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Computation of Radioactive Material Transport Limits Within A1/A2 Working Group at IAEA TRANSSC

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ABSTRACT IAEA's (International Atomic Energy Agency) publication SSG-26 defines a methodology for calculating A1/A2 values. These values were conceived as limits for the transport of radioactive goods, to limit the public's exposure to radiation in the event of an accident. The limits ensure people involved in an accident receive an effective dose of no more than 50 mSv and a skin equivalent dose no greater than 500 mSv. The current values are based on five exposure scenarios taken from the Q-System, described in 1996. In 2013, the IAEA commissioned an international working group to improve the Q-System and calculate new limits for the transport of radioactive material. Within this working group, CERN has developed a set of models and an associated mathematical framework, and compiled them in a single piece of software. The primary purpose of the software is to compute and compare values produced by the different models under discussion. Later, the software could be distributed in a lighter version which will include the agreed upon regulatory model to determine the A1/A2 values.

INDEX TERMS Transport limits for radioactive material, international regulation, IAEA, Q-system, Monte-Carlo simulation, A1 A2 limits.

I. INTRODUCTION

Operation of CERN's accelerators can lead to the activation of equipment, which may require shipping to external workshops, institutes, or repositories for radioactive waste. The IAEA safety standards provide nuclide-specific activity limits, and criteria for the transport of radioactive equipment.

However, the literature lacks data concerning non-standard radionuclides of interest which are produced at CERN's particle accelerators. Such radionuclides are assigned a conservative reference activity limit which needs to be evaluated based on the Q-System. Radiological quantities like external or internal doses must be assessed. In particular, the skin dose originating from beta emitters is difficult to estimate by analytic equations.

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The Q-System [1] considers a series of exposure scenarios in the event of an accident as presented in Figure 1.

CERN previously computed values of the Q-System using the current definition from IAEA SSG-26, and proposed the determination of Q-Values for shipping by the use of transfer functions [2]. The transfer functions are built from data initially calculated with FLUKA Monte-Carlo simulations [3], [4]. The method establishes energy dependent transfer functions from activity to dose, and allows for instantaneous and efficient analytic calculations using a beta spectrum and mono-energetic yields as input data.

This document details how the calculations of these values have been automatized in a C++ tool.

II. CONTEXT OF TOOL DEVELOPMENT

IAEA SSG-26 [1] will be updated by the TRANSSC committee, and the A1/A2 working group has been tasked with

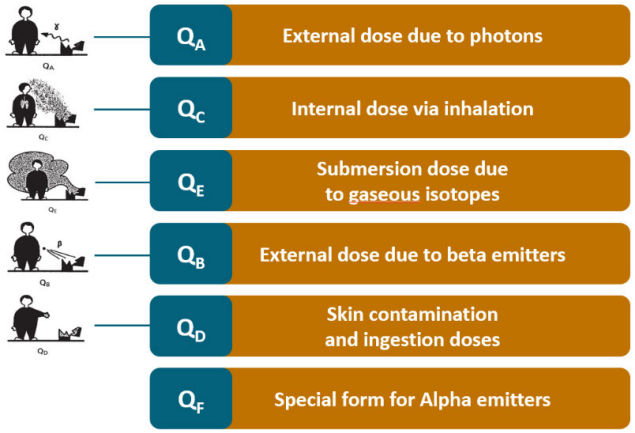


FIGURE 1. Description of Q-Values scenario.

improving the Q-System calculation method. This document provides an overview of a tool developed to compute these values. The software was presented to the IAEA's A1/A2 working group during the TRANSSC-37 meeting. The working group's latest developments in the update of the Q-System are implemented in this software tool. These new developments and their advancements are described in [5]–[13].

IAEA has expressed interest in the software for:

1) Use by the members of the A1/A2 working group to perform comparisons between the studied models in view of selecting the most adequate one. The purpose is benchmarking and standardization of calculations,
2) In the future, possibly distributing a lighter version of this software including the retained regulatory model. Discussions have started to define how to fully transmit the software from CERN to IAEA.

In the next sections, we detail the implementation of the calculations and the use of the software.

III. IMPROVEMENT OF THE A1/A2 METHODOLOGY

The methodology currently being discussed by the IAEA A1/A2 working group is based on the calculation of fluences of particles, according to the different scenarios established for the Q-System. Some new scenarios will be added for example, the consideration of the eye lens dose. The Q-Values are determined by the convolution of calculated fluence with fluence-to-dose coefficients coming from the ICRP-116 publication [14]. These coefficients are geometry-dependent (Antero-Posterior (AP)/Postero-Anterior (PA)/Isotropic (ISO), as described in ICRP publication 116). This establishes dose rates that are then converted into activity limits of a specific radionuclide by convolution with the nuclear decay data available in the nuclear libraries.

The new A1/A2 limits are established using the latest ICRP publications for emission spectra and external dose coefficients. All radiation types (beta+/-, discrete electrons, photons, neutrons) are considered in the respective Monte-Carlo simulations. All these considerations are further detailed in references [5] to [12].

IV. INPUT DATA FOR THE SOFTWARE

The software tool requires two sets of input data files. One is the nuclear data evaluation, containing radionuclide progeny chains, emissions energy and intensity, as well as decay type and half-life. The second is the dose model for the accident scenario considered.

A. NUCLEAR DATA EVALUATIONS

Currently 3 nuclear decay data evaluations are available in SOFT:

- ICRP-107
- ENDFBVIII.0
- JEFF3.3

JEFF3.3 and ENDFBVIII.0 are generated based on the NEA databases and have been set up with the same format as the one related to ICRP-107 with a python script.

The nuclear data is stored inside text files with the format established in ICRP-107:

- A .NDX file contains general information of the radionuclides available, such as half-lives, decay types, but also pointers to the other files lines to easily find values of interest;
- A .BET file contains the beta+/beta− spectrum;
- A .RAD file contains all the discrete radiations emissions and intensities;
- A .NSF file contains the neutrons multigroup spectrum.
- Also, the databases contain a high number of radionuclides which do not have complete decay data. These radionuclides with incomplete information have been excluded from the final database used by the software. The total number of included radionuclides is available in Table 1.

The radionuclides are excluded on the following basis:

- A radionuclide contains a decay mode with no associated radiation type. This is the case in the libraries when the decay mode is known but the spectrum of the radiations is not;
- A radionuclide contains a continuous gamma spectrum;
- A radionuclide contains a continuous beta spectrum without any beta endpoint.

TABLE 1. Number of radionuclides considered in each nuclear data evaluation for the computation of Q-Values.

	ICRP-107	ENDFBVIII.0	JEFF3.3
N. of radionuclides included	1252	1712	1502

B. TRANSFER FUNCTION MODELS

Different transfer function models are implemented in the software since they are still being studied by the IAEA A1/A2 working group. These models are constructed from the following parameters:

- ➢ Irradiation geometry (ICRP-116 coefficients),
- ➢ Output from the Monte-Carlo simulation code, fluence or energy deposited,

- ➢ Simulation Monte-Carlo code used to produce these outputs,
- ➢ Geometry,
- ➢ The nuclear data,
  - used in the simulation code,
  - used for decay emissions,
- ➢ Interpolation methods used:
  - to compute transfer functions from fluences,
  - to interpolate the dose at a specific energy emission,
- ➢ Daughters considerations,
- ➢ Material compositions,
- ➢ Shielding,
- ➢ ...etc.

The principle of using transfer functions has been adopted by the working group and we will refer to this approach as a model. Consequently, a model groups different assumptions, summarized as a transfer function. These transfer functions are then used as input in the software to compute Q-Values under their respective assumptions.

A transfer function describes the dose, or dose rate, relating to one of the scenarios in Figure 1, for one primary particle emitted at a specific energy for the considered geometry.

As the different models consist of transfer functions read from the input files, the general calculation method is similar for all models but the constitution of the transfer functions can differ according the assumptions adopted.

The transfer function database contains all the transfer functions of each scenario. A file is available for each primary particle, each model developed within the working group and for each irradiation geometry conversion factor from ICRP-116 (example of text file name Photon_CERN_ISO). Each file contains columns, the first being the energy in MeV and the others the transfer function value at the corresponding energy for each Q-Quantity (Figure 2).

#Energy	QA	QB	QEYE	QD
#MeV	Sv/prim	Sv/prim	Sv/prim	Sv/prim
1.00E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.00E+00
1.50E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.00E+00
2.00E-02	2.1805E-19	8.5188E-19	1.3132E-18	0.00E+00
2.50E-02	3.2479E-17	7.9430E-17	1.2352E-16	0.00E+00
3.00E-02	3.5395E-16	5.9010E-16	9.2372E-16	0.00E+00
3.50E-02	1.2143E-15	1.6197E-15	2.4902E-15	0.00E+00
4.00E-02	2.4967E-15	2.7484E-15	4.1592E-15	0.00E+00
4.50E-02	3.8697E-15	3.8440E-15	5.6825E-15	0.00E+00
5.00E-02	5.1649E-15	4.6862E-15	6.7828E-15	0.00E+00
5.50E-02	6.3453E-15	5.5060E-15	7.8047E-15	0.00E+00
6.00E-02	7.3650E-15	6.1418E-15	8.5394E-15	0.00E+00
6.50E-02	8.2925E-15	6.8048E-15	9.3752E-15	0.00E+00
7.00E-02	9.1013E-15	7.3781E-15	1.0058E-14	0.00E+00
7.50E-02	9.9183E-15	8.0651E-15	1.0867E-14	0.00E+00
8.00E-02	1.0662E-14	8.7181E-15	1.1595E-14	0.00E+00
8.50E-02	1.1447E-14	9.4705E-15	1.2415E-14	0.00E+00
9.00E-02	1.2187E-14	1.0194E-14	1.3187E-14	0.00E+00
9.50E-02	1.2887E-14	1.0884E-14	1.3916E-14	0.00E+00
1.00E-01	1.3555E-14	1.1545E-14	1.4609E-14	0.00E+00
1.10E-01	1.5083E-14	1.3065E-14	1.6396E-14	0.00E+00
1.20E-01	1.6551E-14	1.4502E-14	1.8137E-14	0.00E+00
1.30E-01	1.7974E-14	1.5893E-14	1.9845E-14	0.00E+00
1.40E-01	1.9361E-14	1.7253E-14	2.1528E-14	0.00E+00
1.50E-01	2.0718E-14	1.8597E-14	2.3190E-14	0.00E+00
1.60E-01	2.2200E-14	2.0016E-14	2.4900E-14	0.00E+00
1.70E-01	2.3672E-14	2.1455E-14	2.6602E-14	0.00E+00

FIGURE 2. Example of transfer function database as input for the software. First line details the scenario (QA, QB...), second line the unit of the values. Then first column described the particle energy, other columns the dose per emitted particle in the corresponding scenario. Each filename is associated to one specific emitted particle and one specific model.

Transfer functions yield the dose for a specific primary particle emitted at a certain energy, considering associated assumptions and scenario. The transfer functions are convoluted with the nuclear decay data as follows:

$$dose_{Qx} = \mathrm{A}\sum_p \left(\int_E \mathcal{H}_p(E,Qx)\xi(E)dE + \sum_E \mathcal{H}_p(E,Qx) * \theta(E) \right)$$

where:

A is a normalization factor

$\mathcal{H}_p\,(E, Qx)$ is the transfer function of the scenario Qx at energy E for a specific particle p (Sv/primary)

$\xi\,(E)$ is the continuous spectrum of the decay at energy E (particles emitted per MeV per nuclear transformation)

$\theta\,(E)$ is the discrete spectrum of the decay at energy E (yeld of the radiation, per nuclear transformation) $dose_{Qx}$ is the dose in the scenario Qx (Sv/h/Bq)

All the interpolations of transfer functions performed in the software are double logarithmic interpolations.

The first paragraph of this section gives a general overview of the general assumptions presently implemented. Then, the other sections describe some of the current models implemented in the software.

1) GENERAL ASSUMPTIONS

Some assumptions have been performed for the construction of the software and must be mentioned here to avoid misinterpretation of the results.

- In ICRP-107, some beta spectra are mixed when they are beta+/beta− emitters. It is impossible to reconstruct the part coming from positron emission and electron emission separately. In this case, these beta spectra from ICRP-107 have been replaced by those from ENDFBVIII or JEFF3.3. The exhaustive list of radionuclides in this case is the following: Ag-106, Ag-108, As-74, Br-78, Br-80, Cl-36, Cs-130, Cs-132, Cu-64, Eu-150m, Eu-152, Eu-152m, I-126, I-128, In-112, In-114, K-40, Mn-54, Rn-84, Rh-102, Sb-122, Tm-168.
- For JEFF and ENDF databases, the generation of the beta spectra with the FERMI equation is performed using BTSPEC tool.[1] We adapted this tool to read today's nuclear data but it can lead to inaccurate values for some radionuclides. The inaccuracies are small but should still be mentioned. These radionuclides are those for which forbidden transitions of types above 3 exist in the frame of beta emissions [15]. For example, this is the case of V-50, Ag-97, In-102, Pa-231. It has been checked by comparison with JANIS4.0 [16] that the impact on the spectra are negligible for our calculations.
- In ICRP-107, some heavy elements like Cf-246 have a beta spectrum tabulated whereas they are not beta emitters. These spectra have been crosschecked with ENDF and JEFF and deleted from ICRP-107 files.
- A radionuclide has been considered as alpha emitter if more than 10^{-3} of its decay are alpha decays. In SSG-26,

[1] http://www.oecd-nea.org/tools/abstract/detail/nea-0866/

it is mentioned that if daughters of a radionuclide have this property, then the radionuclide must be considered as an alpha emitter. However, in Ref. [1] table 1.2, Pb-210 for example, is not considered as an alpha emitter, whereas Bi-210, one of the first 2 daughters, is an alpha emitter. For this work, we have decided not to consider progeny for alpha emitters.

- Submersion and inhalation doses are not yet calculated in the software. They are extracted from the literature. Submersion doses have been considered as described in IAEA SSG-26. No daughters are considered. Inhalation doses are extracted from [1], [17], [18]. The most penalizing value between these three references is considered for 5 μm particles, as suggested in IAEA SSG-26.

2) IAEA2012 MODEL

This model has been developed in coherence with the current IAEA SSG-26 publication. The values and calculation methods are fully described in [2]. The Table 2 below summarizes the characteristics and assumptions of this model.

TABLE 2. Summary of the assumptions to construct a model based on the current regulation (IAEA2012).

IAEA 2012				
	QA	**QB**	**QD**	**QEYE**
Geometry of Monte-Carlo simulation	No geometry. Analytical calculation described in IAEA SSG-26	Isotropic point source surrounded by a 1-meter diameter sphere of skin	Isotropic disk source (radius 7 cm) at contact of skin phantom slab (10x10x10cm3)	-
Skin material	ICRU 51 composition			
Daughters	Considered according to IAEA SSG-26 rule			-
Shielding of radioactive source	No	Calculated according to SSG-26	No	-
MC simulation code	Fluka 2011.2c6			-
Primary particles considered	Photons	Electrons / positrons	Electrons / positrons	-
Secondary particles considered	Photons	Electrons / positrons	Electrons / positrons	-
Scored quantity in Monte-Carlo code	Deposited energy between 0.99 and 1.01 cm of skin	Deposited energy between 50 and 90 µm of skin	Deposited energy in a cylinder between 50 and 90 µm of skin with radius of 0.5642 cm	-
Transfer function generation method	By transforming deposited energy per primary per energy in Sv/h/Bq per primary per energy with a normalization factor		By transforming deposited energy per primary per energy in Sv.m2/s/Bq per primary per energy with a multiplicative factor	-
Energy range of transfer function	1 keV to 12 MeV			-

3) IMPROVED MODEL DEVELOPED AT CERN ACCORDING TO WORKING GROUP DISCUSSIONS

Following the discussion of the working group, it has been decided to build the new transfer functions set by considering irradiation geometries as described in ICRP-116. The construction of emission-to-dose curves from fluence in the case of "CERN AP, PA, ISO" models is performed to simplify the calculations in the software and limit the quantity of input data. It is easier to manipulate emission-to-dose transfer functions instead of fluences and this idea has been adopted by the working group.

With FLUKA, simulations have been performed for different energies of incident particles (photons, electrons, positrons). We consider the fluence $\Phi_{E,p}\left(E', p', Qx\right)$ of particles p' at energy E' for a primary particle p emitted at energy E in the scenario Qx. Secondary photons, electrons and positrons differential fluences as a function of energy have been scored at one meter from the source for 1 keV to 12 MeV photons, electrons and positrons primary emissions. A binning of 1 keV has been selected in order to simplify the integration and increase the accuracy of interpolations in energy. The Figure 3 presents a set of fluences of secondary photons, positrons and electrons, scored at 1 meter from the source in air. This set is calculated with FLUKA for a primary electron emitted at 10 MeV.

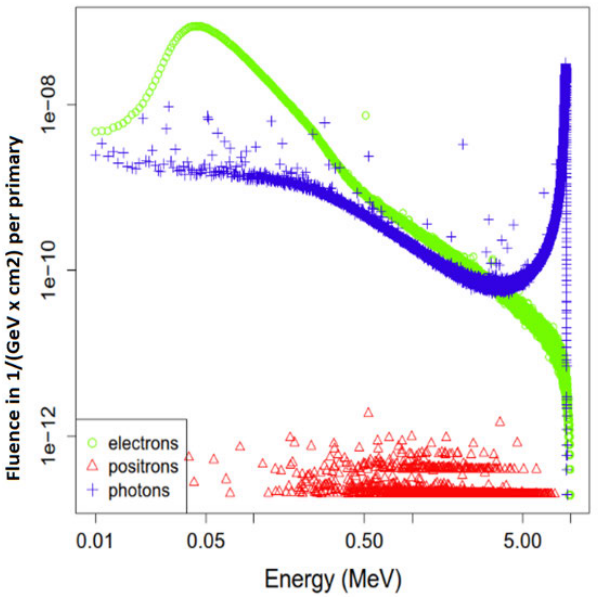


FIGURE 3. Fluences of photons, positrons and electrons for electrons emitted at 10 MeV at 1 meter from the source in air.

Geometry dependent fluence-to-dose coefficients are taken from ICRP-116 to transform fluences into doses. They will subsequently be denoted $C_g\left(E, p'\right)$ for geometry g and particle p′.

The transfer function $\mathcal{H}_{p,g}$ (E,Qx) for particle p emitted at E with the irradiation geometry g in the scenario Qx can be

expressed as follows:

$$\mathcal{H}_{p,g}(\mathrm{E},Qx) = 3600 * 10^3 * 10^{-12} \sum_{p'} \int_{1keV}^{12MeV} \Phi_{E,p}\left(E', p', Qx\right) C_g\left(E, p'\right) dE$$

The factor 10^3 is used to transform the energy unit from FLUKA in GeV to MeV. The factor 3600 allows for transforming the quantity "per primary" into "disintegration per unit time". The factor 10^{-12} comes from the definition of $C_g\left(E, p'\right)$ given in pSv $*$ cm^2. As the energy binning of the fluence data is given in steps of 1 keV, the integral is similar to a summation of the fluence for steps of 1 keV. So,

$$\mathcal{H}_{p,g}(\mathrm{E},Qx) \approx 3600 * 10^3 * 10^{-12} \times \sum_{p'} \sum_{i=1keV}^{12000} \Phi_{E,p}\left(\frac{2i+1}{2}, p', Qx\right) \times C_g\left(\frac{2i+1}{2}, p'\right)$$

Following this equation, the transfer function is built by punctual evaluations of $\mathcal{H}_{p,g}(\mathrm{E},Qx)$, thanks to simulations performed for different primary particles p emitted at different energies E. So, for a particle p emitted for a scenario Qx and considering an irradiation geometry g, we can display the curve of secondary particle doses as a function of energy as shown in Figure 4 below.

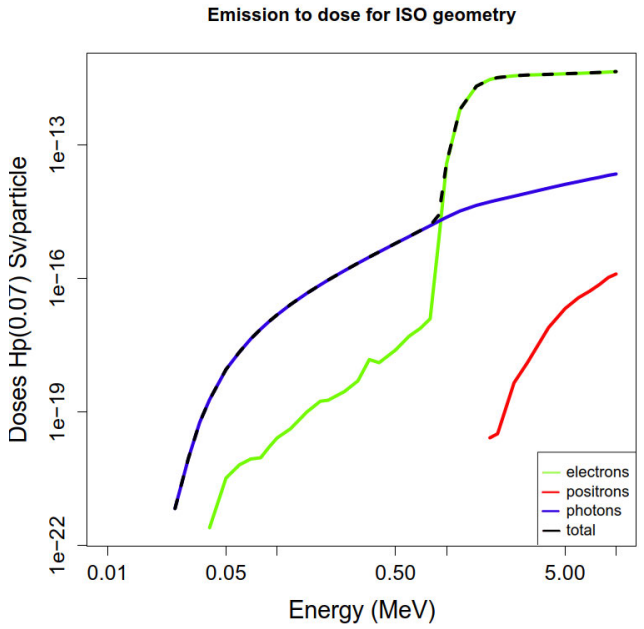


FIGURE 4. Emission-to-dose transfer functions built from fluence data for incident electrons at 1 m from the source (QB scenario) with ISO geometry.

As coefficients from ICRP-116 are not known for each energy, an interpolation is performed to determine values for energies of interest. A linear-linear interpolation has been chosen to avoid issues linked to the fact that some coefficients (e.g. eye lens) have a value of 0.

These models are currently under discussion in the working group A1/A2 [2019]. They are used to discuss the assumptions and compare values coming from the different models developed within the working group.

The Table 3 below summarizes the characteristics of CERN's model.

TABLE 3. Summary of the assumptions associated with improved CERN Q-System model in the current development state for antero-posterior, postero-anterior and isotropic irradiation geometries.

CERN AP/PA/ISO				
	QA	**QB**	**QEYE**	**QD**
Geometry of Monte-Carlo simulation	Isotropic point source in air	Isotropic point source in air	Isotropic point source in air	Isotropic disk source (radius 3.5 cm) at contact of skin phantom slab (10x10x10cm 3)
Skin material	No skin in the geometry. Fluences scored in air			ICRP-110 composition
Daughters	Not considered yet as the way to consider them has not been frozen in the working group			
Shielding of radioactive source	0.5 mm of Steel_316 with 7.8 g/cm3 density and PNNL [19] composition around the source			No
MC simulation code	Fluka 2011.2c6			
Primary particles considered	Photons / Electrons / Positrons	Photons / Electrons / Positrons	Photons / Electrons / Positrons	Photons / Electrons / Positrons
Secondary particles considered	Photons / Electrons / Positrons	Photons / Electrons / Positrons	Photons / Electrons / Positrons	Photons / Electrons / Positrons
ICRP-116 coefficients used for respective particles	Photons: Effective dose Male Table A1 Electrons: Effective dose Male Table A3 Positrons: Effective dose Male Table A4	Photons: Skin Male Table B26 Electrons: Skin Male excel file[2] Positrons: Skin Male excel file	Photons: Eye lens Male Table F1 Electrons: Eye lens Male Table F2 Positrons: Eye lens Male excel file	None
Scored quantity in Monte-Carlo code	Fluence of particles crossing a sphere surrounding the source located at 1m from this one			Deposited energy in a cylinder between 50 and 100 µm of skin with radius of 0.5642 cm
Transfer function generation method	By reconstructing transfer function with ICRP-116 coefficients: -Pointwise data for Photons / Electrons / Positrons -Neutrons not included yet			By transforming deposited energy per primary at energy E in Sv.m2/s/Bq at energy E with a normalization factor
Energy range of transfer function	1 keV to 12 MeV for Photons / Electrons / Positrons			

4) NUMERICAL STEPS FOR CALCULATION OF THE DOSE

Post-processing operations for CERN's models are summarized in Figure 5 and explained in the next paragraph. These

operations are those coded in SOFT for now, but can be modified depending on working group decisions to standardize this process.

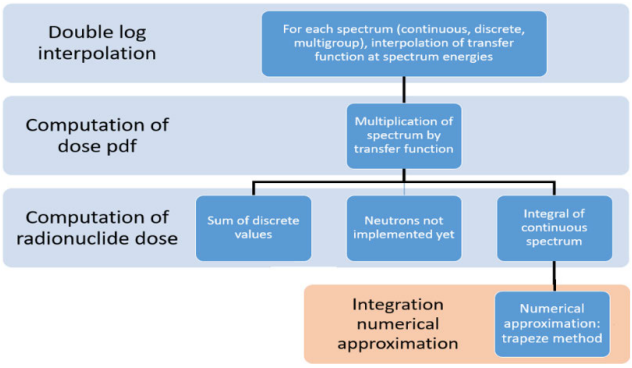


FIGURE 5. Post-processing operations for dose computation.

Interpolations: All the interpolations of transfer functions performed in SOFT are double logarithmic interpolations. For each spectrum from ICRP-107, transfer functions are interpolated at the energy values of the spectrum.

Computation of Dose Probability Density Function (PDF): Spectrums are multiplied by transfer functions to calculate the dose as a function of particle energy emission.

Discrete radiations spectra are stored in ICRP-107.RAD file. The discrete spectra are computed as follows:

$$Dose_{rn,discrete,p,g}(Qx) = \sum_i \mathcal{H}_{p,g}\,(E_i,\, Qx)\; disc\,(E_i,\, p)$$

where

$Dose_{rn,discrete,p}$ is the dose in a specific scenario Qx for a radionuclide rn coming from discrete emissions for a specific particle p calculated with irradiation geometry g.

$\mathcal{H}_{p,g}\,(E_i)$ is the transfer function converting particle p emitted at energy E_i to dose with irradiation geometry g.

$disc\,(E_i, p)$ is the discrete spectrum at energy E_i for particle p.

a: CONTINUOUS SPECTRUM FOR Beta+/Beta−

Beta+/Beta− spectrum are stored in ICRP-107.BET files. Spectrum are described per energy value in MeV from 0 to the maximum beta endpoint. They are normalized per nuclear transformation and the integral of the spectrum takes the value of the decay mode branching ratio.

The current methods used to compute the dose are based on different assumptions having different effects on the final results.

As previously explained, the transfer functions transform a particle emission at an energy to a dose in a specific scenario.

The integral is performed as follows:

$$Dose_{rn,continuous,p,g}(Qx) = \int \mathcal{H}_{p,g}\,(E,\, Qx)\; Sp\,(E,\, p,\, Qx)\; dE$$

where

$Dose_{rn,continuous,p,g}(Qx)$ is the dose in a specific scenario Qx for a radionuclide rn coming from continuous emission for a specific particle p with irradiation geometry g.

$\mathcal{H}_{p,g}\,(E,\, Qx)$ is the transfer function converting particle p emitted at energy E to a dose in scenario Qx with irradiation geometry g.

b: DISCRETE SPECTRUM FOR PHOTONS AND DISCRETE ELECTRONS

$Sp(E, p, Qx)$ is the continuous spectrum value for particle p at energy E in scenario Qx.

Then the trapezoidal algorithm is used for the numerical calculation of the integral.

$$Dose_{rn,continuous,p,g}(Qx) \approx \sum_i (E_{i+1} - E_i) * \frac{\mathcal{H}_{p,g}(E_{i+1},Qx)Sp(E_{i+1},p,Qx) - \mathcal{H}_{p,g}(E_i,Qx)Sp(E_i,p,Qx)}{2}$$

c: CONTINUOUS MULTIGROUP SPECTRUM FOR NEUTRONS

This part concerns neutron decay data that is stored in the ICRP-107.NSF file with the multigroup formalism. No method has been coded yet to compute $Dose_{rn,neutron,g}$.

d: TOTAL DOSE VALUE

The total dose is the sum of all the previous contributions for each particle p emitted for a specific scenario Qx and irradiation geometry g.

$$Dose_{rn,total,g}(Qx) = Dose_{rn,neutron,g}(Qx) + \sum_p Dose_{rn,continuous,p,g}(Qx) + \sum_p Dose_{rn,discrete,p,g}(Qx)$$

5) OTHER MODELS

Other models have been developed by Germany and France. These models are not the subject of this paper but are based on the assumptions described in [12].

V. SOFTWARE DESCRIPTION

The software tool is programmed in C++ displaying a Graphical User Interface (GUI). Different modules are currently included and will evolve during the discussions at IAEA. These modules are described below. The software is available on Linux and Windows and needs approximatively 250 MB of disk space, mainly due to the nuclear data tabulated and 70 MB of Random Access Memory (RAM).

It uses different libraries:

- Graphviz for plotting decay chains,

[2]With ICRP-116 is given an excel sheet including the whole set of irradiation geometry coefficients

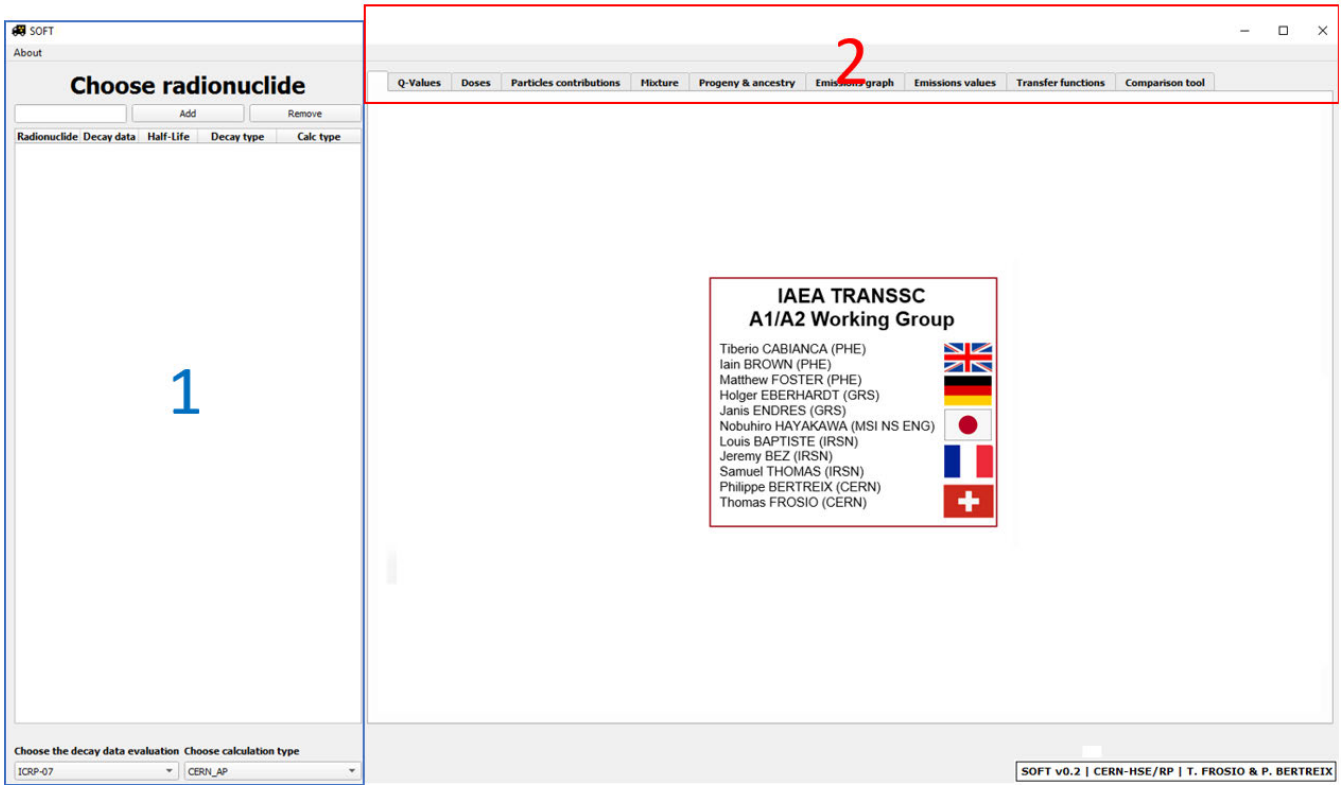
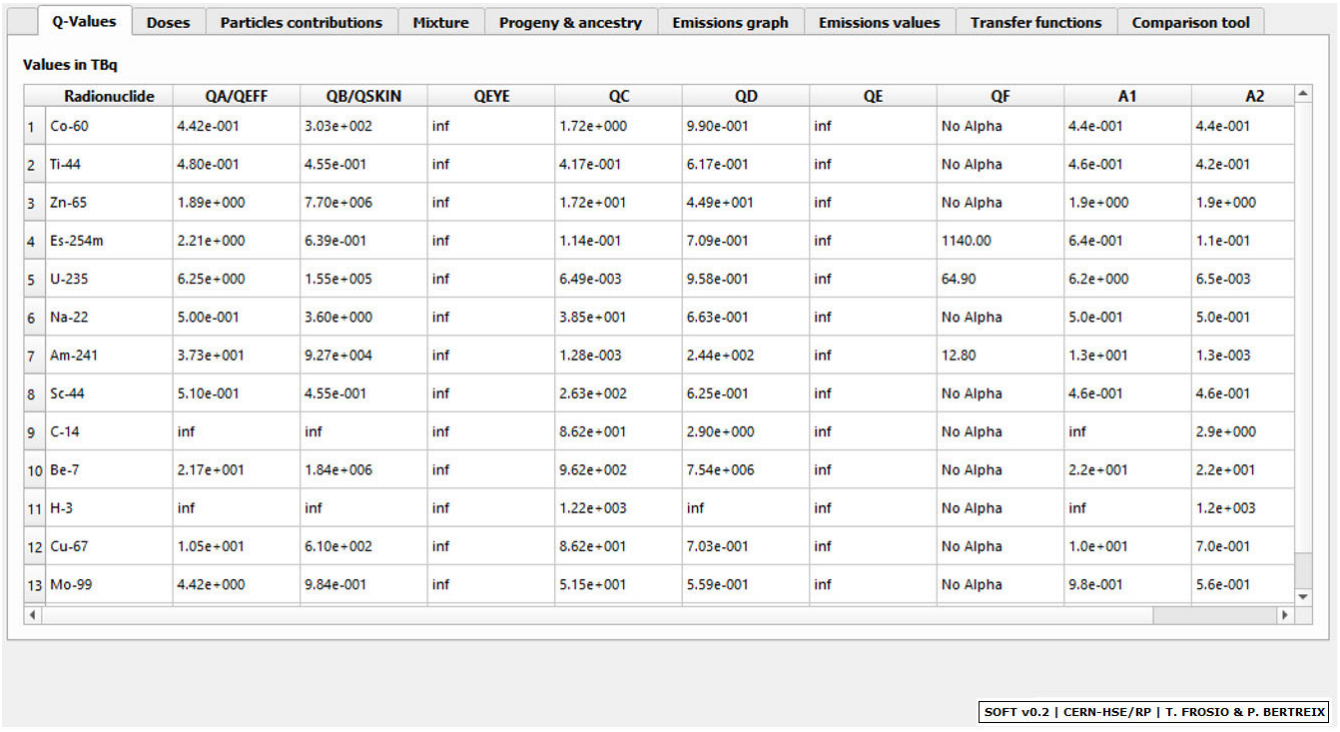


FIGURE 6. Overview of SOFT.



	Radionuclide	QA/QEFF	QB/QSKIN	QEYE	QC	QD	QE	QF	A1	A2
1	Co-60	4.42e-001	3.03e+002	inf	1.72e+000	9.90e-001	inf	No Alpha	4.4e-001	4.4e-001
2	Ti-44	4.80e-001	4.55e-001	inf	4.17e-001	6.17e-001	inf	No Alpha	4.6e-001	4.2e-001
3	Zn-65	1.89e+000	7.70e+006	inf	1.72e+001	4.49e+001	inf	No Alpha	1.9e+000	1.9e+000
4	Es-254m	2.21e+000	6.39e-001	inf	1.14e-001	7.09e-001	inf	1140.00	6.4e-001	1.1e-001
5	U-235	6.25e+000	1.55e+005	inf	6.49e-003	9.58e-001	inf	64.90	6.2e+000	6.5e-003
6	Na-22	5.00e-001	3.60e+000	inf	3.85e+001	6.63e-001	inf	No Alpha	5.0e-001	5.0e-001
7	Am-241	3.73e+001	9.27e+004	inf	1.28e-003	2.44e+002	inf	12.80	1.3e+001	1.3e-003
8	Sc-44	5.10e-001	4.55e-001	inf	2.63e+002	6.25e-001	inf	No Alpha	4.6e-001	4.6e-001
9	C-14	inf	inf	inf	8.62e+001	2.90e+000	inf	No Alpha	inf	2.9e+000
10	Be-7	2.17e+001	1.84e+006	inf	9.62e+002	7.54e+006	inf	No Alpha	2.2e+001	2.2e+001
11	H-3	inf	inf	inf	1.22e+003	inf	inf	No Alpha	inf	1.2e+003
12	Cu-67	1.05e+001	6.10e+002	inf	8.62e+001	7.03e-001	inf	No Alpha	1.0e+001	7.0e-001
13	Mo-99	4.42e+000	9.84e-001	inf	5.15e+001	5.59e-001	inf	No Alpha	9.8e-001	5.6e-001

FIGURE 7. Q-Values module.

- QT for the GUI,
- QCustomPlot for the different graphics that can be produced,
- Boost libraries for a general purpose.

The scope of the software was initially to provide information about doses, Q-Values and data related to radionuclides

produced in some of CERN's installations which are not always tabulated in the dangerous goods regulation for the shipping of radioactive materials [20].

Then, real advantages of using this software within the working group emerged, particularly to compare the different models.

SOFT is currently based on nine modules performing different calculations. Figure 6 shows an overview of the software main window.

The left part of the window (1) is the entry point for the user. It allows the user to add or remove radionuclides. On the bottom of this part, the user can choose which decay database and model (denoted ''calculation type'') they want to use. For each radionuclide added, there is a quick summary giving the decay database, the half-life, the type of decay and the model selected. If a radionuclide doesn't exist in the evaluation or is stable, the following message will appear just above the drop-down menu of the decay database: *Radionuclide: XX-YY not recognized or stable.*

The calculation methods are described in [2] regarding the current regulation limits and in paragraph IV of this document for the on-going work regarding the regulation update. The software will be modified during all the development process of the new models at IAEA, to include the latest decisions. Upon completion, the last release will keep only the model selected by the working group and the associated decay database.

The upper part of the results' view (2) is made of 9 different modules, which show the values/data the user wants to see. These 9 modules are respectively:

- Q-Values: this module provides Q-Values for a given radionuclide, in accordance to the database and the model chosen.
- Dose and dose rate: it gives information of dose and dose rate for a given radionuclide, in the specific scope of the Q-System.
- Particle contributions: this part describes the contribution of each particle to the dose originating from a selected radionuclide, for each Q-Value, in percent.
- Mixture: allows for the computation of radionuclide mixture limits with an overview of the main contributor radionuclides. It also determines if a package can be shipped as Type-A or not.
- Progeny & ancestry: this module generates the progeny's and ancestry's chain of a radionuclide with a graphical representation.
- Emissions graph: all the information regarding the decay emissions (photon / alpha / beta / mono-energetic electrons) are summarized here. This data is directly extracted from decay data evaluations
- Emissions values: shows a table of emission data stored in decay evaluations in text format.
- Transfer functions: provides the curves used to calculate dose and dose rate for a radionuclide.
- Comparison tool: compares different models included in SOFT as well as different libraries, described later in this document

For a radionuclide, the general overview of the Q-Values is shown in Figure 7. To display the Q-Values of a radionuclide, the user double clicks the desired radionuclide in the left column of the software.

Results can be saved in CSV format using the right click button of the mouse.

In case Q-Values and doses of all radionuclides from a database need to be computed, the user can write ''all'' in the radionuclide field.

A. DOSE AND DOSE RATE MODULE

This module calculates all the doses and dose rates useful for the determination of the Q-Values. These doses and dose rates (ept for QA, ebeta for QB, einh for QC, hskin for QD, hesubm and hskinsubm for QE, heye for QEYE) are calculated in accordance with the IAEA SSG-26 publication [1] or the latest statements from the IAEA working group, depending on the model chosen.

Like the Q-Values module, to display the doses and dose rates for a specific radionuclide, the user double clicks the desired radionuclide in the left column of the software. Results can also be saved using the right click button of the mouse. Results can also be computed for all radionuclides as in the previous paragraph. An example of results is shown in Figure 9.

B. PARTICLES CONTRIBUTIONS MODULE

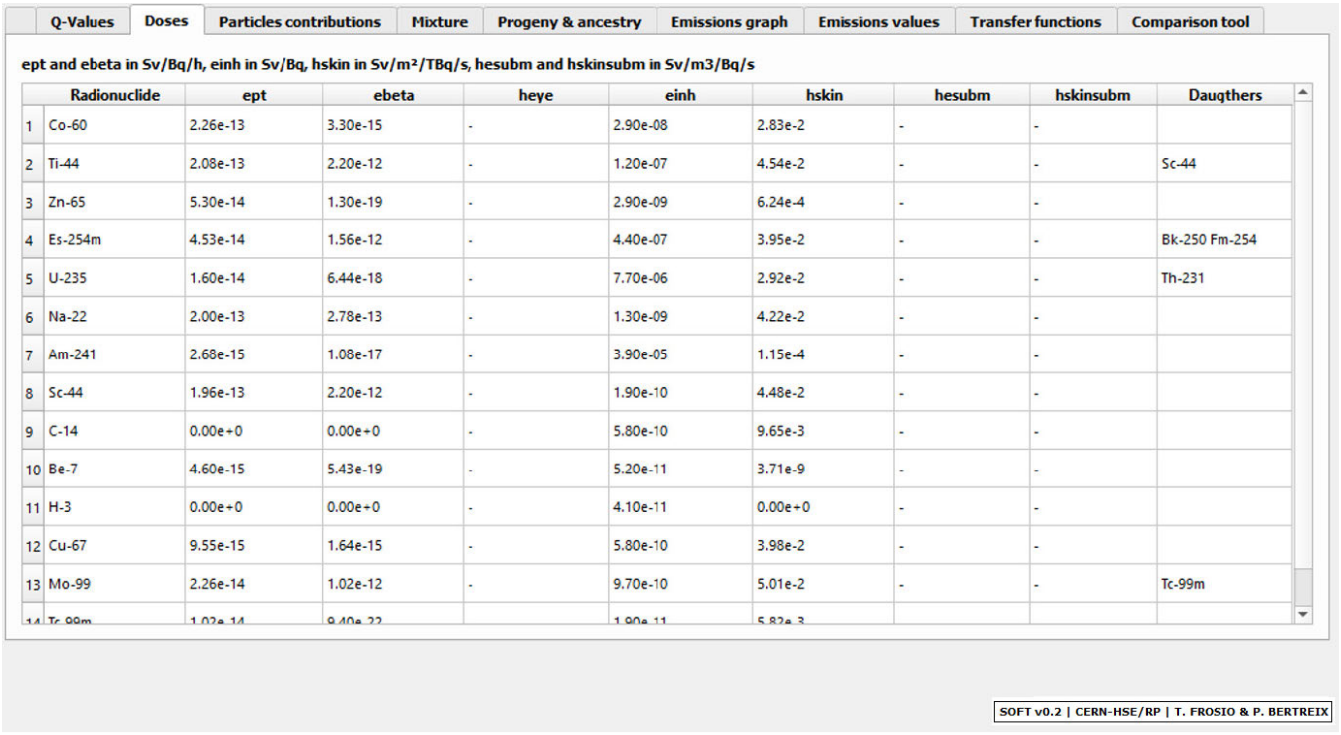
The particle contribution module allows for plotting bar charts in which each particle contribution to the dose is displayed for the scenario linked to QA, QB, QD, QEye. In the example presented in Figure 10, we observe the contributions of particles for Es-254m radionuclide with the ICRP-107 decay database and the IAEA2012 model. For example, in the QB scenario, beta minus radiation is predominant for the dose contribution (78.70 %) and then, the 21.30 % of the remaining dose come from discrete electrons (Auger and Internal Conversion).

C. MIXTURES MODULE

The mixture module allows for computing transport limits for a mixture of radionuclides, according IAEA SSR-6 [2] §405. The user selects the number of radionuclides to add to the package on the right side of the table. Then, they complete the radionuclide names and activities in Becquerel. A preformatted CSV file (radionuclide, activity) can also be downloaded, instead of defining radionuclides one by one (Figure 8).

```
Co-60,0
Ti-44,1E+05
Zn-65,1E+10
Es-254m,800000000
U-235,1E+09
Na-22,100000000
Am-241,1E+09
```

FIGURE 8. Example of.csv file to be read by the software.



	Radionuclide	ept	ebeta	heye	einh	hskin	hesubm	hskinsubm	Daugthers
1	Co-60	2.26e-13	3.30e-15	-	2.90e-08	2.83e-2	-	-	
2	Ti-44	2.08e-13	2.20e-12	-	1.20e-07	4.54e-2	-	-	Sc-44
3	Zn-65	5.30e-14	1.30e-19	-	2.90e-09	6.24e-4	-	-	
4	Es-254m	4.53e-14	1.56e-12	-	4.40e-07	3.95e-2	-	-	Bk-250 Fm-254
5	U-235	1.60e-14	6.44e-18	-	7.70e-06	2.92e-2	-	-	Th-231
6	Na-22	2.00e-13	2.78e-13	-	1.30e-09	4.22e-2	-	-	
7	Am-241	2.68e-15	1.08e-17	-	3.90e-05	1.15e-4	-	-	
8	Sc-44	1.96e-13	2.20e-12	-	1.90e-10	4.48e-2	-	-	
9	C-14	0.00e+0	0.00e+0	-	5.80e-10	9.65e-3	-	-	
10	Be-7	4.60e-15	5.43e-19	-	5.20e-11	3.71e-9	-	-	
11	H-3	0.00e+0	0.00e+0	-	4.10e-11	0.00e+0	-	-	
12	Cu-67	9.55e-15	1.64e-15	-	5.80e-10	3.98e-2	-	-	
13	Mo-99	2.26e-14	1.02e-12	-	9.70e-10	5.01e-2	-	-	Tc-99m
14	Tc-99m	1.02e-14	9.40e-22		1.90e-11	5.82e-3			

FIGURE 9. Doses and dose rates module.

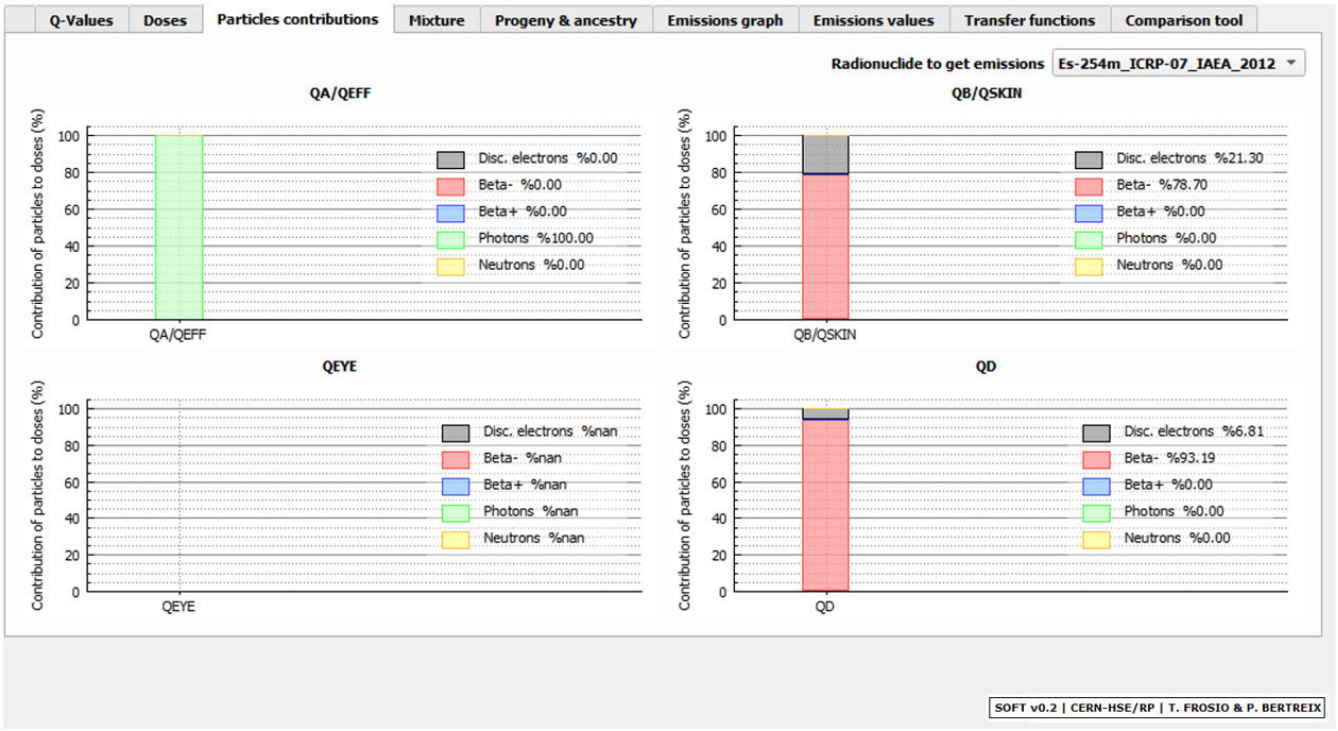


FIGURE 10. Particles contributions to dose module.

The software calculates the A1 and A2 limits of the mixture, as well as the mixture's activity (Figure 11). Then, this activity is compared to the limits. When this activity is below the limit, a message is written in green indicating that the package does not have to be a Type B package. Otherwise, a message is printed in red. The contribution of

each radionuclide to the mixture limit is displayed on the bar charts below the table so that the user can organize its shipping in a more efficient way.

D. EMISSION GRAPH MODULE

This module will plot all the emission data related to the radionuclide selected in the drop-down menu in the top right part of the window. The data coming from ICRP-107, JEFF3.3 or ENDF BVIII can be directly plotted in the software.

As for the progeny/ancestry module, the user can save emission data plotted as an image file for a selected radionuclide or for all the radionuclides selected in the left part (Figure 12). Plots can be saved with a right-click.

E. PROGENY / ANCESTRY MODULE

The progeny / ancestry module generates graphs of decay chains / ancestry chains for a radionuclide. The decay chain goes down until the latest stable nuclides are reached, and the ancestry chain links from all the parents who can at one point generate the specified radionuclide.

The radionuclide chosen is shaped into two circles, and the stable radionuclides are dark-coloured. The type of decay follows a specific colour code to have a better overview of the decay chain. Branching ratios are printed next to the arrow representing the type of decay.

Progeny and ancestry graphs can be generated using all the decay databases (ICRP-107, JEFF3.3 and ENDFBVIII).

If several radionuclides have been chosen by the user, they can display the one desired using the drop-down menu in top-right of the window. Users also have the option to save the decay chain as an image file for a selected radionuclide, or for all the radionuclides in the left part by right-clicking on the decay chain (Figure 13).

F. EMISSION VALUES MODULE

This module provides the emission data for the radionuclides selected using the top-right drop-down menu. It corresponds to data from ICRP-107, JEFF3.3 or ENDF BVIII used in the Emission graph module.

In Figure 14 an example of emission values for Co-60 - decay database ICRP-107 can be seen. The data is divided into emission types (Beta+, Beta-, discrete e-, gamma, alpha). If an emission is present in the decay database, the module will provide: 1) the energy of the emission in MeV, and 2) the intensity.

Data can be saved for a selected radionuclide or for all the radionuclides added in the left part as an html file.

G. TRANSFER FUNCTIONS MODULE

This module allows the user to display the emission to dose transfer function (associated to a model) used to compute

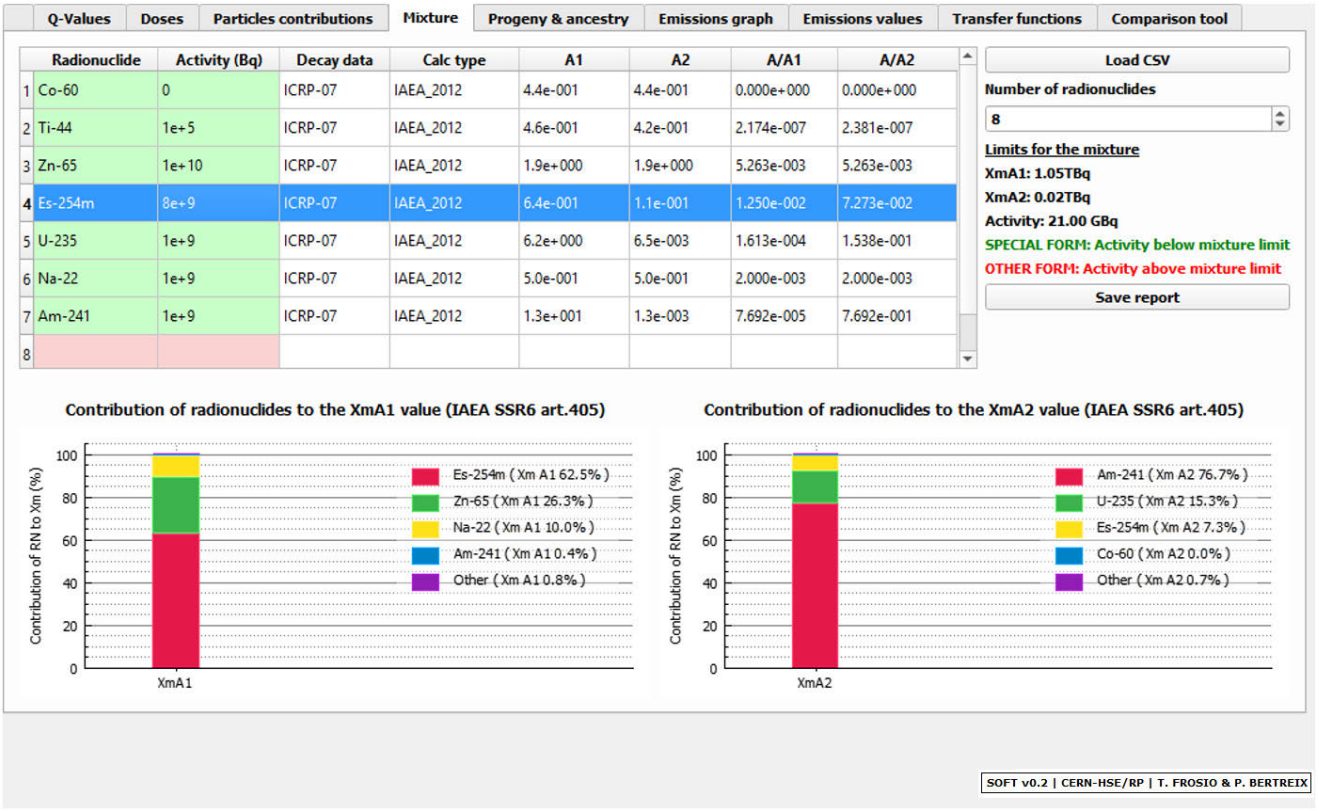


FIGURE 11. Mixture of radionuclides module.

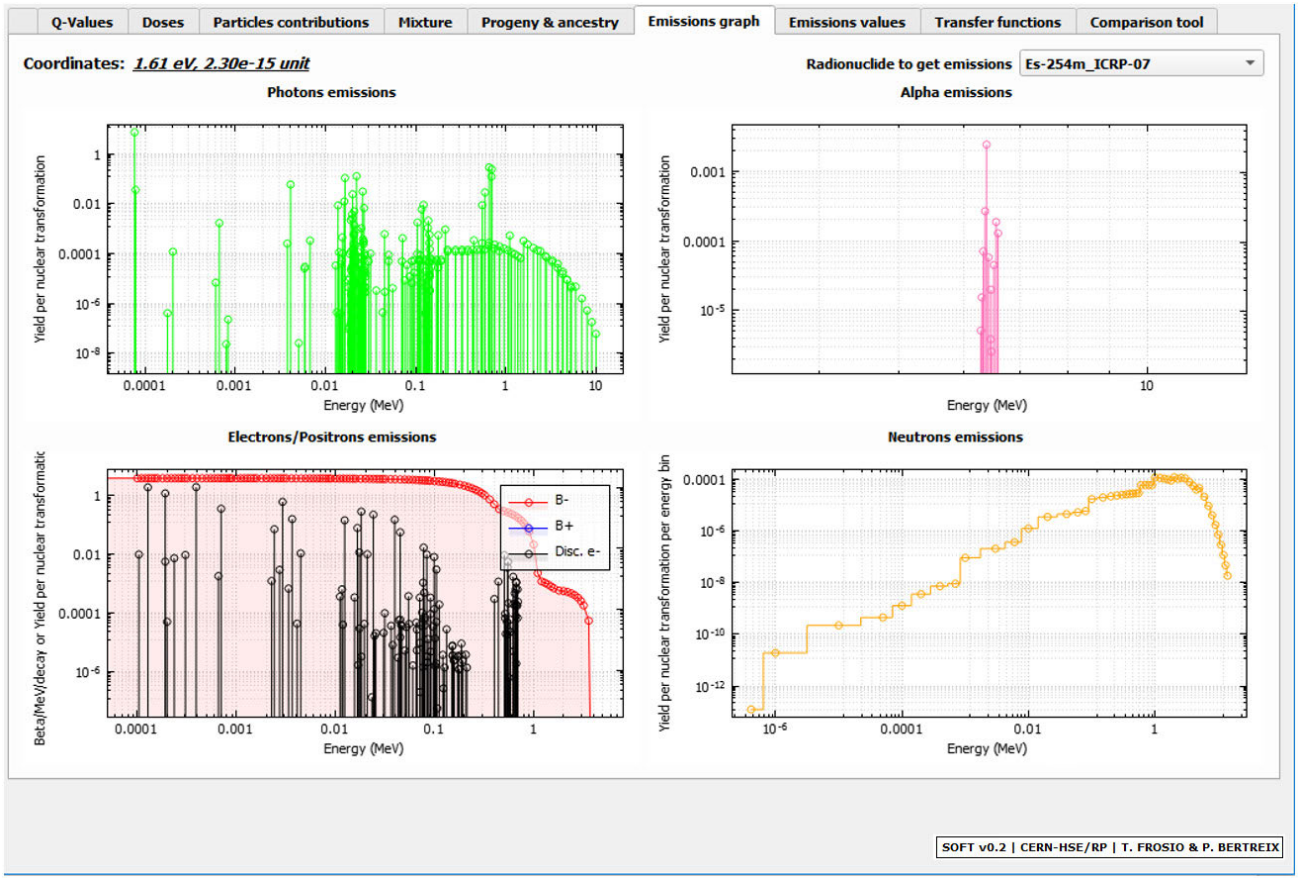


FIGURE 12. Emission graph module.

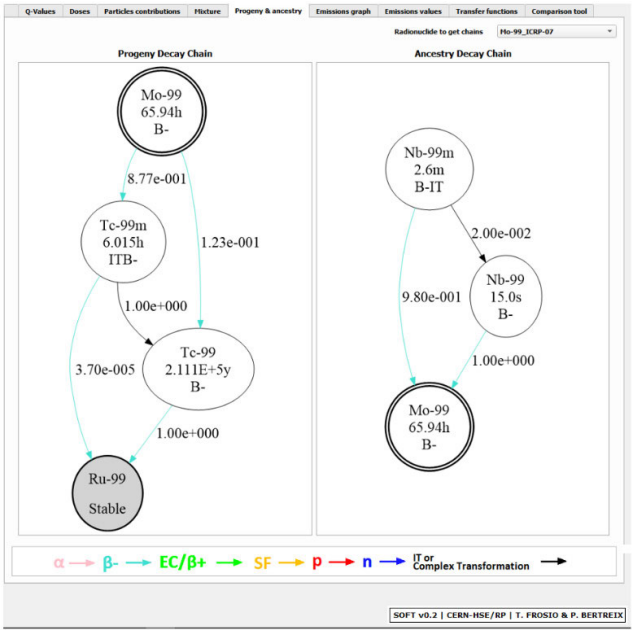


FIGURE 13. Progeny/ancestry module.

values in the Q-Values module and in the dose and dose rate module.

A drop-down menu on the top-right part of the module allows the user to plot transfer functions, including the ones which consider the latest statement of the A1/A2 working group, as shown in Figure 15 (CERN Isotropic model). To get a precise value of the transfer function at a specific energy, the user can move the mouse cursor over the curves. The coordinates of the cursor will be displayed on the top left of the window. The user can also zoom in/out and move the graph to target a specific value.

H. COMPARISON TOOL

The comparison tool compares the dose values coming from the different scenarios, with the different models and nuclear databases. The user selects a radionuclide using the top-left field, the models and the evaluations to compare (Figure 16). Then, they can choose how to compare the results:

- "Doses (Sv/Bq)" compares absolute dose values for the selected models;
- "Particle contribution to dose (%)" evaluates, for each model, the contribution of each particle to the dose;
- "Doses vs model 1" computes the ratio of dose between each model to model 1. The model 1 is defined by the user as the reference model and can be each of the aforementioned model;
- "Particle contribution to dose vs model 1" computes the ratio of the particle dose contribution to model 1.

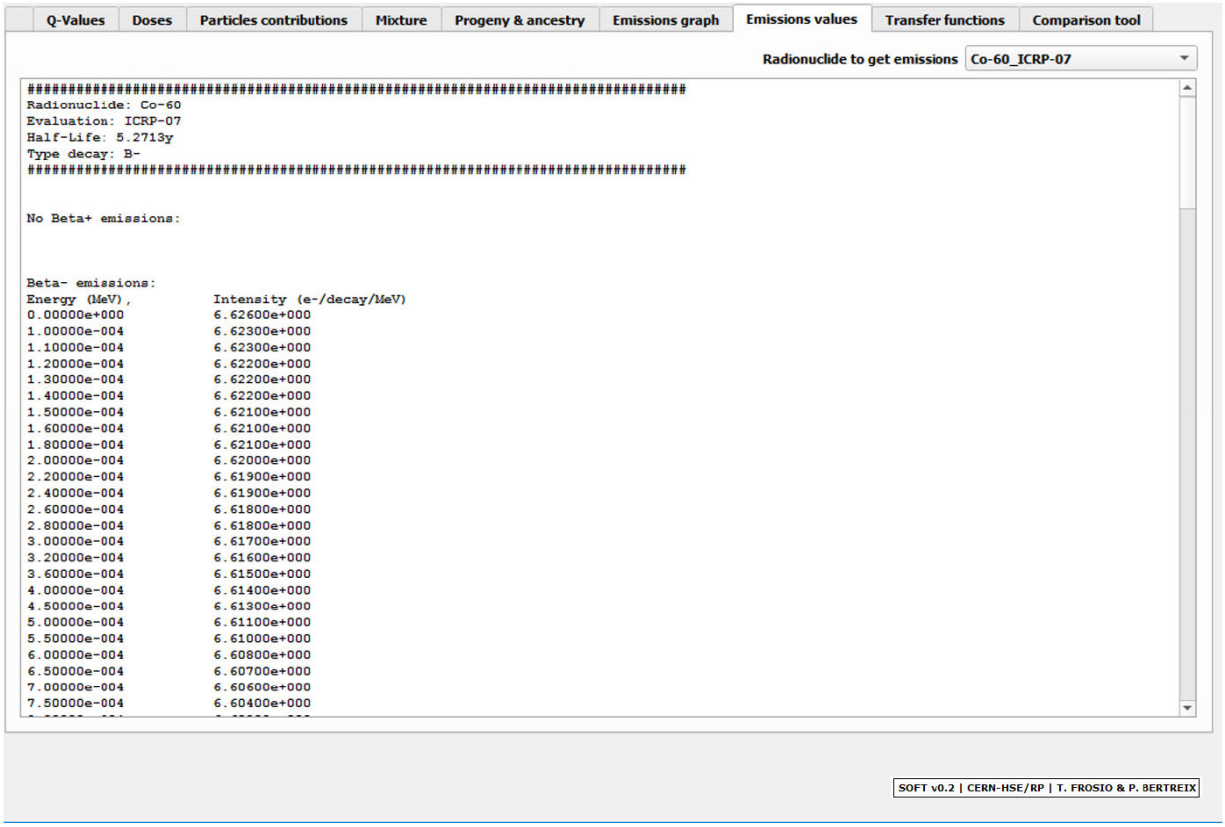


FIGURE 14. Emission values module.

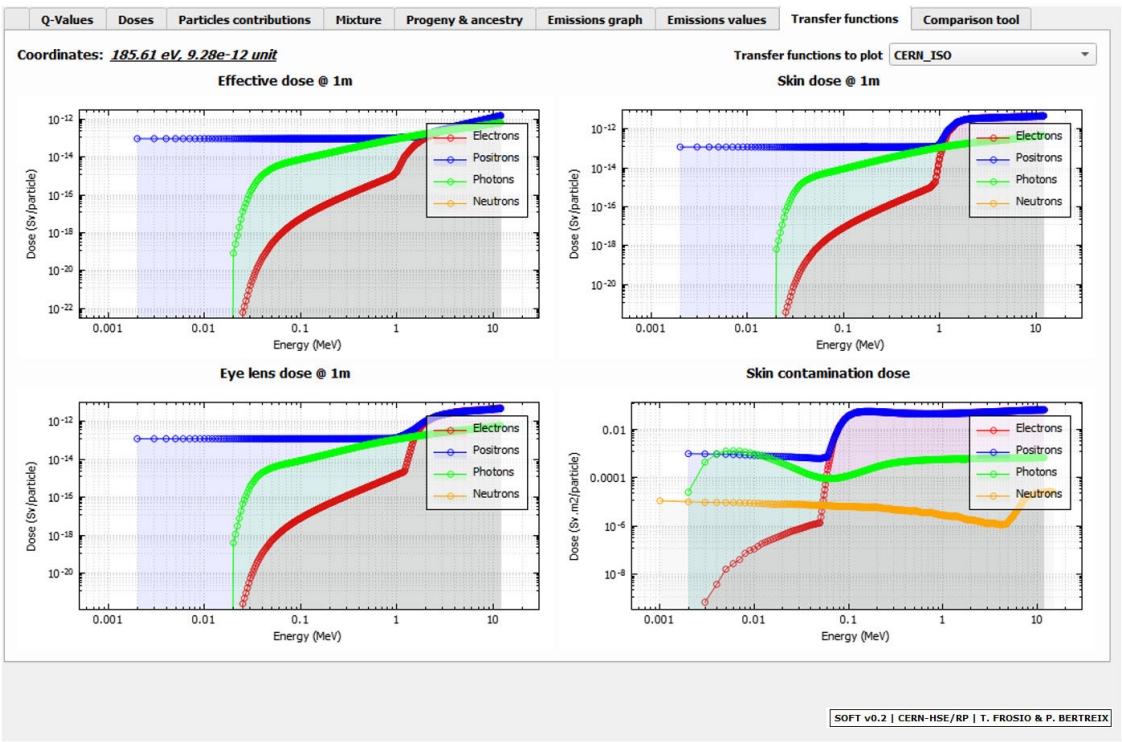


FIGURE 15. Transfer functions module.

All the data are listed in the table below and displayed in the bar charts for the whole set of scenarios. The values are plotted for each particle type which can be selected using the checkbox on top of the bar charts. This module is important to compare model assumptions such as calculation codes, interpolation methods . . . etc.

FIGURE 16. Model comparison module.

VI. CONCLUSION

CERN has developed an efficient software tool to calculate data related to radioactive shipping (Q-values, A1 /A2 limits) for a large scope of radionuclides. An innovative technique of calculation makes the determination of the values simpler, by associating particle/energy/scenario dependent transfer functions with nuclear decay data of a radionuclide. This technique is more efficient and less time-consuming than referring to Monte-Carlo simulations for each Q-Value and each nuclide. Different decay databases (JEFF3.3, ENDFBVIII.0, ICRP-107) can be used, but the IAEA working group recommends ICRP-107. Due to the extensive features exposed in this tool (comparison of different models, free choice of model and database for calculating specific Q-Values, detailed analysis of contributions originating from various particles, mixture of radionuclides etc.) it can be used for carrying out detailed comparison studies very efficiently. This is of high importance for carrying out the standardization process with which the IAEA working group has been mandated.

Later, a lighter version of this software could be produced to be distributed with the then- defined regulation. This step is intended to be discussed once the Q-System review has been completed: currently planned for 2021.

ACKNOWLEDGMENT

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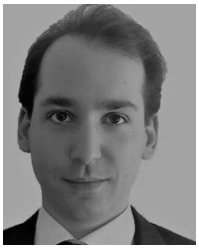

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During his Ph.D., he was working on developing frameworks in order to propagate nuclear and manufacturing data uncertainties on different neutron physics parameters in the coupled numerical simulations transport/depletion (deterministic and Monte-Carlo). He has ten years of experience in various nuclear physics topics. He has been involved with CERN in different topics, since 2017, such as radioactive waste characterization, development of new frameworks for high-performance radio-analytical techniques as gamma spectroscopy. He was leading the pilot project for the first radioactive magnets eliminated at CERN as unitary pieces. He developed a new methodology for material classification at exit of accelerators without requiring sophisticated laboratory analyses. He also contributed to the calculation codes development such as FLUKA (Monte-Carlo) and ActiWiz for which he computed new production cross-sections for low-neutrons energies.

Dr. Frosio is a member of an IAEA, where he is also working to update the international regulation regarding the transport of radioactive material (TRANSSC). He developed the calculation code presented in this article to compute transport limits.

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He has 21 years' of experience in radiation protection. After graduation, he took up a position as an Engineer in radiation protection at CERN, in 1998, where he acquired a first-hand experience in working on the field with particle accelerators. In 2000, he took up the responsibility for the Analytical Laboratory, where he developed a dedicated network connecting the different gamma-spectroscopy installation, and supervised the spectrometry measurements for the dismantling of the large electron positron collider (LEP). For two years, he ensured laser safety for all CERN experiments. He was co-leading a project for designing and testing a radiological gate monitor for the dismantling of CERN experiments. At the same time, he took up the responsibility for the radioactive source service and the radioactive shipping service. In 2003, he improved databases and web interfaces with the RP Group, which permitted the creation of an interface and associated database for managing industrial radiographies performed on site, radioactive sources lent to users, and shipment of radioactive goods by air and road. In 2010, he conceived and developed a software solution for calculating the radiological characterization of packages for the shipment of radioactive material. This software is currently a part of the computation tools available in Nucleonica portal. In 2012, he took a position as a Scientific Assistant to the Head of the radiation protection. He had also the responsibility for the management of electronic documents on a departmental level, as well as for data protection within the RP group. In 2018, he took a position as a Financial Professional and a Scientific Assistant to the Head of the Health Safety and Environment Unit, planning, and control of the material and personnel resources for the entire HSE Unit. He is also the Scientific Secretary for the Tripartite plenary sessions, which held between the OFSP, Switzerland; ASN, France; and CERN.

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Dr. Cabianca is a member of the U.K. delegation at TRANSSC and the Chairman of the IAEA TRANSSC Special Working Group on A1 and A2 values, in the area of transport. He is also the Chairman of the IAEA MODARIA II, Programme

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