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Comparison of MCNP and ERICA codes in two different marine areas

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Abstract

The internal and external dose rates received by a marine organism, were calculated using the MCNP-CP code and the ERICA Assessment Tool. MCNP/MCNPX is a general purpose Monte Carlo code for the transport of all kinds of particles, while ERICA is a more specified software tool for assessing the radiological risk to terrestrial, freshwater and marine biota. A pelagic organism living only in the water medium, was chosen as a start for this comparison. Additionally, two different coastal areas: Stratoni port at Ierissos Gulf, Greece [1] and Shatt al-Arab estuary at Arabic or Persian Gulf [2] were selected. Both areas are receiving the impact of anthropogenic activities as those related with metal mining (Stratoni port) and oil and gas exploration (Arabic/Persian Gulf). The measured concentrations of natural ⁴⁰K, ²¹⁰Pb and ²⁰⁸Tl and artificial (¹³⁷Cs) radionuclides in the surface sediment, were included in the calculations for the estimation of the activity concentrations in the water using the sediment-water distribution coefficient (K_d) of the ERICA database. The preliminary results of MCNP-CP simulations were in good agreement with those of ERICA for all radionuclides.

Keywords ERICA, MCNP-CP, marine organism, radionuclides, dose rates

INTRODUCTION

The scope of this work was firstly to compare the internal and external dose rates obtained by two codes (MCNP-CP code and the ERICA Assessment Tool), in a unreal simple case scenario – a spherical pelagic fish – for some radionuclides observed in the marine environment. Secondly, for the same radionuclides, to estimate the internal and external dose rates inserting experimental data from two different marine areas (Stratoni port at Ierissos Gulf, Greece and Shatt al-Arab estuary at Arabic or Persian Gulf) in the ERICA Tool. MCNP/ MCNPX is a general purpose Monte Carlo code for the transport of all kinds of particles, while ERICA is a more specified software tool for assessing the radiological risk to terrestrial, freshwater and marine biota. A spherical pelagic fish was created in both codes bearing the same characteristics (radius 5.130 cm, density 1 g/cm³, mass 0.566 kg) while the activity concentration of all radionuclides in the water medium was assumed to be 1Bq/L.

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The assumptions and parameters used by the ERICA Tool for the estimation of the dose rates, were included in the dose rate calculations by the MCNP-CP code. The dose rates (in $\mu\text{Gy/h}$) of four representative radionuclides (^{40}K , ^{137}Cs , ^{210}Pb and ^{208}Tl) in the marine environment, of which some are also included as default radionuclides in the ERICA database, were estimated by the two codes. The only exceptions were the ^{40}K and ^{208}Tl radionuclides, as explained below.

METHODOLOGY

ERICA case: In the ERICA whole-body-dose-rate calculations the important parameters of a marine organism to be inserted are: a) the characteristics of the organism (radius (in cm), density (in g/cm^3), mass (in kg)), if a new organism is created, b) the concentration ratio (CR) of the radionuclide of interest, c) the sediment-water distribution coefficients (K_d) of the radionuclide of interest if the organism resides in the seabed and d) the activity concentrations of the media (soil and water for aquatic environments) where the organism resides. The distribution coefficients (K_d) are defined as the quotient of the activity concentration per unit mass of sediment to the activity concentration per unit mass (or volume) of (filtered) water. The concentration ratio (CR) is the ratio of the activity concentration of a radionuclide in the organism whole body over its activity concentration in the seawater (aquatic biota). Additionally, the ERICA Tool includes default marine organisms (e.g. pelagic fish) of ellipsoidal geometry. In the present work the geometry of the pelagic fish was altered from ellipsoid to sphere, to facilitate the MCNP geometries, while the CRs of the default pelagic fish, were inserted in the new geometry.

The Tool assumes secular equilibrium between parent and daughter nuclides, if the half-lives of the latter are shorter than 10 days [3]. This is the case of the dose rate calculation of ^{210}Po (parent nuclide) using the ERICA Tool in the present work. Additionally, weighted total dose rates are estimated by the Tool through the application of weighting factors (dimensionless) for alpha, low beta and high beta-gamma radiation. Default radiation weighting factors of 10 for alpha radiation, 3 for low energy beta ($<10\text{keV}$) and 1 for high energy ($>10\text{keV}$) beta and gamma radiation are applied in the Tool [3].

The ^{40}K and ^{208}Tl isotopes are not included in the default-radionuclides database of the ERICA Tool, however they can be added as described in detail in the Tool manual and briefly mentioned in [3]. In order to use the new isotope subsequent assessment information on transfer parameters including CRs and K_d s were provided manually. The CR and K_d parameters of ^{208}Tl were inserted from the IAEA Technical report [4] for the cases of marine organisms and ocean margin, accordingly. Due to the lack of literature data regarding ^{40}K , potassium was inserted in the ERICA Tool using the CR of Na [4], while the K_d was calculated by measured data of ^{40}K activity concentration in sediment and water of Stratoní port (Ierissos Gulf) [1] and Shatt al-Arab estuary [2].

Monte Carlo case geometry: The MCNP-CP code was used for the simulations of natural radionuclides. The MCNP-CP code, instead of older MCNP versions (e.g. MCNP5) takes

into account the whole cascade scheme of a radionuclide. Two different geometry cases were simulated with the Monte Carlo. In the first geometry the particles (histories) were generated inside the fish volume and the energy deposited in the fish volume (internal) and in the water volume around the fish (external) were recorded using the *F8 tally (Fig.1). In the second geometry the histories were generated in the water volume (around the fish) and the energy deposited inside the fish was again recorded using the *F8 tally (Fig. 2). With the first geometry the calculation of both internal and external dose rates is feasible, while in the second geometry only the external dose rate was calculated. The first geometry approximated the external dose rate calculation of the ERICA Tool, while the second one corresponds to (the definition of) the external dose rate concept. In order to associate the external dose rates of the two geometries, it was essential to keep the (density of) histories that escape the water volume and reach the fish volume in the second geometry to be the same as the (density of) histories that escape the fish volume and deposit their energy in the water volume in the first geometry. Therefore, the ratio of generated histories to the volume of interest (fish volume in the first geometry and water volume in the second geometry) was kept the same in the two geometry cases.

The effective (spherical) water volume – a quasi-infinite homogeneous medium volume, where the organism resides - was calculated using as radius the length attenuation of the highest gamma-ray of the isotope, assuming the loss of 10000 to 1 gamma-ray photons. The generated histories in the fish volume were 10^5 . The energy cutoffs in MCNP-CP for photons were the default ones (1keV) and for electrons, 10 keV or 3 keV to match the ERICA Tool assumptions. The activity concentration in the water was assumed to be 1 Bq/L for all radionuclides. The activity concentration in the fish –for the first geometry case- (calculated using the CRs of the ERICA Tool) was 1 Bg/kg, 84 Bq/kg, 33000 Bg/kg, 33000 Bg/kg and 5000 Bg/kg for ^{40}K , ^{137}Cs , ^{210}Pb , ^{210}Bi , ^{208}Tl , respectively. As mentioned before, the ERICA Tool assumes secular equilibrium between the parent and the daughter nuclides, if the half-life of the latter is less than 10 days, as in the case of ^{210}Pb and ^{210}Bi . Therefore, in the MCNP-CP code these radionuclides were simulated separately.

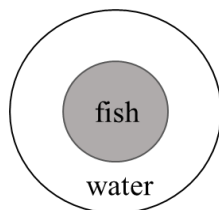


Fig.1. 1st geometry (the gray color represents the generated histories)

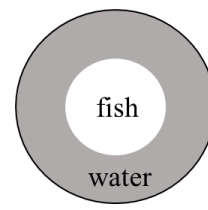


Fig.2. 2nd geometry (the gray color represents the generated histories)

RESULTS AND DISCUSSION

The internal and external dose rates in $\mu\text{Gy/h}$ of ^{40}K , ^{137}Cs , ^{210}Pb and ^{208}Tl radionuclides for the first geometry case are presented in Tables 1 and 2, accordingly. In the tables are presented: a) the radionuclide of interest, b) the estimated dose rate with the ERICA Tool and the Monte Carlo code, c) the ratio of the dose rate estimated by the Tool to the one calculated using the MCNP-CP code and d) the statistical error of the Monte Carlo simulations (in %). The internal dose rates were higher than the external ones, as all radionuclides are characterized by beta decay and emit high energy electrons, X-ray and gamma-ray photons. Additionally, the beta electron range is shorter than the X-ray and gamma-ray photon range and the fish radius, therefore all the beta decay electrons deposit practically their whole energy inside the fish volume, while the X-ray and gamma-ray photons only partially. The highest internal dose rates were attributed to the ^{210}Pb (^{210}Bi) and ^{208}Tl radionuclides, as both emit a large amount of beta-decay electrons comparing to the ^{40}K and ^{137}Cs ones. The internal dose rate results obtained by both codes were in good agreement – within 8% - for all studied radionuclides.

Table 1. Internal dose rates in $\mu\text{Gy/h}$ (1st geometry)

	ERICA	MCNP-CP	Ratio Difference	Error (%)
^{40}K	$3.03 \cdot 10^{-4}$	$2.80 \cdot 10^{-4}$	1.08	0.21
^{137}Cs	$1.53 \cdot 10^{-2}$	$1.58 \cdot 10^{-2}$	0.97	0.12
^{210}Pb	8.35	0.47	1.00	0.21
^{210}Bi		7.90		0.19
^{208}Tl	2.55	2.66	0.96	0.24

The dose rates error is the statistical one of MCNP-CP output

The major contribution in the external dose rates, was observed for the ^{137}Cs and ^{208}Tl radionuclides compared to the one of ^{40}K and ^{210}Pb (Table 2). The ^{137}Cs and ^{208}Tl radionuclides are characterized by medium and high energy gamma-ray photons, therefore the energy deposition of these radionuclides is higher than the energy deposition due to ^{210}Pb . The external dose rate of ^{40}K was also lower than the one of ^{137}Cs and ^{208}Tl , even though ^{40}K is characterized by a high energy gamma-ray (1460keV) emission. This difference is explained through the decay scheme of ^{40}K , as only a branching ratio of 10.7% is followed by the 1460 keV gamma-ray photon. The external dose rate results obtained by both codes were in good agreement – up to 12% - for all radionuclides.

Table 2. External dose rates in $\mu\text{Gy/h}$ (1st geometry)

	ERICA	MCNP-CP	Ratio Difference	Error (%)
^{40}K	$8.87 \cdot 10^{-5}$	$8.77 \cdot 10^{-5}$	1.01	0.88
^{137}Cs	$2.88 \cdot 10^{-4}$	$2.87 \cdot 10^{-4}$	1.00	0.16
^{210}Pb	$4.81 \cdot 10^{-6}$	$9.35 \cdot 10^{-7}$	0.88	1.56
^{210}Bi		$4.53 \cdot 10^{-6}$		2.41
^{208}Tl	$1.78 \cdot 10^{-3}$	$1.78 \cdot 10^{-3}$	1.00	0.07

The dose rates error is the statistical one of the MCNP-CP output

The external dose rates in $\mu\text{Gy/h}$ of the ^{40}K , ^{137}Cs , ^{210}Pb and ^{208}Tl radionuclides for the second geometry case are presented in Table 3. The major contribution in the external dose rates, was observed for the ^{137}Cs and ^{208}Tl radionuclides compared to the one of ^{40}K and ^{210}Pb and this contribution is explained by the decay schemes of each radionuclide (see first

geometry case above). The external dose rate results obtained by both codes were in good agreement – within 6 % - for all radionuclides. In both geometry cases the external dose rate calculations (using the MCNP-CP code) were in good agreement with the ERICA Tool estimations, therefore the external dose rate calculation using these two alternative ways (ERICA approximation and external dose rate concept) proved to be equivalent. The great advantage of the ERICA approximation was naturally the much reduced computational time.

Table 3. External dose rates in $\mu\text{Gy/h}$ (2nd geometry)

	ERICA	MCNP-CP	Ratio Difference	Error (%)
⁴⁰ K	$8.87 \cdot 10^{-5}$	$9.45 \cdot 10^{-5}$	0.94	7
¹³⁷ Cs	$2.88 \cdot 10^{-4}$	$2.72 \cdot 10^{-4}$	1.06	2
²¹⁰ Pb	$4.81 \cdot 10^{-6}$	$7.59 \cdot 10^{-7}$	1.01	2
²¹⁰ Bi		$3.99 \cdot 10^{-6}$		3
²⁰⁸ Tl	$1.78 \cdot 10^{-3}$	$1.80 \cdot 10^{-3}$	0.99	6

The dose rates error is the statistical one of the MCNP-CP output

The internal and external dose rates in $\mu\text{Gy/h}$ of the ⁴⁰K, ¹³⁷Cs, ²¹⁰Pb and ²⁰⁸Tl radionuclides obtained in Stratoní port and Shatt al-Arab estuary are presented in Table 4. In these two areas, sediment samples have been collected, treated and measured via gamma spectroscopy [3],[4]. So, the experimentally deduced values of activity concentration for these radionuclides have been used as input parameters in the ERICA tool and the dose rates received by the pelagic fishes in these two regions, have been estimated. The internal dose rates were higher than the external dose rates in both areas, as explained (in the simple case scenario above). Additionally, the dose rates (internal and external) of ¹³⁷Cs and ²⁰⁸Tl in Stratoní port were higher than those obtained in the Shatt al-Arab estuary, due to the higher activity concentrations in the sediment (and thus in the water medium) measured in Stratoní in comparison with the ones in Shatt al-Arab. The dose rates due to ⁴⁰K were similar in both marine areas, as similar activity concentrations of ⁴⁰K were measured in the sediment and water media of these areas. Generally, the dose rates obtained in those locations, were well below the screening value of 400 $\mu\text{Gy/h}$ adopted for aquatic species by the [5] and [6].

Table 4. Internal and external dose rates in $\mu\text{Gy/h}$ (measured data) estimated using the ERICA Assessment Tool

	Stratoní port		Shatt al-Arab estuary	
	Internal	External	Internal	External
⁴⁰ K	$3.89 \cdot 10^{-3}$	$1.14 \cdot 10^{-3}$	$4.03 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$
¹³⁷ Cs	$3.30 \cdot 10^{-6}$	$6.21 \cdot 10^{-8}$	$1.86 \cdot 10^{-6}$	$3.51 \cdot 10^{-8}$
²¹⁰ Pb	$2.73 \cdot 10^{-3}$	$1.57 \cdot 10^{-9}$	-	-
²⁰⁸ Tl	$3.57 \cdot 10^{-3}$	$2.50 \cdot 10^{-6}$	$1.80 \cdot 10^{-3}$	$1.26 \cdot 10^{-6}$

The screening value of 400 $\mu\text{Gy/h}$ adopted for aquatic species by the [5] and [6].

In the Shatt-al Arab estuary, no experimental data were obtained of ²¹⁰Pb.

CONCLUSIONS

In the present work the internal and external dose rates for a marine organism (pelagic fish) were calculated using two different codes, a general purpose MC code (MCNP-CP) and a more specialized one (ERICA Tool). A good agreement of the calculated dose rates – up to 8% for the internal dose rate and up to 12% for the external dose rate - using the two codes

for a simple case scenario was obtained. Additionally, the external dose rate was calculated using the MCNP-CP code for two different geometry cases, the first geometry case approximated the ERICA Tool external dose rate estimation and the second one was the external dose rate as routinely defined in physics. In both cases the agreement was satisfactory (up to 6%), therefore the ERICA approximation is well established for the pelagic fish case. Furthermore, the internal and external dose rates were estimated using the ERICA Tool in two real cases (Stratoni port and Shatt al-Arab estuary), where the difference of the dose rates obtained between these areas were attributed to the difference in the activity concentrations of ^{40}K , ^{137}Cs , ^{210}Pb and ^{208}Tl measured in the sediment and water media. However, the dose rates obtained in both areas were well below the screening values proposed by [5] and [6].

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