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REVIEW OF THE Q-SYSTEM USING MONTE-CARLO SIMULATIONS

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ABSTRACT

An international working group that is reporting to TRANSSC of IAEA has identified several issues of the current Q-System. The reproduction of some values as well as the calculation of additional nuclides is challenging. Therefore, the working group started reviewing the Q-System on a scientific basis. Even though the scenarios will remain essentially the same, it is necessary to update and improve the calculation procedure. Hence, the calculations used by the working group are based on Monte-Carlo simulations that represents the state-of-the-art of science and technology. For each scenario, the working group aims for an agreement on each relevant parameter. Especially all input parameters for the simulations are defined. In order to reduce uncertainties, several codes are used within the working group and therefore this very detailed coordination is of great importance.

This paper will give an overview of the use of Monte-Carlo simulations for reviewing the Q-System. Advantages compared to the current Q-System will be presented and first preliminary results will be shown. Since secondary particles can be included in the simulations and also all kinds of radiation can be simulated, the impact of this new approach on Q-values will be discussed based on each change compared to the current Q-System.

INTRODUCTION

According to the graded approach of the IAEA transport regulations SSR-6 [1], activity limits for radioactive material in packages are established to limit the radiological consequences during "normal" transport and after an accident, respectively. Especially the activity limitation on the contents of Type A packages (A_1 for special form material and A_2 for material not in special form) for any radionuclide is calculated using the Q-system given in the *Advisory Material for the IAEA Regulations for the Safe Transport of Radioactive Material* SSG-26 [2].

Within the scope of a former research project carried out by GRS, many inconsistencies within the documentation and problematic issues of the Q-System were revealed. At that time, not only GRS but also some other international research groups worked on this topic. Therefore, a meeting with experts in the field of transport of radioactive material was held at GRS Cologne in September 2013. At this meeting, it was decided to further investigate raised issues of the Q-System, and an international working group (WG) was founded. The results elaborated by the WG and discussed issues are regularly reported to TRANSSC. In 2016 the IAEA recognized the WG as a "Special Group". The international WG aims to calculate Q-values considering the state-of-the-art of science and technology. The scenarios of the current Q-System should remain basically the same.

For this purpose, state-of-the-art Monte-Carlo-techniques are used by the members of the working group to calculate values for Q_A, Q_B and Q_D (and Q_E). At GRS the C++ framework Geant4[1] [3] is employed which was developed at CERN[2] for simulating the passage of particles through matter

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[1] **GE**ometry **AN**d **T**racking

[2] ***C****onseil* ***E****uropéen pour la* ***R****echerche* ***N****ucléaire* (European Council for Nuclear Research)

using Monte-Carlo methods. The development, maintenance and user support are taken care of the international Geant4 Collaboration. Initially, the program package was developed for simulating high energy physics processes, but because of its general purpose nature, at the meanwhile, the range of application is extended to nuclear, medical, radiation and space physics. The software is used by a considerable number of research projects around the world.

In addition to Geant4, different Monte-Carlo codes (MCNP [4], PHITS [5]) are used by other institutions in the WG. To assure an effective procedure for comparing and discussing the results obtained by the different institutions, the WG decided to define a short list of nuclides (F-18, Co-60, Kr-85, Sr-90, Tc-99m, Ru-106, Cs-134, Cs-137, Eu-154, Ir-192) which were analyzed in detail.

RELEVANT ASPECTS OF THE CURRENT Q-SYSTEM

In the scope of the Q-System, a series of exposure pathways are considered which lead to five (or six) so-called Q-values:

- Q_A: external photon dose
- Q_B: external beta dose
- Q_C: inhalation dose
- Q_D: skin and ingestion dose due to contamination transfer
- Q_E: submersion dose
- (Q_F: “special case” of Q_C for alpha emitters)

The A_1-value is applicable for special form radioactive material and is defined as the lesser of the two values Q_A and Q_B. The A_2-value is applicable for non-special form radioactive material and is understood as the least of the A_1-values and the remaining Q-values.

Boundary conditions of the Q-System are, e.g.:

- a distance of 1 m to the source (for Q_A and Q_B)
- an exposition time: 0.5 h (for Q_A, Q_B, Q_C, (and Q_E)), 5 h (for Q_D)
- dose limits: 50 mSv (eff. Dose), 500 mSv (skin dose), 150 mSv (dose of the lens of the eye)
- an absorber of 150 $mg \cdot cm^{-2}$ (for the calculation of Q_B)

SIMULATION OF Q_A

By means of state-of-the-art Monte-Carlo-methods, it is possible to consider all kinds of particles for calculations of the Q_A-values. That means that the Q_A-value, defined initially only for the external effective dose due to photons, now can be defined for the external effective dose due to all types of radiation (γ, e+, e-, n). Furthermore, for consistency reasons, the WG decided to consider an absorber (originally only applied for Q_B) also for the calculation of Q_A. Concerning this matter, the WG deemed it as reasonable to consider a shielding thickness of 0.5 mm of stainless steel for all radioisotopes when evaluating the Q_A (and Q_B) values. Further details on the calculation conditions can be found in [6].

The general geometry for the simulation of Q_A (and Q_B) is shown in Figure 1. To avoid significant changes compared to the current Q-System, a point source is assumed, and the distance of the source to the exposed person is assumed to be 1 m. A sphere surface with a radius of one meter is used as detector.

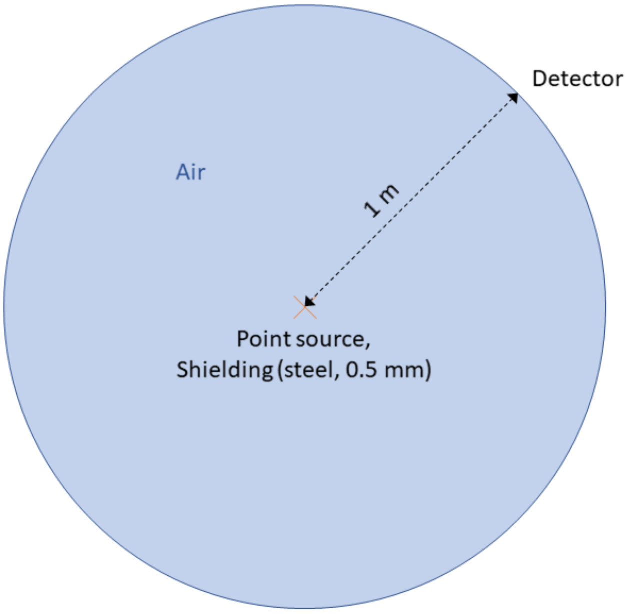

Figure 1: General geometry for the simulation of Q_A (and Q_B)

Table 1 shows preliminary results of the GRS-calculations for Q_A considering the short list of nuclides (see above) and compared with the current Q-values [2]. For the majority of nuclides (seven out of ten), the results agree within 10 %. The differences in the results of the three remaining nuclides can be analyzed in detail.

Table 1: Preliminary results for Q_A compared with the current Q-System

Nuclide	**Q_A (Current)**	**Q_A (Geant4)**	**Ratio (Geant4 / Current)**
	(TBq)	**(TBq)**	
Co-60	4.5E-01	4.4E-01	98%
Cs-134	6.9E-01	6.8E-01	96%
Cs-137	1.8E+00	1.9E+00	100%
Eu-154	9.0E-01	8.7E-01	96%
F-18	1.0E+00	1.0E+00	93%
Ir-192	1.3E+00	1.3E+00	100%
Tc-99m	9.8E+00	9.3E+00	93%
Kr-85	4.8E+02	3.0E+02	63%
Ru-106	5.3E+00	1.3E+00	25%
Sr-90	1.0E+03	5.4E+00	0%

To investigate the impact of the new approach, including particularly the contribution of all types of radiation and interactions as well as secondary particles like bremsstrahlung, a detailed analysis can be performed. In case of significant changes in the values compared to the current system, the acceptance of authorities and the industry will depend strongly on clear documentation and justification. The origin of changes should be demonstrated. Hence, the analyzing tools have been developed using the advantage of Monte-Carlo simulations which offer the possibility of enabling or disabling individual processes such as interactions of interest (e.g. bremsstrahlung) or the discrimination of individual particles. This analysis allows for a subdivision of all contributions to the corresponding Q-value. In the following, the deviation of the Q_A-values from the values of the current Q-System for the three nuclides Kr-85, Ru-106, Sr-90 will be discussed.

By calculating the Q_A-value for Kr-85 without simulating the (bremsstrahlung) contribution of the primary electron, a Q_A-value of 4.7 E+02 TBq is obtained. Thus, an agreement of 98 % compared with the value of the current Q-System is found.

Similarly, if only the primary photon contribution is considered while calculating Q_A for Ru-106, a Q_A-value of 5.2 E+00 TBq is obtained and again an agreement of 98 % in comparison to the value of the current Q-System is found.

For Sr-90 the value of the current Q-System is obtained by applying an artificial cut-off at 1.0E+03 TBq (without documentation in the current Q-System). If this value is recalculated using the formalism of the current Q-System, Q_A equates to 1.0E+06 TBq. In comparison, the Geant4-simulation of this value (not taking into account the bremsstrahlung contribution) leads to Q_A=4.0E+07 TBq, which is at least a better agreement than shown in Table 1.

This discussion clearly demonstrates the analyzing power of the new approach. For any nuclide, the impact of every new assumption can be investigated, and a scientific justification for a change of values can be documented.

SIMULATION OF Q_B

As was the case with Q_A, it is possible to consider all kinds of particles when calculating the Q_B-value. This means that the Q_B-value, originally defined only for the skin-equivalent dose due to electrons, now can be defined for the skin-equivalent dose due to all types of radiation (γ, e+, e-, n). As described above, the WG considers a shielding thickness of 0.5 mm of stainless steel for all radioisotopes when evaluating the Q_B (and Q_A) values. For comparison, in the current Q-System, an absorber of 150 mg/cm² was assumed, which corresponds to a thickness of steel of 0.2 mm. Further details on this topic can be found in [6].

The general geometry for the simulation of Q_B is basically the same as for the simulation of Q_A (see above).

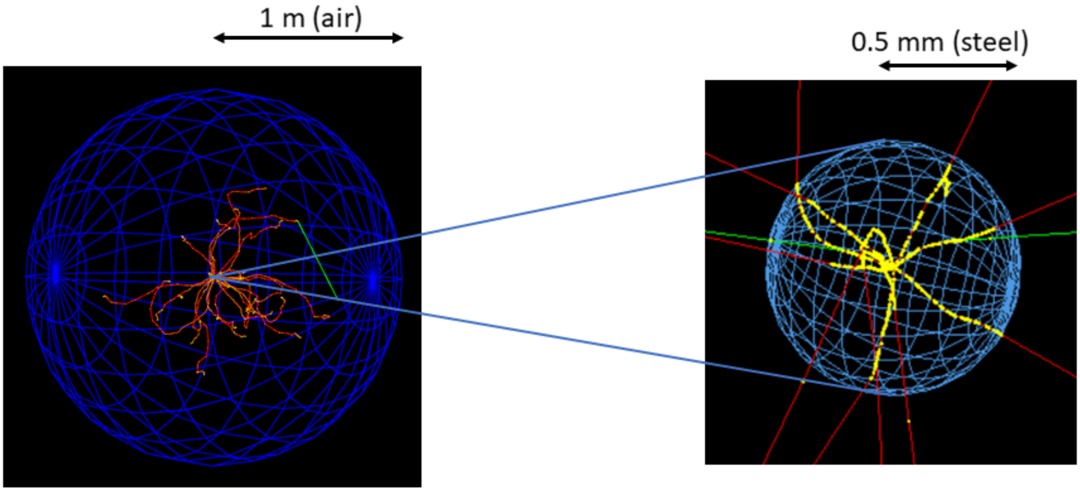

Figure 2: General geometry as implemented in Geant4 (left) and zoom into the center of the sphere to show the implemented shielding (right).

Figure 2 shows the implementation of the geometry within the framework of Geant4. Electron-trajectories are shown in red, γ-trajectories (arising due to bremsstrahlung) are shown in green. One can see that primary electrons can generate bremsstrahlung in the air inside the sphere as well as in the implemented shielding of 0.5 mm stainless steel surrounding the point source.

Preliminary results of the GRS-calculations for Q_B are given in Table 2 for the short list of nuclides (see above) and compared with the current Q-values [2]. The comparison with the current Q-System shows that only for five nuclides there is an agreement within 35 %. For the remaining five nuclides, there is no reasonable agreement.

Table 2: Preliminary results for Q_B compared with the current Q-System

Nuclide	Q_B (Current) (TBq)	Q_B (Geant4) (TBq)	Ratio (Geant4 / Current)
Co-60	7.3E+02	1.8E+00	0%
Cs-134	3.6E+00	2.4E+00	67%
Cs-137	8.2E+00	6.1E+00	74%
Eu-154	1.6E+00	2.1E+00	131%
F-18	2.8E+01	3.6E+00	13%
Ir-192	4.6E+01	5.4E+00	12%
Tc-99m	1.0E+03	7.5E+01	8%
Kr-85	1.4E+01	1.3E+03	9286%
Ru-106	2.2E-01	1.6E-01	73%
Sr-90	3.2E-01	2.7E-01	84%

The main differences of the calculation methods which result in these deviations are given above. In order to reproduce the Q_B-values of the current Q-system, a simulation without assuming a shielding has been performed and the contribution of the primary photons have not been considered in the calculations. The shielding factor of the current Q-system was based on an absorber of 150 mg/cm² and is given in [7] as a function of the maximum beta energy. By assuming this shielding factor, Q_B-values as shown in Table 3 can be obtained. For seven out of ten nuclides, the results agree within 20 %.

Table 3: Preliminary results for Q_B by adapting the calculation (see text) compared with the current Q-System

Nuclide	Q_B (Current) (TBq)	Q_B (Geant4, adapted) (TBq)	Ratio (Geant4 / Current)
Co-60	7.3E+02	4.0E+02	55%
Cs-134	3.6E+00	3.3E+00	92%
Cs-137	8.2E+00	3.5E+00	43%
Eu-154	1.6E+00	1.6E+00	100%
F-18	2.8E+01	3.3E+01	118%
Ir-192	4.6E+01	3.8E+01	83%
Tc-99m	1.0E+03	3.6E+09	3.6E+06%
Kr-85	1.4E+01	1.5E+01	107%
Ru-106	2.2E-01	2.1E-01	95%
Sr-90	3.2E-01	2.8E-01	88%

While the differences of the results for the nuclide Co-60 also improved significantly, there is no strong impact for Cs-137. It has to be emphasized that recalculating these values using the formalism of the current Q-System, values of 5.5E+02 and 6.6E+00 respectively, are obtained. This is a deviation of 25 % to the current Q-system for both nuclides and shows that the calculation procedure and documentation of the current Q-system is partly not consistent as already mentioned in the introduction.

The difference of the result for Tc-99m can be explained by the artificial cut-off at 1.0E+03 TBq which is implemented in the current Q-system.

These results demonstrate that the differences to the current Q-system are understood and that a scientific justification for a change of values, using the new approach, can be documented.

PRELIMINARY RESULTS (A_1)

The preliminary results for the A_1-values, i.e. the lesser of the two values Q_A and Q_B, for the short list of nuclides, are shown in Table 4 and compared with the current values. Most of the values (nine out of ten) can be reproduced but for one nuclide there is no reasonable agreement.

As shown above, the differences can be principally explained by the modified definitions of Q_A and Q_B and by the changed assumptions for the thickness of the shielding.

Table 4: Preliminary results for A_1 compared with the current Q-System

Nuclide	A_1 (Current)	A_1 (Geant4)	Ratio (Geant4 / Current)
	(TBq)	(TBq)	
Co-60	4E-01	4E-01	100%
Cs-134	7E-01	7E-01	100%
Cs-137	2E+00	2E+00	100%
Eu-154	9E-01	9E-01	100%
F-18	1E+00	1E+00	100%
Ir-192	1E+00	1E+00	100%
Tc-99m	1E+01	1E+01	100%
Kr-85	1E+01	3E+02	3000%
Ru-106	2E-01	2E-01	100%
Sr-90	3E-01	3E-01	100%

SIMULATION OF Q_D

The method used to calculate Q_D in the current Q-System is based on spectrum data given in ICRP 38 [8] and dose coefficients taken from [9]. The approach employs an MC method to calculate dose distributions due to beta contamination on an air-water interface. In the mentioned publication, doses are evaluated at a water depth of 70 µm (integrated dose between 60 µm and 80 µm) for a target surface area of 1 cm² and a contamination area of 100 cm² located at the air-water boundary.

As stated above, the scenarios of the current Q-System should remain basically unchanged. Nevertheless, to meet the current state-of-the-art in science and technology, the updated spectrum data given in ICRP 107 [10] are used instead of those given in ICRP 38. The general geometry of the model currently used by GRS for the calculations is shown in Figure 3. It is comprised of a cylinder ($100\ cm^2$ * 5 cm) of air on top of a cylinder ($100\ cm^2$ * 5 cm) of skin material (as defined in [11]). The target geometry is chosen as defined in [9] ($1\ cm^2$ * 20 µm at 70 µm depth) and consists of skin material. The contamination area of 100 cm² located at the air-skin boundary is also consistent with the specifications given in [9].

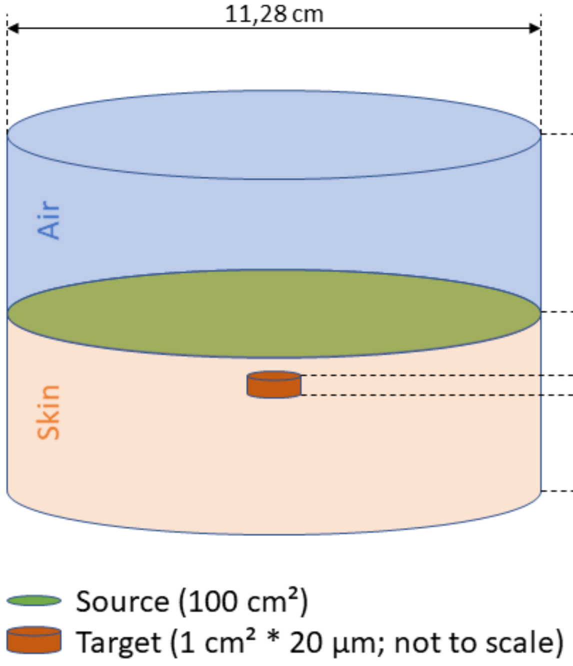

Figure 3: General geometry for the simulation of Q_D

Preliminary results of the GRS-calculations for Q_D are given in Table 5 regarding the short list of nuclides (see above[3]) and compared with the current Q-values [2]. For this short list, the results of the calculations are consistent with the current Q-System within 15 %.

Table 5: Preliminary results for Q_D in comparison to the current Q-System

Nuclide	Q_D (Current) (TBq)	Q_D (Geant4) (TBq)	Ratio (Geant4 / Current)
Co-60	1.05E+00	9.70E-01	92%
Cs-134	9.45E-01	9.20E-01	97%
Cs-137	6.77E-01	6.30E-01	93%
Eu-154	6.05E-01	5.50E-01	91%
F-18	6.74E-01	5.80E-01	86%
Ir-192	6.45E-01	6.10E-01	95%
Tc-99m	4.26E+00	4.30E+00	101%
Ru-106	5.65E-01	5.70E-01	101%
Sr-90	3.22E-01	3.10E-01	96%

SUMMARY AND CONCLUSIONS

This publication gives an overview of ongoing calculations regarding a review of the Q-system. An international working group performs Monte-Carlo simulations to develop a basis for a revised Q-

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[3] Kr-85 is not listed in Table 5 because it is not estimated in the current Q-System. Instead, for Kr-85 and other noble gases, Q_E is calculated.

System which conforms to the current state of scientific and technical knowledge. The calculations of Q_A, Q_B and Q_D, using the Geant4 software toolkit are presented, and preliminary results regarding a short list of nuclides are shown. For an investigation of the impact of this new approach, the analyzing options are discussed which allow for a clear identification of the origin of changes in the final values.

Concerning Q_A and Q_B the values obtained within the current Q-System were reproduced, or the differences between the values can be understood at least in a qualitative manner. For Q_D, all presented values for the short list are consistent with the current Q-System within 15 %.

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