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Modelling and assessment of ^{137}Cs and of heavy metals impact on marine ecosystems

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Abstract

Modelling is an important and useful tool for predicting the behaviour and the impact of pollutants on the local ecosystem parameters. More specifically, simulation and computational methods can be used for estimating the environmental impact on marine ecosystems.

The paper presents a three-dimensional general deterministic model, developed to simulate and study the time-dependent behaviour of ^{137}Cs in marine environments. The model capabilities are demonstrated by applying it at the northeast region of the island of Lemnos, in the NE Aegean Sea, Greece. Full Navier-Stokes equations for transient, three-dimensional turbulent flow, heat and mass transfer are solved numerically. The solution method is the finite-volume method and the general CFD code in which the present model is implemented is Phoenixics.

Keyword : Modelling, CFD, turbulence, radionuclides, impact assessment, doses, finite-volume method.

1. Introduction

The present paper describes the use of environmental modelling for dose- effects estimations and impact assessment of (mainly) ^{137}Cs on marine organisms of the greek marine ecosystems. Furthermore, practice of the behaviour of selected heavy metals based on their concentrations in sea water are included in this study. The impact assessment for a selected area near the north-east coast of Lemnos island (in the North Aegean sea in Greece) is carried out based on gamma spectrometry (for the

winter (01/12/2005) and summer (23/06/2006) measurements together with published data of radionuclide concentrations in sea water and sediment by the NCSR “Demokritos”, Institute of Nuclear Technology-Radiation Protection, Environmental Radioactivity Laboratory.

The North Aegean Sea is exposed to the influence of Black Sea discharges Chernobyl contamination mainly during the purification processes of the Black Sea through Dardanelles Straits.

2. The physical issue

A three dimensional general deterministic model developed to simulate the time-dependent behaviour of ^{137}Cs in the Aegean Sea. The model simulates the hydrodynamic dispersion and the turbulence diffusion (sea surface, water column) of ^{137}Cs (activity concentrations Bq m^{-3}). Use of experimental data in a limited depth of the water column during winter and summer time period. Estimation of dose rates. Estimation of possible effects. The pollutants, are subjected to various weathering and turbulent processes of the hydrodynamic field considering a NW and a NE wind of 8m/s and a time period of one month. For estimations and modeling of the dose rates for the radiological impact on marine organisms, a region around the surface measurement station is used taking into account the curves of equal concentrations of ^{137}Cs (at the surface and throughout the water column). Also, estimations of the behaviour of selected heavy metals based on their concentrations in sea water are included in this study [1-7].

3. The mathematical formulation

The flow problem is considered to be three-dimensional in space, transient in time, and turbulent. The basic equations are the Full Navier-Stokes equations for transient, three-dimensional turbulent flow, heat and mass transfer. The model utilizes an Eulerian flow approach [1-2,4,8-9].

All differential equations can be cast in the following general form:

$$\frac{\partial}{\partial t}(r_i \rho_i \phi_i) + \text{div}(r_i \vec{V}_i \rho_i \phi_i - \Gamma_{\phi_i} \text{grad}(r_i \phi_i)) = S_{\phi_i} \quad (1)$$

where ϕ_i is the dependent variable is the dependent variable for phase i (i.e. r_i, u_i, v_i, w_i, h_i and 1 for continuity equation).

The surface wind may be given by the following simple expression:

$$U_{sa} = 0.01 \exp(1.03 + 0.14) U_\alpha \quad (2)$$

where U_{sa} is the wind speed measured above the mean sea level (usually 10 m).

The calculation formulae for the external dose rates received per habitat of the marine organisms of the area are as follows [1-2,4,8-9]:

Sea water

$$D = 9.58 \times 10^{-14} A_s (137Cs) \text{ Gy/s} \quad (3)$$

where : $A_s(137Cs)$ is the Activity Concentration of 137Cs in sea water (Bq/l)

Sediment – sea water intermediate phase

$$D = 4.79 \times 10^{-14} [A_s(A)137Cs + A_s(B)137Cs] \text{ Gy/s} \quad (4)$$

where $A_s(A)137Cs$ is the Activity Concentration of 137Cs in seawater (Bq/l) and

$A_s(B)137Cs$ is the Activity Concentration of 137Cs in sediment (Bq/kg)

Sediment

$$D = 9.58 \times 10^{-14} A_s(137Cs) \text{ Gy/s} \quad (5)$$

where : $A_s(137Cs)$ is the Activity Concentration of 137Cs in sediment (Bq/kg)

The dose rates in the marine ecosystem of the area of interest ($\mu\text{Gy h}^{-1}$) are as follows [10-12]:

a) 137Cs gamma-radiation- summer

Seawater–air intermediate phase	Seawater
$0.002 \cdot 10^{-4} - 0.004$	$0.015 \cdot 10^{-4} - 0.002$

b) 137Cs gamma-radiation -winter

Seawater–air intermediate phase	Seawater (Depth 0m)	Seawater (Depth 20m)
$0.008 \cdot 10^{-4}$	$0.025 \cdot 10^{-4}$	$0.012 \cdot 10^{-4}$

c) Natural gamma-radiation in the marine ecosystem in the Greek marine environment.

Seawater–air intermediate phase	Seawater
0.002• 10 ⁻⁴ – 0.004	0.015• 10 ⁻⁴ – 0.002

The calculation formula for the exposure of swimmers and divers is as follows [13]:

$$D=0.576CE \quad (6)$$

where :D is the dose rate in water, C is the radionuclide concentration including the contribution from the suspended particulate material,E is the photon energy per decay.

For the area of interest the results are as follows:

$$D(\text{summer})=0.005\mu\text{Gy/h}$$

$$D(\text{winter})=0.003\mu\text{Gy/h}$$

The calculation formula for the internal dose rates estimations to human due to consumption of fish is as follows:

$$D = 0.5 \cdot \sum_{j=1}^m DCF_j \cdot CF_j \sum_{i=1}^n A_i \int_0^T C_{ij}(t) dt, \quad (7)$$

where [0, T] is the time interval (y); DCF_j (Sv/Bq) is the dose conversion factor for radionuclide j ($j = 1, 2, \dots, m$); CF_j (m³/t) is the concentration factor for radionuclide j in fish; A_i (t/y) is catch of fish in the model compartment i ; ($i = 1, 2, \dots, n$); C_{ij} (Bq/m³) is the concentration of radionuclide j in filtered seawater in model compartment i ; and 0.5 is the edible fraction for fish.

For the pelagic fish of the area of interest the results are as follows:

Pelagic fish

$$\text{a) (Winter)} \quad = 0.010\text{mSv}$$

$$\text{b) (Summer)} \quad = 0.017\text{mSv}$$

The calculation formula for heavy metals concentration is as follows [14-15]:

$$C_f = C_{tc}/C_e \quad (8)$$

where: C_f , concentration factor, C_{tc} , metal concentration in a trophic component
 C_e , metal concentration of abiotic environment

The finite-volume method was implemented for the numerical solution of the above system of equations in sections, together with the auxiliary equations. The differential equations are integrated over control volumes and the final general form of the discretized equations is as follows [16]:

$$a_p \phi_p = a_N \phi_N + a_S \phi_S + a_E \phi_E + a_W \phi_W + a_H \phi_H + a_L \phi_L + a_T \phi_T + \text{source terms} \quad (9)$$

where the coefficients a_i represent effects of convection and diffusion added together (in a form that depends on the difference scheme used), for finite-difference node P and all neighbouring nodes (N,S,E,W,H,L), and T for the old time -step:

The central coefficient a_p is as follows:

$$a_p = a_N + a_S + a_E + a_W + a_H + a_L + a_T \quad (10)$$

i.e. it is the sum of all neighbours to p .

The algorithm used for the solution of the equations is IPSA (Interphase Slip Algorithm). The above model is implemented in the CFD code PHOENICS which utilizes IPSA to solve the Navier-Stokes equations for transient, two phase, three-dimensional turbulent flow.

A time step of 750s proved to be adequate for time-step independent solutions while using 100 iterations per time step. Grid-independency runs were also performed to obtain grid-independent results, for both test cases considered.

There exist several turbulence models in literature, the most widely used being the $k\sim\epsilon$ model, that solves two differential equations, one for the turbulence kinetic energy, k , and the second for the energy dissipation rate ϵ . Preliminary computer runs by the authors using various other models, revealed that the more recent “Renormalization group $k\sim\epsilon$ model” (RNG- $k\sim\epsilon$ model) [17], may be a better choice and as such it was adopted for the present study.

The full set of equations of the above model is as follows:

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right\} + P_k - \varepsilon \quad (11)$$

$$\frac{\partial \varepsilon}{\partial t} + u_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left(\nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right\} + (c_{\varepsilon 1} P_k + c_{\varepsilon 2} G) \frac{\varepsilon}{\kappa} - \frac{c_\mu \eta^3 (1 - \eta / \eta_0)}{1 + \beta_1 \eta^3} \frac{\varepsilon^2}{k} \quad (12)$$

where:

$$\nu_t = c_\mu \frac{k^2}{\varepsilon}, \quad P_k = \nu_t \frac{\partial u_i}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad \eta = \frac{S k}{\varepsilon}, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right),$$

$$G_b = - \frac{g}{T_0} \frac{\nu_t}{\sigma_T} \frac{\partial T}{\partial y}, \quad S = (S_{ij} S_{ij})^{1/2}$$

where T is temperature and σ_T the Prandtl number.

An optimization of the constants involved for well-known test cases leads to the following values:

c_μ	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$	$c_{\varepsilon 3}$
0.0845	1.42	1.68	$\tanh \mu / \nu $

σ_k	σ_ε	n_0	β_1
0.719	0.719	4.38	0.012

Finally, the effective viscosity is as follows:

$$\mu_{eff} = \mu + \mu_t \quad (13)$$

where μ the molecular viscosity and $\mu_t = \frac{c_\mu \rho k^2}{\varepsilon}$.

The runs were performed on a Silicon Graphics Origin 200 machine (4 CPU R 10000). A typical run using a 120x95x16 grid for 20 time steps (15000 secs real time) requires 12 hrs CPU time on the above machine using UNIX and 5 hrs using LINUX on a Pentium IV, 2.4 GHz, 512 MB.

4. Results and Discussions

The model capabilities are demonstrated by applying it to the southeast coast of the island of Lemnos (Fig.1), in the Aegean Sea, considering a surface of $11.5 \times 9.0 \text{ km}^2$ and a maximum depth of 70m.

Fig.1 The map of the region

Fig. 2 presents the model results based on the summer data of ^{137}Cs activity concentrations.

Fig.2 The model vertical profile for ^{137}Cs (summer)

Fig. 3 presents the model results at the surface based on the winter data of ^{137}Cs activity concentrations.

Fig.3. The model vertical profile for ^{137}Cs (winter)

The probabilistic data using the ERICA Tool¹ are as follows:

Fig. 4. External dose rates-pelagic fish (probabilistic data summer)

Fig.5 Internal dose rates-pelagic fish (probabilistic data summer)

Statistic	Result
Mean	3.45E-
Variance	6.84E-6
5 th Percentile	6.83E-4
25 th	1.64E-3
Median	2.97E-3
75 th Percentile	4.68E-3
95 th Percentile	8.91E-3
Minimum	1.72E-4
Maximum	1.74E-2

Statistic	Result
Mean	2.01E-1
Variance	1.58E-1
5 th Percentile	1.13E-2
25 th	4.18E-2
	9.46E-2
75 th Percentile	1.89E-1
95 th Percentile	7.16E-1
Minimum	1.71E-3
Maximum	4.15E0

Fig.6. External dose rates-benthic fish (probabilistic data-summer)

Fig.7 Internal dose rates-benthic fish (probabilistic data-summer)

¹ The ERICA Tool is a computerised, flexible software system that has a structure based upon the ERICA Integrated Approach to assessing the radiological risk to biota. The Tool guides the user through the assessment process, recording information and decisions and allowing the necessary calculations to be performed to estimate risks to selected animals and plants [18].

Statistic	Result
Mean	2.04E-3
Variance	2.28E-6
5 th Percentile	3.94E-4
25 th Percentile	9.44E-4
Median	1.72E-3
75 th Percentile	2.70E-3
95 th Percentile	5.14E-3
Minimum	9.90E-5
Maximum	1.00E-2

Fig.8. External dose rates-pelagic fish (probabilistic data-winter)

Statistic	Result
Mean	2.04E-3
Variance	2.28E-6
5 th Percentile	3.94E-4
25 th Percentile	9.44E-4
Median	1.72E-3
75 th Percentile	2.70E-3
95 th Percentile	5.14E-3
Minimum	9.90E-5
Maximum	1.00E-2

Statistic	Result
Mean	1.16E-1
Variance	5.28E-2
5 th Percentile	6.54E-3
25 th Percentile	2.42E-2
Median	5.46E-2
75 th Percentile	1.09E-1
95 th Percentile	4.13E-1
Minimum	9.87E-4
Maximum	2.40E0

Fig.9. Internal dose rates-pelagic fish (probabilistic data –winter)

Statistic	Result
Mean	1.16E-1
Variance	5.28E-2
5 th Percentile	6.54E-3
25 th Percentile	2.42E-2
Median	5.46E-2
75 th Percentile	1.09E-1
95 th Percentile	4.13E-1
Minimum	9.87E-4
Maximum	2.40E0

Fig.10. External Dose rates-benthic fish (probabilistic data-winter)

Fig.11. Internal Dose rates-benthic fish (probabilistic data-winter)

Statistic	Result
Mean	1.84E-3
Variance	3.66E-6
5 th Percentile	3.17E-4
25 th Percentile	7.35E-4
Median	1.22E-3
75 th Percentile	2.33E-3
95 th Percentile	5.19E-3
Minimum	9.27E-5
Maximum	1.64E-2

Statistic	Result
Mean	9.97E-2
Variance	2.09E-2
5 th Percentile	5.16E-3
25 th Percentile	1.91E-2
Median	4.91E-2
75 th Percentile	1.09E-1
95 th Percentile	4.09E-1
Minimum	6.16E-4
Maximum	1.10E0

The mean total dose does not exceed the screening dose rate 10μGy/h

The 5% value means that there is a 95% chance the dose rate is greater than this value. The 95% value means there is a 5% chance the dose rate is greater than this value. There is no need to check effects database, but for methodology reasons we present here the closer example for the results of the present study from Frederica database².

Notes	Effect value:
Number of larvae hatched	31.5
Total eggs and larvae died	74
Mortality of eggs during first 6 days	60
Notes	Effect value:
Number of larvae hatched	44
Mortality of eggs during first days 6	60.5
Total eggs and larvae died	45
Radionuclide reported:	137-Cs
Wildlife group:	Fish
Species name(latin)	Pleuronectes platessa
Fedorov, A.F. Podymakhin, N.N. Skhitenko, N.T. and Chumachenko, V.V., (1964), The effect of slight radioactive contamination of water on the development of the plaice (pleuronectes plates L), Voprosy Ikhtiologii, 3, (32)	
Specific endpoint descriptor	Mortality of eggs and larvae

Different exposure rates (infinitive and semi-infinitive) in sea water, sediment , and seawater-sediment interface respectively are used for the external dose rates estimations to natural marine biota of the area. The simulation data are evaluated in terms of the conceptual model (Polikarpov model)³ of dose rates effects and our published data of the cytogenetic effects of radionuclides on natural marine organisms

³ Polikarpov model zones

Uncertainty zone (2.7 10 ⁻² -1 10 ⁻¹ μGy d ⁻¹)
Natural background – zone of radiation well being (0.11 – 14 μGy d ⁻¹)
Physiological masking zone (14 – 137 μGy d ⁻¹): minor radiation effects at the individual level occur
Ecological masking zone (137 – 10958 μGy d ⁻¹): effects of radiation at the population level are detected
Obvious action zone (> 10958 μGy d ⁻¹): obvious radiation action (reduction in the number of organisms, elimination of radiosensitive species impoverishment of communities and degradation of ecosystems.

and the results are in the zone of no detected effects. Fig.12 and Fig.13 present the results of the model for ¹³⁷Cs at the surface and throughout the water column (examples for 10m depth) with the relevant distance from the coast for summer and winter, respectively.

Fig.12.

The model results for ¹³⁷Cs (summer)

Fig.13

The model results for ¹³⁷Cs (winter)

For the better environmental impact analysis of the studied area, the action of conventional pollutants and especially of heavy metals pollution has been taken into account [19]. Figs.14, 15, 16 present the model results (mg/kg) for Cu, Mn, Ni, respectively, at the surface-in 10m depth- at various distances from the shores (summer).

Fig.14

Model Cu concentrations

Fig.15

Model Mn concentrations

Fig.16

Model Ni concentrations

Figs.17, 18, 19 present the model results for the Cu, Mn, Ni concentrations in pelagic fish.

Fig.17. The model results for Cu concentrations in pelagic fish

Fig.18. The model results profile for Mn concentrations in pelagic fish

Fig.19. The model results profile for Ni concentrations in pelagic fish

Figs.20, 21, 22 present the model results for the Cu, Mn, Ni concentrations in human.

Fig.20. The model results for Cu concentrations in human

Fig.21. The model results for Ni concentrations in human

Fig.22 The model results for Mn concentrations in human

5. Conclusions

The effects of the exposure dose rates received by marine biota depend on the radiosensitivity of the exposed organism. For an integrated radiological analysis the modelling of the effects of radioactivity at molecular level is necessary. Furthermore, studies of the organisms' "adaptive reaction" when they are exposed to the radioactive fields and mixture toxicity effects have to be taken into account.

The combined methodology of model and dose rates estimation results to the prediction of the radiological impact. Model values are in accordance with the measured values. Also, the model it has a general structure that can accommodate any other processes deemed necessary.

The present model can therefore respond to the demand for predictions and support the decision makers for the countermeasures to be taken when necessary. It is feasible to estimate the ecological and environmental risk, keeping in mind that the synergetic action of conventional pollutants has to be taken into account.

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References

- [1] Psaltaki M. Florou H.and.Markatos N.C,”A model of the behaviour of Caesium-137in Marine Environment (A Finite-Volume Method Implementation)”,Proc.of the 1st WSEAS International Conference on Finite-Differences-Finite Elements-Finite Volumes, Malta, 11-13, pp.74-78 September,2008.
- [2] Psaltaki M., Markatos N.C.” Implementing the Finite-Volume method in simulating the behaviour of pollutants in marine environment” proc. Of the 4th IASME/WSEAS International Conference on CONTINUUM MeCHANICS (CM’09),Cambridge,UK pp.187-199 February 24-26, 2009.
- [3] Psaltaki M.,Florou H.,Trabidou G.,and Markatos N.C. “Modelling and the assessment of anthropogenic impacts on marine ecosystems” Book of Abstracts of the 2nd International Conference on “Environmental Management , Engineering Planning and Economics (CEMEPE) &SECOTOC Conference, p.83 Mykonos,June 21-26, 2009.
- [4] Psaltaki M.,Florou H.,Trabidou G.,and Markatos N.C. « Modelling and assessment of pollutant impact on marine environments», 2nd WSEAS International Conference on Computer Engineering and Applications (CEA ’10),Harvard University, Cambridge USA, p.p. 176-180, January 27-29, 2010.
- [5] H. Florou, M. Psaltaki, G. Trabidou, N. Evangeliou, N.C. Markatos, «A preliminary study on the use of modeling of ¹³⁷Cs distribution in seawater for radiation dose assessment to natural organisms”, poster presentation, Environmental Radioactivity Conference, 25th-27th October 2010, Rome.
- [6] Florou H. ¹³⁷Cs Measurements in the Aegean and Ionian Sea, Greece. Radiation Protection 70. The radiological exposure of the population of the European Community to radioactivity in the Mediterranean Sea. Marina – Med Project Report EUR 15564. Proceedings of Seminar held in Rome at the European Nuclear Energy Agency headquarters from 17 to 19 May 1994.
- [7] Florou H., Chaloulou Ch. Fish as bioindicators of radiocaesium pollution in aquatic environment in Greece. Fresenius Environment Bulletin 6: 009-015 (1997).

- [8] Spalding D.B. (1981), "A general purpose computer program for multi-dimensional one- and two -phase flow". *Maths and Computers in Simulation*, North Holland Press, Vol. 13 pp.267-276.
- [9] AS.V.Patankar and D.B.Spalding,(1972) -"A calculation procedure for heat, mass and in three-dimensional parabolic flows", *Int.J.Heat Mass Transfer* 15,1787.
- [10] Tsytsugina V.G.,Polikarpov G.G. "Radiological effects on population of Oligochaeta in the Chernobyl contaminated zone *J.Environ.Radioactivity*, 66 (2003) 141-154.
- [11] Trabidou G. Radiological study in radioactive spring areas. Ph. D. Thesis University of Athens, Athens; 2004.
- [12] Trabidou G. Radiological study in radioactive spring areas. Ph. D. Thesis University of Athens, Athens; 2004.
- [11] Launder B.E., and Spalding D.B., (1974) "The numerical computation of turbulent flows", *Comput.MethodsinMech.eng*.Vol.3, pp. 269-289 .
- [12] Launder B.E., and Spalding D.B., (1974) "The numerical computation of turbulent flows", *Comput.MethodsinMech.eng*.Vol.3, pp. 269-289
- [13] G.J.Hunt "Simple models for prediction of external radiation exposure from aquatic pathways" *Radiation Protection Dosimetry*, (1984) Vol.8, No.4, p.215-224.
- [14] Sven Erik Jorgensen,, "Modelling the distribution and effect of heavy metals in an aquatic ecosystem", *Ecological Modelling*, 6(1979),199-222.
- [15] R. Dallinger, F.Prosi, H.Segner,and H.Back, "Contaminated food and uptake of heavy metals by fish a review and a proposal for further research" *Oecologia (Berlin)* (1987),73:91-98.
- [16] <http://www.cham.co.uk>
- [17] Yakhot V.and S.Orszag, S.Thangam, T.B Gatski and. C.G.Speziale (1992) "Development of turbulence models for shear flows by a double expansion tech-nique",*Physics of Fluids A*,Vol. 4,No 7 .
- [18] <https://wiki.ceh.ac.uk/x/5gHbBg>
- [19] C. Zeri and F. Voutsinou - Taliadouri. Processes affecting the distribution of dissolved trace metals in the North Aegean Sea (Eastern Mediterranean). *Cintinental Shelf Research*, Vol. 23(9) , pp. 919 -934, 2003.