Consequence Analysis – A state-of-the-art Public Dose Calculation Tool

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The European Spallation Source (ESS) is one of the largest science infrastructure projects being built in Europe today. Based in Lund, Sweden, its purpose is to generate neutron beams for science. Lloyd's Register is supporting ESS to perform consequence analyses and to estimate activity transport and doses to the public. This is one of the requirements imposed by the Swedish Radiation Safety Authority (SSM) for the ESS facility. To demonstrate compliance with acceptance criteria issued by SSM, a state-of-the-art tool for dose calculations – ESS Doctor – has been developed by Lloyd's Register.

Based on various accident sequences, ESS Doctor was developed for calculating activity concentrations and doses to workers and to the public, and to produce lists of the nuclides that dominate in contributing to the doses. This paper presents the methodology adopted for the dose calculations in ESS Doctor. An overview is given of the development and the analysis steps; for example, accident sequence characterization, modelling, calculation of activities and doses, identification of dominating nuclides, and contributions in terms of inhalation, external cloud, external ground, and ingestion. ESS Doctor can also be utilized in Emergency preparedness by calculating doses during an emergency.

Keywords: Consequence analysis, dose calculations, radiation, accident, ESS Doctor, emission, public, accelerator, radiation safety.

1. Introduction

The radioactive material that may be available for release and emission to the environment, following an accident, is located in systems and rooms surrounded by other rooms and spaces. The release path to the outside through the facility may thus be fairly complex, and depending on the volumes and flows, the transport and emission of the activity may take some time.

Most of the analysed accident scenarios have very short delays between the initiation of the event and the start of the emission of activity to the environment, and thus also a very short time to actuate any mitigating actions for the public.

Doses are calculated for a representative person of the public, which is an adult and a one-year old child living on a farm approximately 300 m from the main stack of the facility. Due to the relative position of the farm and the assumed release points at ESS, this distance is a good approximation for all releases considered the analysis. The dose results are presented to SSM for the adult representative person of the public.

The exposure paths include inhalation, external radiation from the radioactive cloud passing the representative person (cloud shine), external radiation from the activity deposited on the ground when the radioactive cloud passes (ground shine), and ingestion of food and water contaminated by the emitted radioactivity.

A common basis to calculate the doses is the activity concentration at the position of the representative person. It is calculated for each nuclide by multiplying the emitted integrated activity of the nuclide with the relative concentration, where

- The emitted activity of each nuclide is calculated by considering the activity and half-life of the nuclide, released or to be released from the source at the beginning of the accident, and performing transport and decay calculations as the nuclide follows the release path to the outside.
- The relative concentration is a factor connecting the activity emission rate and the activity concentration at the position of the representative person. It depends mainly on the height of the emission point, the weather conditions (wind speed, stability, and inversion height), the duration of the emission, and the distance between the emission point and the representative person. The relative concentration is calculated with the program Lena.

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The respective dose is then calculated by multiplying the time-integrated activity concentration with relevant constants like dose coefficients, breathing rate, deposition rates and ingestion rates of different food. This is comprehensively described in an ESS report [Spanier L., 2019].

For the doses to the workers, the time-averaged activity concentration during the exposure time is also calculated by considering the activity and half-life of the nuclide released from the source; and performing transport and decay calculations as the nuclide passes the different rooms in the facility. The inhalation dose is then calculated by multiplying the average activity concentration with the corresponding exposure time, the breathing rate and the inhalation effective dose coefficient. All source nuclides with half-lives of ten seconds or longer are included in the calculation.

Doses are calculated for four different emission heights e.g. 10 m, 20 m, 30 m and 45 m (main stack height) and two different weather situations i.e. median weather, P50%, and the 95 % percentile weather, P95%. The doses calculated with the P95% weather are used when comparing with the acceptance criteria for the different accident scenarios. The P50% weather is given for comparison with earlier results.

A new tool for calculating activity concentrations and doses to workers and to the public, based on accident sequence specifications given by ESS, has been developed by Lloyd's Register (LR): ESS Doctor (ESS Dose calculation tool – rapid). It also produces lists of the nuclides that dominate in contributing to the doses.

2. Development objectives

The development of the new dose calculation tool for ESS was based on the methodology adopted in the dose calculations currently performed for ESS [Spanier L., 2019]. The methodology rests on a solid theoretical foundation, has been accepted by SSM, and is therefore used as a roadmap for the development.

The calculations have traditionally been performed using multiple applications – Mathcad for transport and decay calculations, and several Excel workbooks for calculations of doses and dominating nuclides; requiring detailed knowledge of Mathcad modelling and data processing in and between Excel sheets. The objectives for developing ESS Doctor were to

- automate many steps, and reduce the large number of manual actions needed to obtain the final results,
- reduce the susceptibility to manual errors,
- increase user-friendliness using an intuitive interface,
- reduce the time needed to obtain results,
- facilitate calculations by ESS, and
- facilitate traceability.

The new tool was realized as a single program with an interactive user interface guiding the user through the calculation. Manual data handling is limited to providing input to the calculation as given by ESS, as well as evaluation of intermediate results when needed. All steps previously performed with Mathcad and Excel are implemented in the new program. As far as achievable, the calculations are automated. The tool is developed in the programming language Python in the Windows environment.

The program is able to handle input from and produce output to external files, which thereby can be edited and processed as needed outside the program, e.g. for other applications. Thereby the analysis prerequisites supplied by the experts can be entered either through the user interface or by input files. Examples of such externally stored input data are

- flows,
- volumes,
- source inventories,
- weather data,
- exposure cases.

Output examples are

- doses to the public,
- doses to workers,
- customized dose results by extracting data from calculation results, e.g. doses from iodine to the thyroid gland for a 1-year old child,
- external source terms,
- listings of the input prerequisites, as received from ESS and as formatted for the calculation in the program.

The latter is thereby providing an account for how the original input is used in the program to obtain the output. Since the format used by the tool is clearly defined, the ESS experts providing inputs can use this as a template and supply the analysis prerequisites already in the format expected by the program, to reduce the time needed for the dose calculations.

The handling of external files includes version control for each file, with unique identifiers for traceability. Thereby users can work in parallel, paying attention to (e.g.) the version of the nuclide list that must be adopted as input to the calculations.

Modular programming facilitates replacing one method to solve a part of the analysis sequence with another method. The first version of the software relies closely on the calculation principles as adopted in the previous calculations.

However, the following serve as examples on potential future replacements or additions in the code, allowed by the modular structure:

- Accounting for the decay during transport: Replacement of a Weibull function adopted to model activities as results of 20 nuclide half-lives (elaborated in section 4.3), with (i) interpolation (more half-lives), or (ii) calculations of activities for *all* nuclides in the activity sources.
- Expanding the number of nuclides.
- Including daughter nuclides.
- Quick choices of previously calculated or pre-defined leak paths.
- Sensitivity analysis.
- Extended user guidance.

Quality assurance (QA) was achieved by verifying that the program reproduces dose results obtained with the previously used tool. The results from calculations performed with ESS Doctor version 1.0 were benchmarked against results from calculations utilizing Mathcad 15.0 and Microsoft Excel.

3. Analysis principles

3.1 *Analysis prerequisites*

A prerequisite for a dose calculation is the delivery of an accident sequence specification table from ESS. This consists of results from thermodynamic analyses of the accident sequence:

- activity release dynamics from the activity source (or sources),
- gas flows between the rooms and spaces in the emission path of the activity, and
- other quantities such as the volumes of the affected rooms.

Some of the accident sequences analysed are called unmitigated because no safety systems are credited in the calculations. In the safety analyses of ESS, reported to SSM, the doses are one of the inputs used in the process to define the safety systems. When safety systems are credited in the calculations, the sequences are called mitigated.

3.2 *ESS Doctor transport model*

The parameters to be given to the calculation engine in ESS Doctor, through the interface, are determined by interpreting the data in the table delivered by ESS. The parameters are entered in a format that is applicable to the model of the facility used in ESS Doctor. Therefore, an understanding of the following quantities defined in the model is needed.

3.2.1 *Volumes (rooms or other spaces)*

These are connected sequentially from the first to the last volume.

The main volumes V0, V2 and V4 are the actual physical volumes shown in Fig. 1.

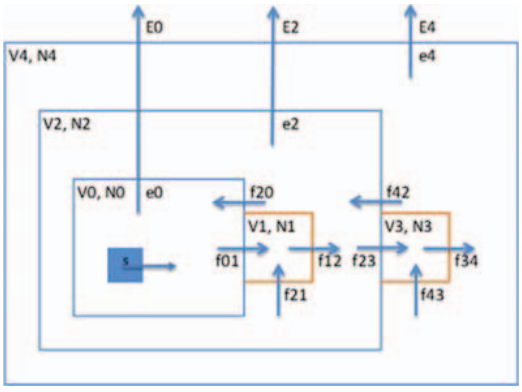

Fig. 1. General transport model including imaginary dose control volumes V1 and V3, and backflows.
V# = volumes (m^3)
f# = flows between volumes (m^3/s)
e# = emission flows (m^3/s)
s= source (nuclei/s)
N# = numbers of nuclei in volumes
E# = emitted numbers of nuclei

In addition, there are imaginary dose control volumes V1 and V3 – to enable calculation of doses to workers in the main rooms, being exposed to activity by inhalation.

If a worker is close to the flow path entering a room, the activity concentration in that position may be underestimated because the model assumes the activity to be instantly dispersed in the whole volume. Therefore, in the model, the gas passes the volumes V1 and V3 in which the workers are assumed to be, before entering the main volumes V2 and V4. Each of V1 and V3 are 56 m^3.

Since V1 and V3 are relatively small, the activity concentrations will be larger than in V2 and V4. As V1 and V3 are also imaginary, there is a back flow modelled into them from V2 and V4, and after some time, the activities will decrease until reaching equilibrium with V2 and V4, respectively.

If doses to the public are to be calculated instead of worker doses, V1 and V3 are not relevant and are set to 1 m^3, since a very small volume facilitates quick transport through the volumes.

3.2.2 *Gas flows, from one volume to the next*

The flows between volumes are designated f01 (from V0 to V1), f12, f23 and f34.

In the ESS Doctor interface, the flow leaving volume V0 and entering the next physical volume V2 is designated f01, reflecting that there is an imaginary dose control volume V1 in the model. Nevertheless, this is the same flow as f02 in the accident specification.

The back flows to enable equilibrium between main and imaginary volumes are denoted f21 and f43. The back flows from one main volume to the previous one are denoted f20 and f42.

The flows to the environment from the main volumes are denoted e0, e2 and e4.

3.2.3 *The source of activity*

This is placed in the first volume (V0) and there are two modelling options:

- A specific number, s, of radioactive nuclei at the beginning of the event ("instant release").
- An activity source generator, s(t), releasing a number of radioactive nuclei per second into V0. The source generator may vary with time and typically becomes zero after some time. It is possible to model continuous varying sources as well as energetic sources such as explosions or pipe breaks.

3.2.4 *Numbers of radioactive nuclides*

These are calculated in ESS Doctor as a function of time. The amounts in the different volumes are denoted N0, N1, N2, N3 and N4, while the amounts emitted to the environment are called E0, E2 and E4 (also designated N5, N6 and N7).

3.3 *Analysis steps*

The initial work aimed at creating a beta version of the program that included all calculation steps needed to obtain the doses, and a graphical user interface that guides the user through the different steps:

- Step 1: Entering or reading volumes, flows, activity source parameters, and other input. Presentation of the input as perceived by the program.
- Step 2: Performing transport and decay calculations – solving a system of differential equations for numbers of nuclei and activities in different volumes, and emitted to the environment, as functions of nuclear half-lives. Check of calculation stabilities.
- Step 3: Establishing functions for activities as results of nuclide half-lives.
- Step 4: Establishing data needed for the dose calculations – scaling of inner source terms with given activity source data. Calculation of activities in rooms, and released to the environment, for the final dose calculations.
- Step 5: Calculation of doses to workers and/or the public. Sorting for dominating nuclides. Compiling and exporting results and applied inputs.

The program also provided the possibility to change other inputs like dose coefficients, nuclides to calculate the dose from, and the volatility/chemical state of different chemical elements (typically Gas, Volatiles, Aerosols, Others). Such data can be placed in external files.

4 Realization of the technical specification – analysis example

A number of different hypothetical accident scenarios were considered to formulate a detailed technical specification for the development of the tool, and to verify that the outcome, e.g. ESS Doctor, would produce results as expected for these scenarios [Klug J., 2019]. This section accounts for the actual outcome of the development, by showing how the tool appears to the user and by elaborating in more detail on the five analysis steps discussed in section 3.3. A hypothetical accident scenario is used as an example; with the leak path LP-101B, i.e. leak through the beam pipe, the accelerator tunnel and the klystron galleries, ending in a release to the environment via the stack; mitigated after 40 seconds.

The accident includes four different activity sources with different amounts of radioactive material and release dynamics. Material from the helium coolant and the filter particles are released during the first ten seconds, from the moderator water the duration of the release is 20 000 s, and from the tungsten target it is 1000 s. The activity release dynamics are different enough for the four sources to be handled in different calculations. However, since the helium coolant and the filter particles have the same release time, three separate transport calculations have to be done (instead of four).

4.1 *Step 1. Accident sequence characterisation*

After starting a new analysis in the user interface, metadata and other parameters such as volumes, flows and activity source data for the specific calculation are entered after interpretation of the specification given by ESS. Fig. 2 shows the first input panel.

The three fields for exposure time are used when calculating worker doses – hence three different time periods, during which a worker is assumed present in the room traversed by the gas flow, can be treated in the same calculation. The default values are 120 s, 600 s and 14 400 s.

When deciding on the number for the imaginary volume size, it can be noted that,

exceptionally, there are accidents with only one room from which there is a time-dependent emission flow.

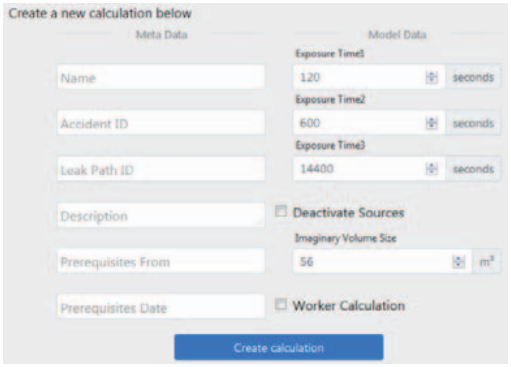

Fig. 2. Metadata entry fields.

Only in a case where there is no source releasing material for a certain time, but all activity is instead assumed present in the inner volume at the beginning of the accident ("instant release"), the "Deactivate Sources" box must be checked.

Even though the aim of a calculation may be to obtain public doses, both worker doses and public doses are being calculated in ESS Doctor version 1.0. This means that the worker dose results must be disregarded since the Imaginary Volume Size is set to 1 m^3. For worker dose results, a separate calculation must be made, where the Worker Calculation box is checked, and the Imaginary Volume Size is set to 56 m^3.

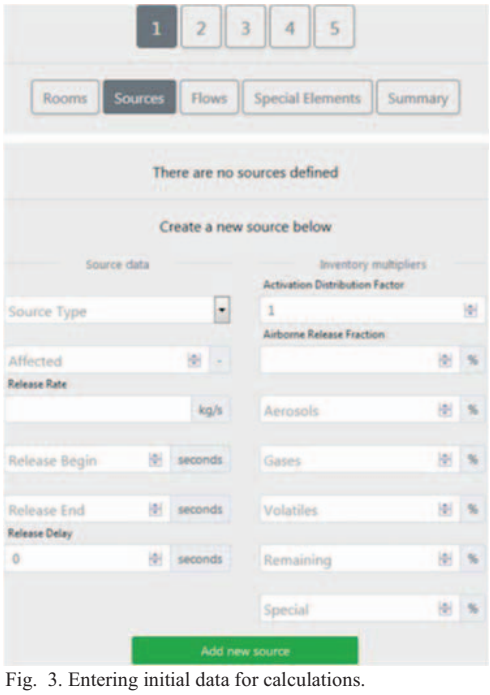

Fig. 3. Entering initial data for calculations.

By pressing "Create calculation" (see Fig. 2), the current analysis Step 1 in the calculation sequence is invoked, where initial data are to be entered as shown in Fig. 3. Throughout the analysis, an upper row of boxes numbered 1-5 indicates the five main steps that must be carried out to obtain

Fig. 4. Step 1 – Input as perceived by the program.

the final doses. Below that, one or more additional rows of boxes indicate which sub-steps that must or may be addressed within that main step. The current step and sub-step are represented by filled boxes.

ESS Doctor compiles the data entered through the interface, and the user can verify that the data to be used for the subsequent calculations are perceived appropriately, see Fig. 4.

4.2 *Step 2. Performing transport and decay calculations*

In this step, transport calculations are performed for each activity source. Eight dependent ordinary differential equations describing the gas flow in the system are solved with respect to the dependent variables N0 to N7, i.e., the numbers of nuclei in the different volumes or emitted to the environment. This results for the activity source presently analysed in:

- The number of nuclei in each volume as a function of time.
- The average activity concentration in every volume for three exposure times, normalized to a total initial source of one Becquerel.
- The emitted activity to the environment at the end of the accident, normalized to a total initial source of one Becquerel.
- The times when certain fractions of the activities are emitted.

The physical quantity having an influence on the number of nuclei that will reach the different volumes and the environment in a certain accident sequence is the decay during the transport, governed by the half-lives ($t_{1/2}$) of the nuclides released from the activity source. For nuclides with $t_{1/2}$ shorter than the transport time through the facility, the numbers of emitted nuclei go down as $t_{1/2}$ decreases. For nuclides with $t_{1/2}$ much longer than the transport time through the facility, the numbers of emitted nuclei do not depend on $t_{1/2}$. For nuclides with $t_{1/2}$ between these extremes, the numbers of emitted nuclei change in a continuous way and go up with longer $t_{1/2}$. Thus, in principle, the transport equations should be solved for every nuclide present in the source.

The normalization to a total initial source of 1 Bq is achieved as ESS Doctor specifies the activity A0 in the source at t = 0 to 1 Bq. The number of nuclei N0 at t = 0 is then obtained using the decay constant λ; $N0 = A_0 / \lambda$. In the analysis step following the transport calculations, the normalized activity concentrations in the volumes or the normalized emitted activities will be fitted as functions of $t_{1/2}$ (depending on whether doses to workers or to the public are to be calculated). Thereafter, these functions will be used together with the specific activities of all nuclides in the activity source (given at t = 0) to obtain the actual activities needed to calculate the doses.

For those of the four activity sources listed in Fig. 5 that have different active time periods, separate transport and decay calculations have to be performed. Knowing that the helium loop gas and the filter sources have the same active period (10 s), this means that it is only necessary to perform the calculations for the helium loop gas, the moderator water (active for 20 000 s), and the tungsten target (active for 1000 s).

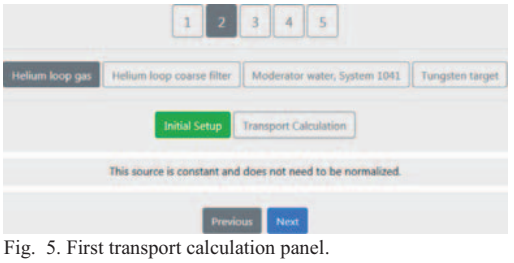

Fig. 5. First transport calculation panel.

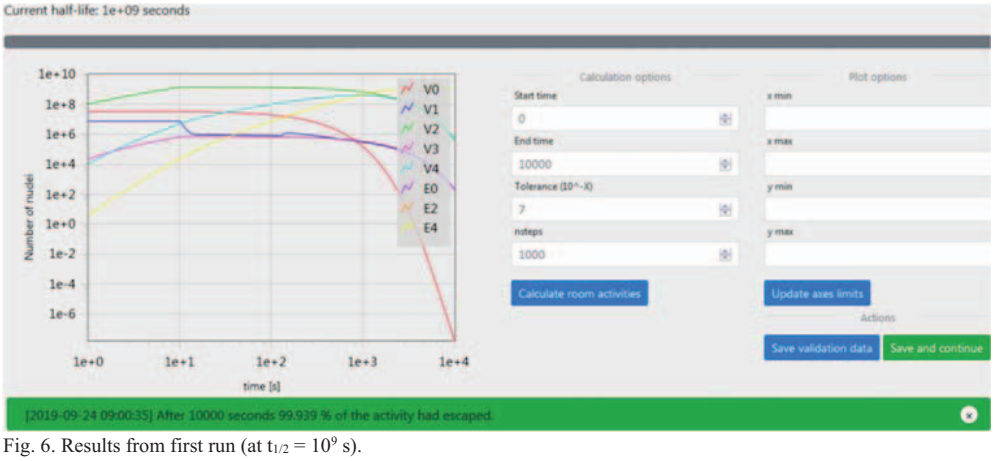

Fig. 6. Results from first run (at $t_{1/2} = 10^9$ s).

As the source helium loop gas has a constant release rate, ESS Doctor identifies that a normalization is not needed.

The graph in Fig. 6 shows the numbers of nuclei in each volume (V0-V4) and emitted to the outside (E0-E4), as a function of time.

- As the source emits nuclei at a constant rate from 0 to 10 s, the curve representing the number of nuclei in V0 drops off after 10 s.
- The change in flow at 10 s (from 18 m^3/s to a lower rate) is reflected in the changes of the graphs for V1-V3.
- The end of turbulent conditions at 130 s, i.e. 120 s after the change in flow at 10 s, is also reflected in the change of the graph for V1.
- Eventually, the numbers of nuclei in each volume (V0-V4) drop off as the transport to the outside continues, and the number emitted to the outside (E4) converges to a maximum.
- There are no nuclei emitted to the outside via emission paths E0 and E2.

As more than 99 % of the activity has escaped, the calculation end time does not need to be increased. The transport calculations are performed following the same principles for all activity sources.

4.3 *Step 3. Fitting activities as functions of $t_{1/2}$*

The function used in the fits to $t_{1/2}$ is the Weibull function

$$W(x) = a - b \cdot e^{-c \cdot x^d},$$

and ESS Doctor calculates the numerical values of the parameters a, b, c, and d (Fig. 7). The procedure is applied to the activity data of every volume or emission point for which doses are to be calculated. The parameters are fitted by minimising the sum of squares of the differences between the Weibull function and the values based on the solutions of the transport equations. The result is the numerical values of the parameters a, b, c, and d.

4.4 *Step 4. Calculating inner and outer source terms*

To obtain the inner source terms, the source activities read from external files are multiplied with the fractions of the activity source inventories that are subject to transport through the facility, and with the airborne release fractions of the chemical elements present in the source materials. The release fractions depend on whether the chemical elements have been classified as Gas, Volatiles, Aerosols, Remaining, or Special; and on the numerical fraction values specified for each group (and special elements, if existing).

The outer source terms are the nuclide inventories released to the environment, needed for calculation of doses to the public. They are established by combining the activities of the nuclides in the inner source terms with the decay along the transport through the facility, modelled with the Weibull function.

4.5 *Step 5. Calculating worker doses, public doses and lists of dominating nuclides*

In this final step, the following are calculated and presented (see Fig. 8):

- Worker doses
- Public doses
- Lists of the nuclides that contribute most to the doses compiled into a single Excel file.

5. Benchmarking and conclusion

For five accident scenarios, benchmarking calculations [Klug, J., 2019] have been performed with ESS Doctor version 1.0 against calculations performed previously, utilizing Mathcad 15.0 and Microsoft Excel.

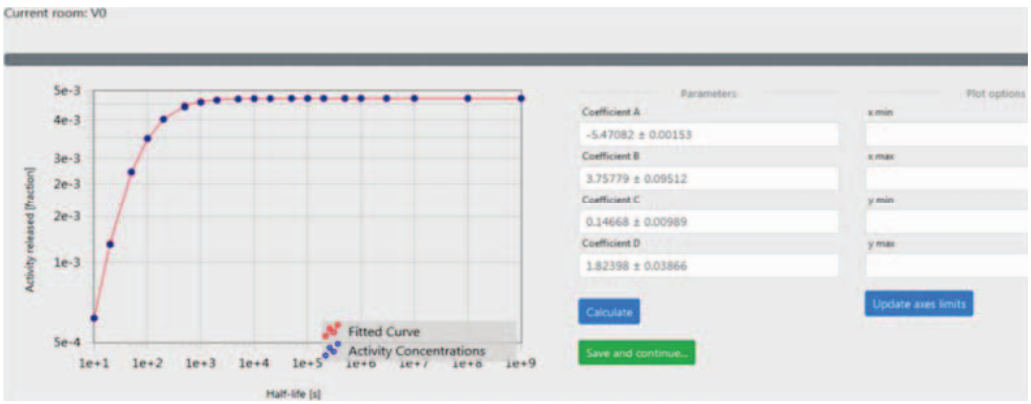

Fig. 7. Weibull fit.

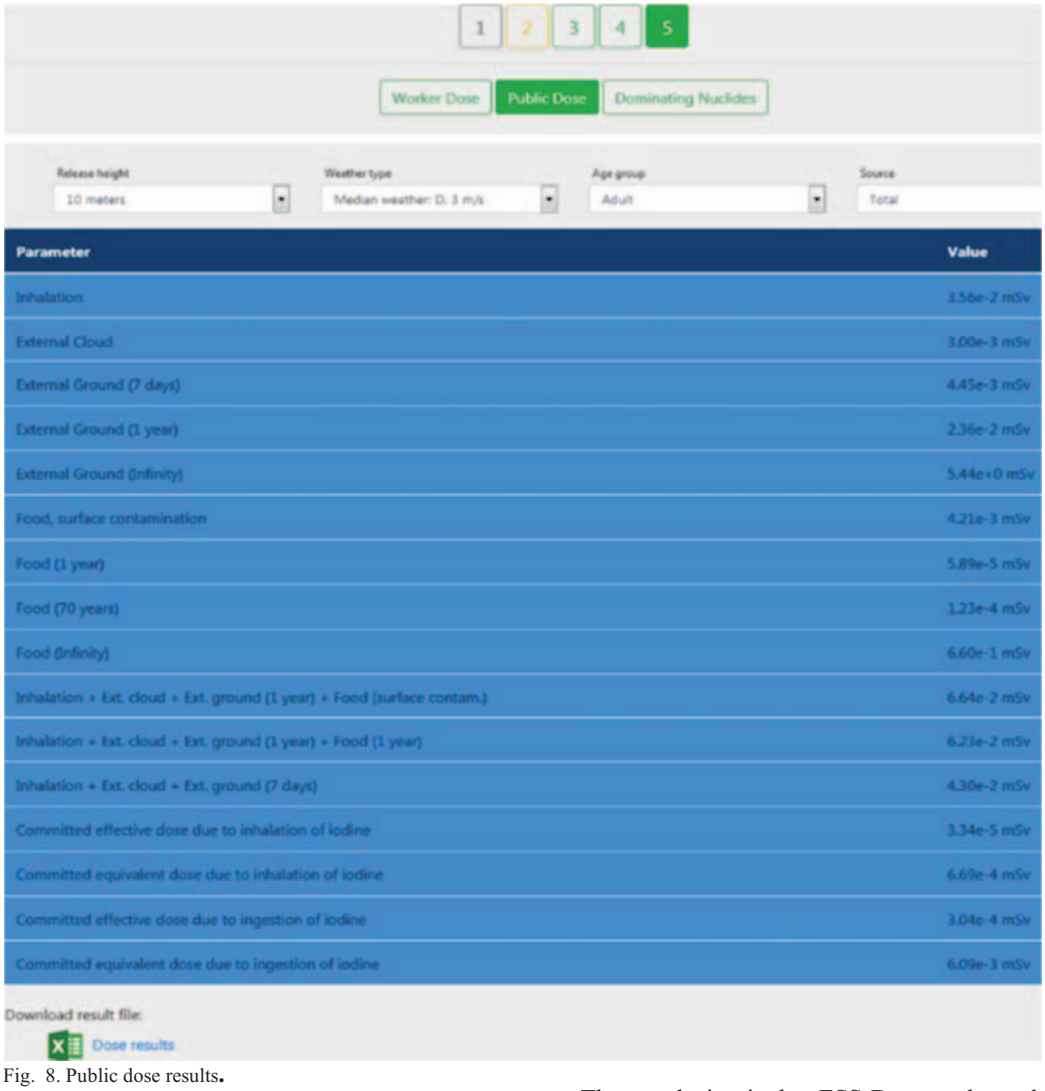

Fig. 8. Public dose results.

The five tests represent a range of different analysis prerequisites that ESS Doctor must be able to handle. The major findings in the benchmarking come from a very complex accident and leak path with eight different activity sources releasing radioactive isotopes, and where one of the sources becomes active relatively late after the beginning of the accident due to deflagration of hydrogen.

The final results in all benchmark tests for public doses, worker doses, dominating nuclides and committed effective and equivalent doses from iodine to the thyroid gland for a one-year old child have differences in the sub-percent range when compared to previously obtained results.

The conclusion is that ESS Doctor adopts the established methodology and reproduces the results much faster, and as perfectly as can be expected. The same approach can be utilised in Emergency dose calculations.

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