{(2\pi)^2}\int_{v_1}^{v_2}f_v(v)dv\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-i(xs_1+ys_2)}\cdot\varphi_0\left(\sqrt{s_1^2+s_2^2}\right)\cdot I_0\left(tv\sqrt{s_1^2+s_2^2}\right)ds_1ds_2.$$

Rewriting this formula in polar coordinates, we get

$$f_t(x,y)=\frac{1}{\sqrt{2\pi}}\int_{v_1}^{v_2}f_v(v)dv\int_0^{\infty}\rho\cdot\varphi_0(\rho)\cdot I_0(vt\rho)\cdot I_0\left(\rho\sqrt{x^2+y^2}\right)d\rho. \tag{2.2}$$

Now consider the following cases, important in practice:

1) Let ψ be distributed uniformly in $[0,2\pi]$ and ξ_0 be normally distributed:

$$f_0(x,y)=\frac{1}{2\pi\sigma^2}e^{-\frac{x^2+y^2}{2\sigma^2}},\qquad \varphi_0(s_1,s_2)=e^{-\frac{\sigma^2}{2}\left(s_1^2+s_2^2\right)}.$$

By virtue of (2.2)

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$$f_t(x,y)=\frac{1}{\pi\sigma^2}e^{-\frac{x^2+y^2}{2\sigma^2}}\int_{v_1}^{v_2}e^{-\frac{v^2t^2}{2\sigma^2}}\cdot I_0\left(\frac{vt\sqrt{x^2+y^2}}{\sigma^2}\right)f_v(v)dv\ . \tag{2.3}$$

2) Let ψ and ξ_0 be uniformly distributed in $[0,2\pi]$ and in the circle with radius r respectively. We have

$$\varphi_0(s_1,s_2)=\frac{2}{r^2}\int_0^r \lambda I_0(\lambda\sqrt{s_1^2+s_2^2})d\lambda=\frac{2I_1(r\sqrt{s_1^2+s_2^2}\ )}{r\sqrt{s_1^2+s_2^2}},$$
$$f_t(x,y)=\frac{1}{\pi r}\int_{v_1}^{v_2}f_v(v)dv\int_0^\infty I_1(r\rho)\cdot I_0(vt\rho)\cdot I_0(\rho\sqrt{x^2+y^2})d\rho. \tag{2.4}$$

3) Let ψ and v be uniformly distributed in the intervals $[\psi_1,\psi_2]$ and $[v_1,v_2]$ respectively, ξ_0 be normally distributed. By virtue of (2.1) we have

$$f_t(x,y)=\frac{1}{2\pi\sigma^2\Delta v\Delta\psi}\int_{v_1}^{v_2}\int_{\psi_1}^{\psi_2}e^{-\frac{(x-vt\cos\psi)^2+(y-vt\sin\psi)^2}{2\sigma^2}}dvd\psi\ . \tag{2.5}$$

Using polar coordinates $x=R\cos\theta,\ \ y=R\sin\theta$, we get

$$f_t(R,\theta)=\frac{e^{-\frac{R^2}{2\sigma^2}}}{2\pi\sigma^2\Delta v\Delta\psi}\int_{v_1}^{v_2}\int_{\psi_1}^{\psi_2}e^{-\frac{t^2v^2}{2\sigma^2}}\cdot e^{-\frac{Rtv\cos(\psi-\theta)}{\sigma^2}}dvd\psi. \tag{2.6}$$

4) Let ψ and v be the same as in previous case and ξ_0 be uniformly distributed in the circle with radius r. Then, using (2.1), we have

$$f_t(R,\theta)=\frac{1}{\pi r^2\Delta v\Delta\psi}\int_{v_1}^{v_2}\int_{\psi_1}^{\psi_2}dvd\psi\cdot\begin{cases}1,\ if\ R^2+v^2t^2+2vtR\cos(\psi-\theta)\le r^2,\\ 0,\ if\ R^2+v^2t^2+2vtR\cos(\psi-\theta)>r^2.\end{cases} \tag{2.7}$$

Two last cases are most interesting in practice. Let's see where the density function attains its maximum. It is easy to see, that for any R the maximum with respect to θ is attained when $\theta=\frac{\psi_1+\psi_2}{2}$. If $\Delta\psi$ is sufficiently small ($\Delta\psi<<2$), then the maximum with respect to R is attained when $R=\frac{v_1+v_2}{2}t.$

Note that all the expressions above are valid and simpler when v or ψ, or both together are constants.

Example. Take $M=10000kg$. Let the centre of the pollution be the origin of coordinate system, the initial distribution be normal with parameter $\sigma=10/3$, ψ and v be distributed uniformly in the intervals $[0,2\pi]$ and $[1,2]$ respectively. This case corresponds to (2.5).

The distribution of mass in the concentric shells $(S_k,k=1,\dots 6)$, surrounding the circle of radius $R=10m,(S_0)$ with step $r=5m$ r = 5m at certain moments of time $t(\sec\times10^{-4})$ is given by the Table 2.1 and in Fig. 2.1.The model was numerically implemented by means of MATLAB (function **dblquad**).

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Table 2.1. The distribution of mass in the shells ($M\times10^{-4}$)

S_k / t (sec.)	S_0	S_1	S_2	S_3	S_4	S_5	S_6	out of shells
0	1	0	0	0	0	0	0	0
5	0.82853	0.15786	0.0134	0.00016	0.00002	0	0	0.00003
10	0.46874	0.25804	0.19893	0.06841	0.00566	0.0001	0	0.00016
15	0.31252	0.17458	0.16997	0.16598	0.12918	0.04395	0.00358	0.00024
20	0.23439	0.13098	0.12746	0.12643	0.12585	0.12307	0.09654	0.03528
25	0.18755	0.10473	0.102	0.10118	0.10072	0.10015	0.09795	0.20572
30	0.15629	0.0873	0.08501	0.08424	0.08393	0.08347	0.08131	0.33845
35	0.13397	0.07486	0.07281	0.07221	0.07198	0.07186	0.0693	0.43301
40	0.11718	0.06549	0.06379	0.06319	0.06292	0.06283	0.0609	0.5037
45	0.10417	0.05821	0.0567	0.05622	0.05588	0.05585	0.05427	0.5587
50	0.09376	0.05247	0.05099	0.05053	0.05037	0.05012	0.04878	0.60298

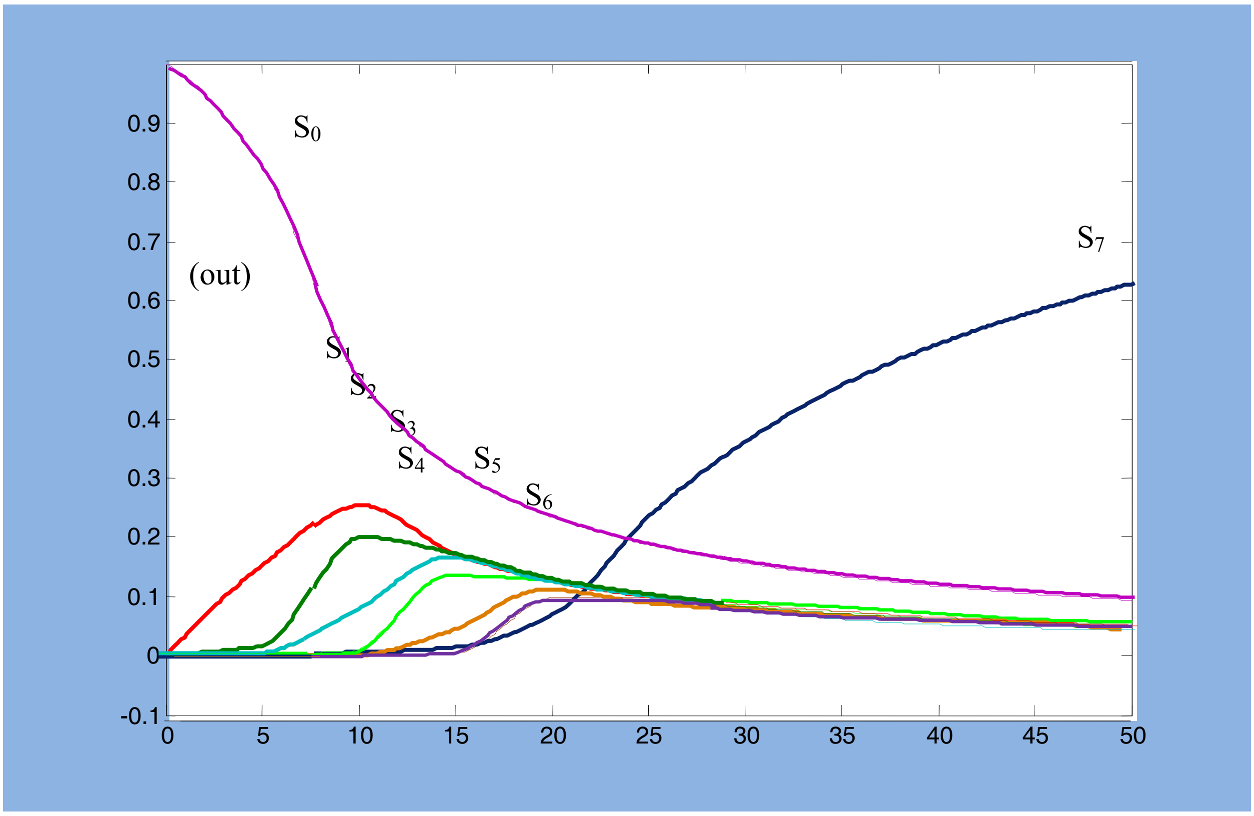

Fig. 2.1. The distribution of mass in the shells

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Finally note that both models can be applied to the coast pollution process, but we don't discuss it here, because it is a partial case.

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