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Title page

Redesigning the FDMT food chain transfer model: Now probabilistically enabled and fully flexible

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Abstract

In Europe, the two main nuclear accident response decision support systems in use are ARGOS and JRODOS, both of which make use of the FDMT (Food Chain and Dose Module for Terrestrial pathways) model to simulate the transfer of radioactivity along terrestrial food chains and to predict radionuclide activity concentrations in human foodstuffs. FDMT was originally developed in the early 1990's for Southern German agricultural conditions. Its application to other geographical settings has raised concerns regarding its fitness for purpose. Furthermore, the FDMT model in its original format lacks transparency, flexibility and the possibility to be run probabilistically. In order to improve FDMT's fitness for purpose and overcome its main shortcomings it has been implemented in a new modelling platform which incorporates powerful numerical solvers and renders uncertainty and sensitivity analysis possible. The modelling structure of FDMT has been re-configured and a library configuration has been introduced which offers flexibility in working such that model components can be tested, modified or replaced easily. The new FDMT allows for the consideration of case/region specific issues and to make predictions which are of more relevance and of better use with regards to decision making and management of risk. Furthermore, the default databases of FDMT have been updated and wherever possible PDFs have been assigned. In this paper, the transition of FDMT from old to new modelling structure is presented along with a demonstration of developments achieved.

Key words: Nuclear accident, human exposure, food chain, process-based modelling, decision support system

1. Introduction

Following the Chernobyl and Fukushima accidents, the need of fit for purpose radioecological models to predict radionuclide activity concentrations in human foodstuffs has become widely acknowledged [1-4]. After an accidental release, the transport of radionuclides from the source and their dispersion within the environment trigger concerns related to the risk for humans and the environment. These concerns may result in actions to minimise the impact of an accident (i.e. reduce exposure, produce foodstuffs with radionuclide activity concentrations below intervention limits etc.). Decisions about such actions are aided by the assessment of the possible impact of the release on human health through estimating likely exposures. However, adopting an optimal radiation protection strategy requires identification of where resources are likely to be spent most effectively.

Quantification of the risk associated with a release of radioactivity requires an understanding of the many processes involved in transport and transfer of radioactivity and the ability to translate that understanding into a mathematical model [5,6]. In developing models, we make judgements and assumptions which reflect our state of knowledge at the time [7]. Usually, this state changes as we get more data or insight into the problem. As our knowledge changes we need to revisit our models and their underlying science and assumptions to update them accordingly. However, development and modification of models through iteration has an important prerequisite: that models are set up in such a way that readily allows for such updating. This means that they should be flexible enough to allow for new knowledge to be incorporated easily and with minimal effort. Additionally, the models ideally ought to provide the option to incorporate variability and uncertainty, which is a necessary step in conducting sensitivity and uncertainty analysis [8]. The latter is important in order to evaluate the degree of confidence that can be placed in the risk estimates we make and to minimise the chance of overstating or underestimating risk [8].

In reality the estimation of exposures following a large-scale accidental release is complicated because of the interaction of many factors such as the relative contributions of dry and wet deposition, the time of the year, the agricultural conditions in a region affected, living habits, and the fraction of the diet that is produced locally. However, the ICRP [9], suggest that if no protective measures are taken, it is likely that, doses from ingestion of contaminated food will comprise the largest contribution of the projected doses over the first year after an accident.

Several models have been developed to simulate the transfer of radionuclides to terrestrial food products, such as FARMLAND [10], TRANFOOD [11] and SYMBIOSE [12]. The FDMT (Food Chain and Dose Module for Terrestrial pathways) is another such model [13], and is integrated into two main European decision support systems (ARGOS - Accident Reporting and Guiding Operational System [14] and JRODOS - Real-time On-line Decision Support System [15]), where it can be run deterministically. FDMT is based on the ECOSYS-87 model to simulate the transfer of radioactive material in food chains, and for assessment of doses (individual as well as collective) to the population [16]. However, because ECOSYS-87 was developed in the early 1990's it did not consider the large numbers of radioecology studies prompted by the 1986 Chernobyl accident and subsequent compilations of model parameters [17]. Furthermore, the original parameter collation was mainly specific to Southern German agricultural conditions [18].

One of the characteristic features of an emergency is the urgent need for making decisions under highly dynamic and uncertain circumstances. In general, uncertainties involved can be ascribed to two categories: those belonging to the ongoing emergency situation, which can be unique and specific, and those which have a more general nature and are not situation specific. The main difference between these two groups is in the amount of work we can do beforehand in dealing with them. Potentially, an extensive collation of data pertaining to models can be conducted prior to an accidental release. More data can reduce uncertainties associated with our lack of knowledge of underlying processes. There is also uncertainty related to the inherent randomness and heterogeneity of environmental processes. This is manifested as variability in data, which is not reducible, but can be better characterised and represented through further analyses [19].

A key observation of the recent EC funded CONFIDENCE project considering uncertainties in modelling and decision making after nuclear accidents [20] was that uncertainty management for simulation models in decision support systems (such as ARGOS and JRODOS), was far from satisfactory [21]. One of the key problems identified was the current inability to incorporate process-based models (i.e. models who's parameterisation take into account soil and potentially plant characteristics [2]), in the context of simulating food-chain transfer, to potentially reduce the uncertainties associated with the existing empirical ratio-based transfer approaches. Raskob and Duranova [21] considered quantification and reduction of uncertainties to be an essential step towards improving decision making to protect affected populations and minimise the disruption of normal living conditions.

The reliability of support systems used for decision making depends on the robustness of their underlying sub-systems/modules; the same holds for any improvement of such systems. According to the internationally agreed research agenda for radioecology [22, 23], focus should be placed upon development of process-based transfer and exposure models, better parametrisation and assessment of associated parametric uncertainty in such models. Addressing these key research requirements should lead to the reduction in uncertainties in radionuclide transfer/food chain modelling.

The present study is a direct response to these research needs and the requirement to improve our modelling capacity for better decision making. The main objective is to further improve the FDMT model and make its application more user friendly. In this paper, the approach taken to achieve this objective will be presented along with a demonstration of developments achieved.

2. Methods

Knowing that FDMT's fitness for purpose should be improved such that better and more robust estimates could be made, a systematic method was needed to identify which parts of the model need to be modified/improved, in which order and how. In this regard, a sensible first step was the identification of FDMT's limitations through a review of the reported works in which the FDMT model has been applied and by conducting a gap analysis.

A literature review was conducted to make use of what had already been identified as limitations and potential areas for further improvement of the FDMT model [24-28]. Furthermore, data were extracted from published reviews and available literature to populate the FDMT's default databases.

The gap analysis was conducted based on considerations regarding the application of FDMT to the Nordic conditions. The FDMT's approaches for modelling radionuclide transport as well as its default food chains and parameters were then compared with the identified needs.

Following the gap analysis and the literature review it was clear that, FDMT, in its original format, suffers from three types of limitations; structural, conceptual and specificity. Regarding the former, being originally implemented within Microsoft EXCEL™ and then later as an integrated module within ARGOS and RODOS, flexibility is limited to changes of parameters and not the underlying models [39, 30] and there is little transparency with regards to the underlying calculations. Conceptual limitation refers to the science underlying the FDMT's governing equations which is, as considered below, in many cases an oversimplification of reality and neglects important influences such as chemical forms of radionuclides in soils [31] as well as soil chemistry [32]. The specificity limitation arises because FDMT has been parametrised for conditions that are largely for Southern Europe and, for the example considered here, likely not relevant to other areas (including Nordic agricultural practices as considered in the scenario we have used to illustrate the ECOLEGO FDMT implementation) [33].

2.1 FDMT

The FDMT model can be used, among other things, for the prediction of radionuclide activity concentrations in various, mainly agricultural, food products for given inputs of radionuclides into terrestrial systems. The starting point for FDMT calculations is the outputs from atmospheric dispersion models (as also implemented within and connected to the ARGOS and RODOS systems). The main input quantities for subsequent calculations within FDMT are:

- the date of the deposition (day, month)
- the time-integrated radionuclide activity concentration in near ground air
- the activity deposited by precipitation per unit ground area
- the amount of precipitation (for wet deposition)

In cases where the measured activity in air and the wet deposition are not available, the model provides alternative options for estimating the required inputs.

Based on these limited input data, the transfer of radionuclides through food chains is quantified by modelling various processes including: the deposition and interception of radionuclides on vegetation/crop surfaces; the loss from vegetation/crops (via weathering); the change in radionuclide activity concentrations in vegetation/crops via biomass dilution; foliar and root uptake of radionuclides by vegetation/crops; intake of contaminated foodstuffs by farm animals and radionuclide-specific equilibrium transfer factors and biological loss rates for these animals.

After inserting the above-mentioned input values into FDMT, the next step would be simulation of dry and wet deposition of radionuclides. The output from these simulations forms the basis for most of the subsequent calculations performed within FDMT.

Deposition and interception are key initiating and seminal processes that dictate the levels of radionuclides that are used in subsequent parts of the FDMT model. In order to emphasise their importance and their complexity, in the following, it is first shown the way these are modelled in FDMT and later argued why these have to be reconsidered/remodelled.

2.1.1 Deposition in FDMT

In FDMT dry and wet deposition are considered separately. The dry deposition to different plant species is calculated from the time-integrated air concentration using a deposition velocity which depends on the plant type:

$$D_i = v_i \cdot C_{air}, \qquad (1)$$

with

D_i = dry deposition onto plant type i ($Bq \cdot m^{-2}$),

v_i = deposition velocity for plant type i ($m \cdot s^{-1}$),

C_{air} = time-integrated activity concentration (for a specified radionuclide) in air ($Bq \cdot s \cdot m^{-3}$).

The deposition process has a pronounced seasonality which is location specific [24]. In the FDMT model, this has been taken into consideration by defining deposition velocity at the time of deposition (v_i) as a function of the leaf area index (LAI), which is defined as the ratio of the (single-sided) leaf area to the soil area [24]:

$$v_i = v_{i,max} \cdot \left({LAI_i}/{LAI_{i,max}} \right), \qquad (2)$$

where

$v_{i,\,max}$ = the maximum deposition velocity for the given plant type i, assuming fully developed foliage,

LAI_i = the leaf are index of plant *i*, at the time of deposition, and

$LAI_{i,max}$ = the corresponding leaf area index for the fully developed plant.

The deposition velocity depends on the chemical form of radionuclides and size of aerosols [34]. However, in FDMT all aerosols are treated the same, regardless of their size; the model only distinguishes between elemental, organic bound and aerosol bound iodine. If the default values of FDMT are not changed to adequately represent aerosol size the deposition estimates can be wrong by several orders of magnitude [24].

2.1.2 Interception in FDMT

In FDMT, the interception of wet deposited radionuclides is expressed as function of LAI, the total amount of rainfall and the water storage capacity of the plants' leaves without considering any aerosol particle features such as size. The interception fraction, f_i, for plant type i is quantitatively expressed as:

$$f_i = \frac{LAI_i S_i}{R}\left(1 - exp\left(\frac{-ln2}{3S_i} R\right)\right), \qquad (3)$$

with

$f_{,i}$ = interception fraction for plant type *i*,

S_i = retention coefficient (mm) of plant type *i,*

R = amount of rainfall (mm) of a rainfall event.

If application of this equation results in an interception fraction greater than 1.0, $f_i = 1.0$ is assumed. Three groups of elements are differentiated with regards to retention coefficients: *I)* Ce, Cs, Mn, Na, Nb, Pu, Rb, Ru, Sb, Te, Zr; *II)* Ag, Am, Ba, Cm, Co, La, Mo, Nd, Np, Pr, Rh, Sr, Y and *III)* I, Tc. For all other elements, as a default, it is assumed that they behave similarly to cesium [13]. Furthermore, the current interception model in FDMT does not consider the influence of particle size. Although this has been shown to have a substantial effect on interception [35].

2.2 Adaptation of a new modelling platform

After identifying the limitations in FDMT we need to decide how to address them in a proper and logical order. From the three main limitations outlined above, the one associated with the structure of FDMT was considered as the most fundamental shortcoming of the model. Dealing with this limitation required a new modelling platform, which allowed for changes to be performed easily and in a straight-forward manner. The desired platform had to provide transparency, flexibility and for the option of conducting probabilistic modelling. The latter is beyond the FDMT model's currently available deterministic approach and hence a clear improvement could be introduced by allowing sensitivity and uncertainty analyses to be performed. To fulfil these requirements, we used the modelling platform ECOLEGO [36].

2.3 ECOLEGO

The ECOLEGO modelling platform [36, 37] is developed for creating dynamic models and performing deterministic or probabilistic simulations (making use of Monte Carlo or Latin Hypercube sampling). The software incorporates numerical solvers for complex and dynamic systems, i.e. solver for ordinary differential equations including 'stiff' problems.

2.4 Implementation of ECOSYS87/FDMT in ECOLEGO

The FDMT model has been implemented using the ECOLEGO software package. The implementation has covered the entire suite of radionuclides and exposure pathways to humans that were included in the original ECOSYS-87 model although subsequent focus, in relation to collation of revised parameters, has been placed on the food-chain transfer component of the model as opposed to the (human) dose calculation module. Default parameters are essentially those presented in the earlier version of the model [16, 38].

The FDMT model is a compartment model consisting of a system of Ordinary Differential Equations (ODE) that are solved mainly analytically, although some equations are solved through integration using the trapezoidal method. In ECOLEGO, the same system of ODEs was implemented using specialized blocks called compartments. Each ODE compartment was then defined by adding specialized ECOLEGO blocks representing transfers between compartments, sources from outside the modelled system and sinks to outside the system. The equations corresponding to the different blocks (compartments, transfers, sources, sinks etc.) were written using the library of functions available in ECOLEGO. Once the model is implemented, ECOLEGO then integrates the whole system of ODEs, using the numerical method selected by the user from those available in the software.

The FDMT model within ECOLEGO can be graphically viewed either as an interaction matrix or as a more traditional compartmental model as shown in Fig. 1. The model is organised into different subsystems corresponding to different types of target environment, such as 'Grass Intensive', 'Grass Extensive', etc. Within each sub-system the relevant blocks can be viewed, i.e. the user can view all ODEs and other equations used in the model. The user can modify and add equations without any need for programming.

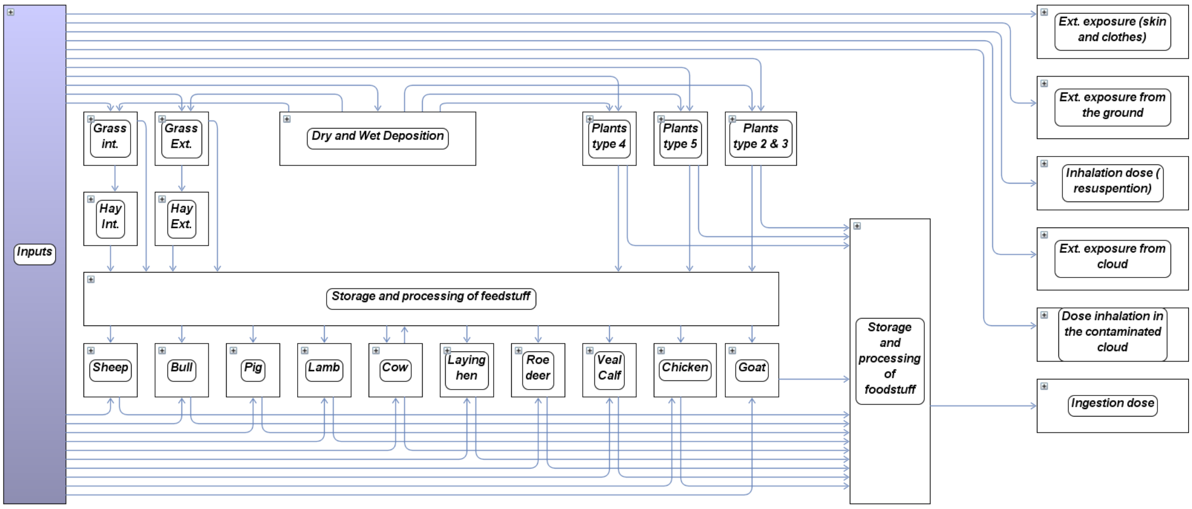


Fig. 1 The setup of FDMT as modelled in the ECOLEGO platform.

3. Results and discussion

The main findings of the gap analysis indicated modification of model features and parameter values was needed for the FDMT model to be more widely applicable. As an example, Nielsen and Andersson [24, 25] demonstrated the sensitivity of FDMT's outcomes to a number of site-specific input parameters, such as soil type, sowing and harvesting times, feeding regimes for animals and human consumption habits. The same studies also showed that many of the FDMT/ECOSYS default parameters values need to be updated and suggested that several new parameters (e.g. particle size and soil characteristics) should be included. As an example, several important regional foodstuffs (e.g. for Nordic or Mediterranean countries) are not part of the default diet list of ECOSYS. For instance, reindeer and brown (or whey) cheese are not included in the default list of foodstuffs of FDMT. However, these are not only two important foodstuffs in the Norwegian diet, but both are also prone to accumulating radiocaesium [25, 39].

It, therefore, goes without saying that any attempt to improve the fitness for purpose of FDMT should take place at two levels in parallel: modifying sub-model components and parameter updating. Regarding the former (i.e., modifying the modelling structure and underlying components), despite the requirement being identified in several earlier studies [24, 25, 28], no substantial improvements have previously been made. In contrast, the issue of parameter updating has received more attention (e.g. [24, 25, 28, 40]). For instance, as an attempt to include the option of modelling radionuclide transfer to reindeer, Staudt [40] included reindeer as an animal category for boreal and alpine radioecological regions in a demonstration of regionalising FDMT. However, the model was re-parameterised by adopting the feed to animal transfer factor (d kg^{-1}) for beef cattle. There was no evidence provided to support the efficacy of so doing and indeed given that the transfer factor is dependent upon the daily dry matter food intake rate the assumption is unlikely to be valid. Ideally, a bespoke model for reindeer based on, for example, the analyses conducted by Åhman [41] would be more appropriate or perhaps the application of a generic dietary concentration ratio rather than using/having to derive an animal specific transfer factor (see discussion in [17, 42].

3.1 General limitations and shortcomings of FDMT

3.1.1 Lack of relevance and transparency

As noted above, the radioecological parameters in FDMT were originally derived for Southern German agricultural conditions and in many cases not relevant for other environments/production systems. Furthermore, the parameter values originate from before the wealth of radioecological studies prompted by the 1986 Chernobyl accident and also international initiatives to collate transfer parameter data (i.e. IAEA [43] subsequently superseded by IAEA [17]). Consequently, there has been criticism that FDMT is not using state-of-the-art knowledge (e.g. Nilsen and Andersson [25]). In many cases, FDMT has default transfer parameter values that are not based directly on empirical data. For some animal products, Müller and Pröhl [16] describe how such values were derived; for example, if transfer factors were not available for sheep and goat milk a value 10-times higher than that for cow milk was assumed. However, there are many cases where it is not clear how the default parameter values have been derived when data were not available (see Brown et al. [44]). Hence, greater transparency is required on how these values have been derived and indeed they should potentially be revisited taking into account the latest IAEA handbook [17] and possibly also the recent consideration given to extrapolation approaches to derive missing radiological data (e.g. [42, 45, 46]).

3.1.2 Being deterministic

The current version of FDMT in the ARGOS and JRODOS decision support systems utilises discrete parameter values and allows for deterministic calculations. From one perspective, this might not be considered a major limitation and might even be deemed an advantage for being straight-forward and easily implementable. However, from an alternative viewpoint, this might result in assigning an unwarranted certainty to the outputs as the approach does not allow account to be taken of uncertainty in the simulation output despite the knowledge that large uncertainties exist in many of the parameters used in the calculation. The importance of adequately characterising variability and uncertainty in exposure assessments for human health risk assessments has previously been highlighted [12, 47, 48].

3.1.3 Not feasible for conducting sensitivity analysis

Another limitation is that the existing version of the model does not permit a robust sensitivity analysis. It is a fact that uncertainties are an inherent part of all modelling processes. Identifying the uncertainties that influence model outcomes most (either qualitatively or quantitatively) and communicating their importance is essential for proper integration of information from models into the decision-making process [7].

Müller and Pröhl [16] do present an initial consideration of uncertainty of the default ECOSYS-87 parameter values (some of which were relatively site specific) and identified the 21 most sensitive parameters from a total of more than 400 parameters. This work has limitations, mainly in relation to the specificity of the calculation and simplicity of assumptions regarding underlying statistical distributions that were made. Furthermore, it is self-evident that the greater number of data that are now available enable a more refined statistically based parameterisation.

3.1.4 Cannot handle complex dynamic systems

FDMT is not currently set up to allow the user to solve complex dynamic systems – essentially analytical solutions are provided for basic differential equations and simplifying assumptions are made with respect to, inputs to and losses from, various components of the modelled system.

However, if it is desirable to move towards a more process-based modelling approach or to consider more complex and dynamic systems, it would be a great advantage if the model was linked to software packages which make use of numerical solvers.

3.1.5 Lack of flexibility

There are components of ECOSYS-87/FDMT where there are concerns over the robustness of the approach (e.g. Nielsen and Andersson [26, 27]) and where external (sub) models are available/published that may be considered as viable alternatives. An example can be given by the equations used to determine the concentration of bio-available radionuclide activity in the root zone of soil. There are more sophisticated models available than the simplified approach described in FDMT where generic fixation and desorption rates are used across all soil types and migration/leaching rates vary between pasture and agricultural soils only because the depth of the rooting zone is assumed to be different. The 'Absalom model' [49], for example, allows the radiocaesium bioavailability to be determined specifically as a function of soil clay content, exchangeable K^+ status, pH, NH_4^+ concentration and organic matter content. In the latest version of this model [50] the number of required input parameters has been reduced by excluding NH_4^+ concentration. Accounting for such soil parameters enables predictions to vary according to soil type.

3.2 Testing of the new FDMT

After implementing ECOSYS-87 into ECOLEGO, it was necessary to test that the results generated by ECOSYS-87 could be reproduced acceptably by the ECOLEGO implementation.

Two scenarios involving dry and wet deposition were adapted from Søvik et al. [51] for this model-model comparison. Deposition date was selected to be 1st August and the magnitude of deposition was 1000 Bq m^{-2} for four radionuclides (Cs-134, Cs-137, Sr-90 and I-131). Table 1 shows the input parameters considered in the two scenarios.

Table 1 Input parameters specified in the scenarios used to test the ECOLEGO implementation of FDMT.

Input parameter	Dry deposition Case	Wet deposition case
Calculated activity concentration in air (Bq h/m^3)	140	0.55
Wet deposition (Bq/m^2)	0	1000
Total deposition to vegetated soil (Bq/m^2)	1000	1000

The original ECOSYS-87 in EXCEL™ and the new implementation in ECOLEGO were run for a 5-year period, using default parameter values. The endpoints compared were predicted radionuclide activity concentrations in winter wheat (whole grain), leafy vegetables, milk (cow), beef (cow) and lamb.

The outputs from the ECOLEGO and EXCEL™ implementations of ECOSYS-87 were compared for both wet (assuming 3 mm of rainfall) and dry depositions and showed good agreement. In most cases, the values corresponded exactly or were within a few percent of one another (at very worst the deviation was not greater than ~7 %). Hence, we could conclude that ECOSYS-87 has been implemented correctly into ECOLEGO. Fig. 2, shows the outputs from both ECOSYS-87 in EXCEL™ and ECOLEGO for Cs-137 and the wet deposition scenario as an example.

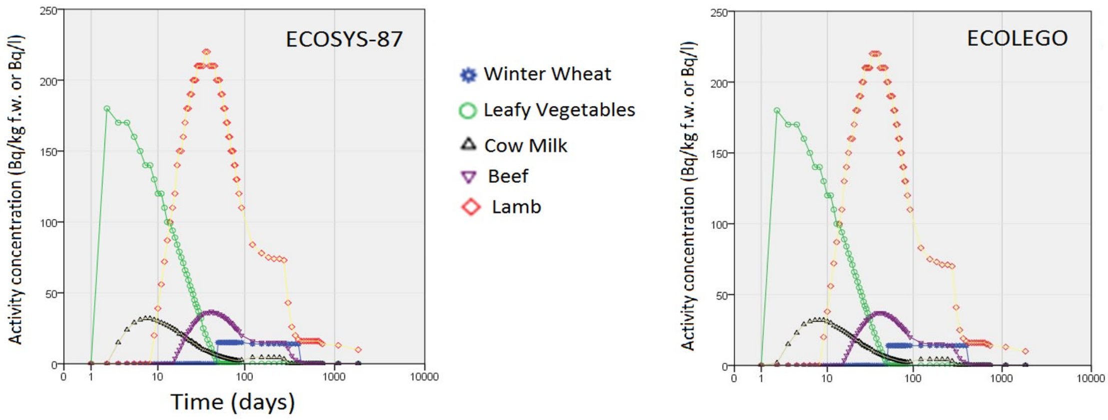


Fig. 2 Concentration of Cs-137 in foodstuffs obtained with ECOLEGO and ECOSYS-87 for the wet deposition scenario.

3.3 Updating databases and collation of underlying statistical datasets

In parallel with the ECOLEGO implementation, FDMT's default databases have been repopulated using data extracted from recently published reviews and available literature. The selection of parameters to collate was dictated by the scenarios outlined above. The collation of underlying statistical data was restricted to the four radionuclides considered in the scenarios, although the coverage was extended to all crop and animal derived food product types. The goal was to cover as many parameters as practicable but certain constraints were introduced by the consideration that underpinning data were sometimes unavailable or the set-up of the model limited the statistical treatment of a given parameter. To explain this last point, it should be noted that some of the time-dependent parameters, such as Leaf Area Index (LAI) and translocation factors, in the ECOLEGO version of FDMT are included as 'look-up' tables for which only single data values are provided for each discrete time-point. It was, therefore, impracticable to assign distributions to these parameters. This issue could be improved and might be considered in the next phase of this work.

As noted elsewhere [12, 52], it was considered that transfer factors result from the multiplication of a large number of unknown positive parameters and that their PDFs might be suitably characterised by log-normal distributions. It was, therefore, considered appropriate to allocate log-normal distributions to the default transfer factors collated in the present analysis. In other cases, the coverage of the data was simply not comprehensive enough to allow a detailed PDF to be characterised. In such cases, uniform distributions were typically employed allocating equal probability to the sampling of all quantities within the range defined by minimum and maximum values. In several additional cases where a range of values and best estimate value were available, the selection of triangular distributions was considered appropriate. The configuration of the default databases for this work on FDMT-ECOLEGO has drawn heavily on recent collations of radioecological parameter (most notable with regards to soil to plant transfer factor, and feed transfer coefficients for animal products) by the IAEA [17, 34]. Detailed descriptions on our data collation (giving information on their provenance and derivation) can be found in Brown et al. [44].

Table 2 shows old and new values for the soil to plant transfer factors along with the assigned distributions for the two crops used in abovementioned scenarios. Complete tables of transfer factor values for caesium, strontium and iodine for all crop types considered by FDMT can be found in the Appendix.

Table 2 Soil to plant transfer factor (TF, unitless) (new values from IAEA [34]).

	Plant	**New default (old default)**	**Distribution***	
			Arithmetic mean	**STD**
Caesium	Leafy_vegetables	6.0E-3 (2.0E-2)	1.7E-2	2.1E-2
	Winter_wheat	2.6E-2 (2.0E-2)	6.7E-2	1.3E-1
Strontium	Leafy_vegetables	7.6E-02 (4.0E-1)	1.9E-1	1.8E-1
	Winter_wheat	9.7E-02 (2.0E-1)	1.6E-1	1.7E-1
Iodine	Leafy_vegetables	6.5E-04 (1.0E-1)	1.6E-3	2.9E-3
	Winter_wheat	5.5E-04 (1.0E-1)	1.2E-4	2.5E-3

*Assumed to be untruncated log-normal distribution

We have focussed on these three elements and their radioisotopes as these will likely present the main causes of concern with respect to food chain transfer following an accidental release from a nuclear facility. The geometric means from the abovementioned data compilations are used as the new default parameter values for deterministic runs, as these values provide the best indication of central tendency for log-normally distributed data, whilst the arithmetic mean and associated pdf, from the same compilations, are used for probabilistic modelling.

3.4 Probabilistic model runs

Following the implementation of FDMT into ECOLEGO and assignment of distributions to various model parameters by updating its default databases, FDMT could be run probabilistically.

To demonstrate this new functionality, the new FDMT was applied to the scenarios described above (i.e. those used for the model testing considering wet and dry deposition cases). Using a Monte Carlo sampling method, 500 iterations were made for each run. The choice of 500 iterations was based on practical considerations, as a higher number of iterations required considerably longer simulation time. For each iteration, ECOLEGO takes a random sample from the PDF of each varied model parameter and performs a simulation for the set of parameters corresponding to this iteration. As a result, a set of model endpoint values is obtained for each iteration. The values obtained from all iterations, in this case 500, are then used to obtain different statistics of the model endpoints, such as the mean value, the median, the 5^{th} and 95^{th} percentiles.

The resulting simulations are for: cow milk, beef and lamb; dry and wet depositions; and Sr-90, I-131 and Cs-137. Deposition occured on1^{st} August, i.e. at Julian day = 213. For each run mean, 5^{th} and 95^{th} percentiles were obtained over a period of 5 years. The outputs from two such probabilistic runs are shown in Figs. 4 and 5 for activity concentration of Cs-137 in cow milk and meat.

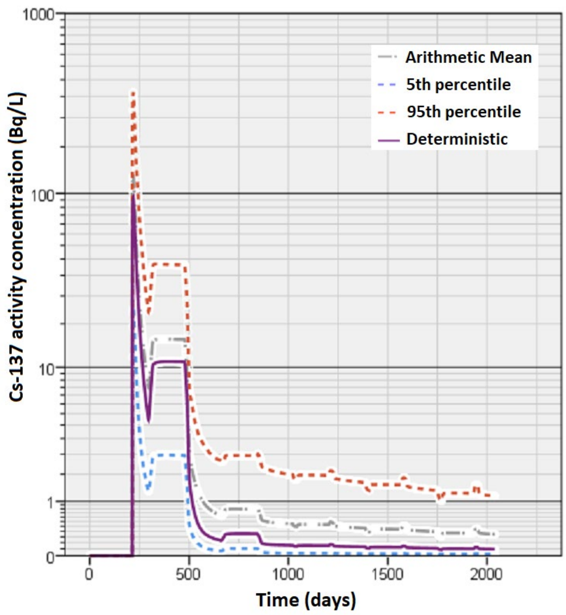


Fig. 4 Probabilistic simulation of activity concentration of Cs-137 in milk (cow) for the dry deposition scenario. In addition to 5th percentile, mean and 95th percentile, the output from deterministic run (based on using default new best estimate value) is also shown.

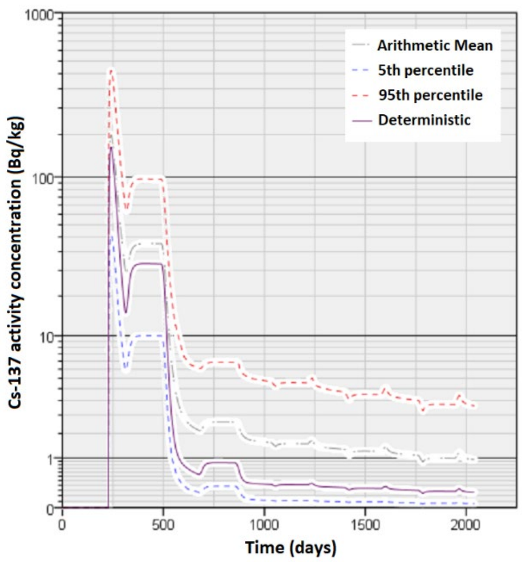
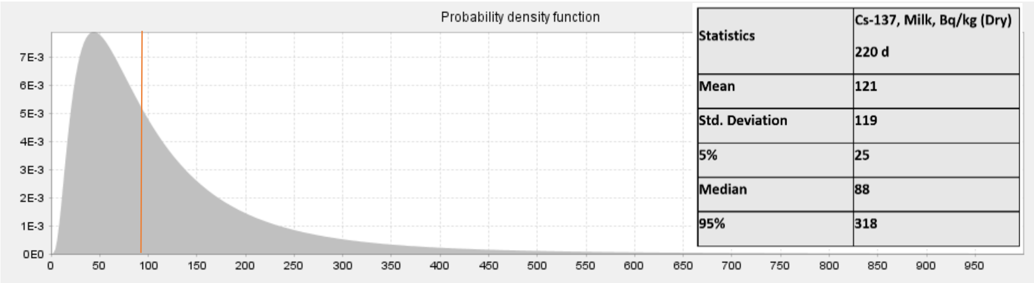


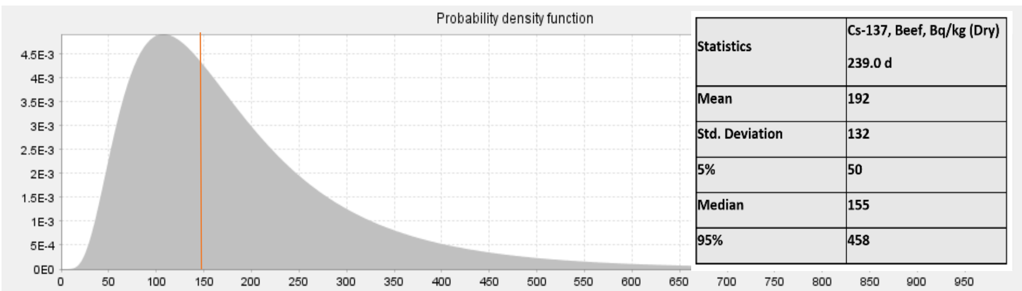
Fig. 5 Probabilistic simulation of activity concentration of Cs-137 in beef (cow) for the dry deposition scenario. In addition to 5th percentile, mean and 95th percentile, the output from deterministic run (based on using default best estimate value) is also shown.

As shown in Figs. 4 and 5, for the case of cow milk and beef, the deterministic predictions are comparatively low and close to 5th percentile values. Furthermore, the span between 5th and 95th percentiles is relatively narrow; the ratio of the 95th to 5th percentile falls generally around 10 and up to two-orders of magnitude at the most. Should the span between 5th and 95th percentiles have been much larger, e.g. the 95th to 5th percentile ratio reaching many orders of magnitude, problems may arise in specifying anything concrete when making a prognosis; at the low end of the prediction impacts might be negligible whereas at the high end, impacts may be dramatic. However, these kinds of considerations require extra information which is only possible to obtain by running the model probabilistically. Figs. 6 and 7 are shown here to illustrate the point that a probabilistically enabled FDMT is capable of producing results which are more detailed and informative as opposed to information obtained when running the model deterministically



Statistics	Cs-137, Milk, Bq/kg (Dry) 220 d
Mean	121
Std. Deviation	119
5%	25
Median	88
95%	318

Fig. 6 PDF and statistics for activity concentration of Cs-137 in cow milk for dry deposition scenario at day 220 (7 days after initial deposition). The vertical line indicates the value obtained upon running FDMT deterministically.



Statistics	Cs-137, Beef, Bq/kg (Dry) 239.0 d
Mean	192
Std. Deviation	132
5%	50
Median	155
95%	458

Fig. 7 PDF and statistics for activity concentration of Cs-137 in beef (cow) for dry deposition scenario at day 239 (26 days after initial deposition). The vertical line indicates the value obtained upon running FDMT deterministically.

The obtained confidence intervals illustrate the amount of uncertainty involved in each time step and provide useful information relevant in the process of making decisions. For example, regulatory standards can be compared with lower and upper confidence limits (such as 5^{th} and 95^{th} percentiles) to decide whether a standard will be violated or not. Regarding how to make use of the information obtained from a quantitative uncertainty analysis in decision making Hammond et al. [8] provide the following guidance: "if a 5% lower confidence limit is above a regulatory standard of concern, then it is likely that the standard will be violated. If the 95% upper confidence limit is below the standard, it is likely that the standard will not be violated. If the 95% upper confidence limit is above the standard, but the 50^{th} percentile is below the standard, further study should be recommended on those parameters that dominate the overall uncertainty. However, if the 50^{th} percentile is above the standard, further study may still be recommended, but under some circumstances one may opt to proceed with regulatory action depending on the cost-effectiveness of measures for risk reduction.".

In the present work, we have focused on model parameter uncertainties and the estimated endpoint uncertainties do not reflect the overall uncertainties associated with estimated concentrations, but only uncertainties related to the limited number of parameters that have been considered in these runs. Furthermore, in addition to parameter uncertainties there are other sources / types of uncertainties which could contribute to the total uncertainties associated with a model's output. These can be related to the conceptual and mathematical model, scenario and input data used to make the assessment [53]. It is important to have these considerations in mind when analysing estimated uncertainties of outputs of probabilistic runs.

3.5 Sensitivity analysis

Sensitivity analysis assesses how sensitive the model output is to changes in model inputs/ parameters [54]. It can be used to determine, for instance:

a. the parameters that contribute most to the output variability;

b. the model parameters (or parts of the model itself) that are insignificant;

c. if and which (groups of) parameters interact with each other.

The last point is related to correlation which might exist between various parameters and is often ignored, mostly due to computational challenges. Addressing the interaction between parameters requires computation of higher order sensitivity indices and in ECOLEGO there exists functionality for such considerations. Nonetheless, it was considered premature in this study to apply this option without a more detailed knowledge about the relationships between FDMT model parameters. The issue of correlation between input parameters and how this may affect model outputs has been considered elsewhere [55, 56].

The sensitivity analysis in this work was done for the case study described above for the wet deposition scenario and considers the same endpoints of radionuclide activity concentrations (^{90}Sr, ^{131}I and ^{137}Cs) in winter wheat (whole grain), Leafy vegetables, Cow milk, Cow meat and Lamb meat. The simulation period was extended to explore the influence of some parameters which are expected to play a role only after a prolonged period. Various time points were selected, namely : 1 day, 1 week, 2 weeks, 1 month, 2 months, 1 year, 10 years, 25 years, to account for the dynamics of the system and also to reflect the fact that the sensitivity of the model output to any given parameter might have a time dimension. The approach taken was as follows:

1. Probabilistic simulations – 5000[1] iterations by Monte Carlo sampling (random sampling) from the probability distributions assigned to several model parameters.

2. The probabilistic results were used for calculating different correlation and regression coefficients for the untransformed and ranked variables (this means that model inputs and outputs are ranked).

3. An algorithm named EASI (Effective Algorithm for Computing Global Sensitivity Indices) was applied [57]. This variance decomposition method is model independent. The calculated sensitivity index for each uncertain parameter represents the first order contribution of this parameter to the variance of the output.

[1] The choice of iteration numbers is somewhat arbitrary, the number of iterations for sensitivity analysis selected as being a factor of 10 higher than probabilistic runs. The common factor in both cases was that enough iterations were selected to ensure that the statistical information being generated could be deemed reliable.

In principle, for this study the EASI method alone was sufficient for ranking the model parameters by sensitivity, however, this method does not show if the parameter has a positive or negative effect on the output. On the other hand, although the Spearman Rank Correlation Coefficients (SRCC) do not give a quantitative measure of the contribution of the parameters to the variance of the outputs, they show the direction of the effect of the parameters on the output of interest. The outcomes from both analyses have therefore been used in tandem (Figs. 8 and 9).

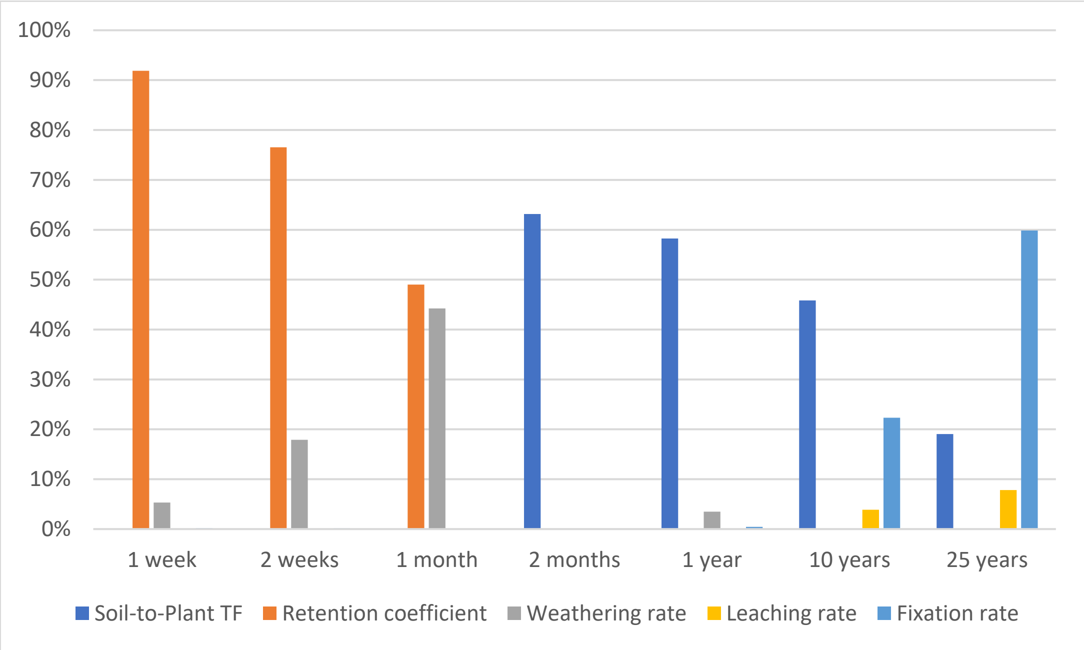


Fig. 8 Sensitivity indices (as calculated by EASI method) as function of time for Cs-137 concentrations in leafy vegetables.

The results from the analysis intuitively make sense. In the initial period of the simulation, up to the first month or so, the retention coefficient and (loss from vegetation) weathering rate constitute those parameters which predominate in terms of their contribution to the variance observed in Cs-137 activity concentrations in leafy vegetables. In later stages of the simulation, 10 to 25 years, the uncertainties associated with processes influencing the behaviour of Cs-137 in soil start to have a major influence upon the variance observed in the model output.

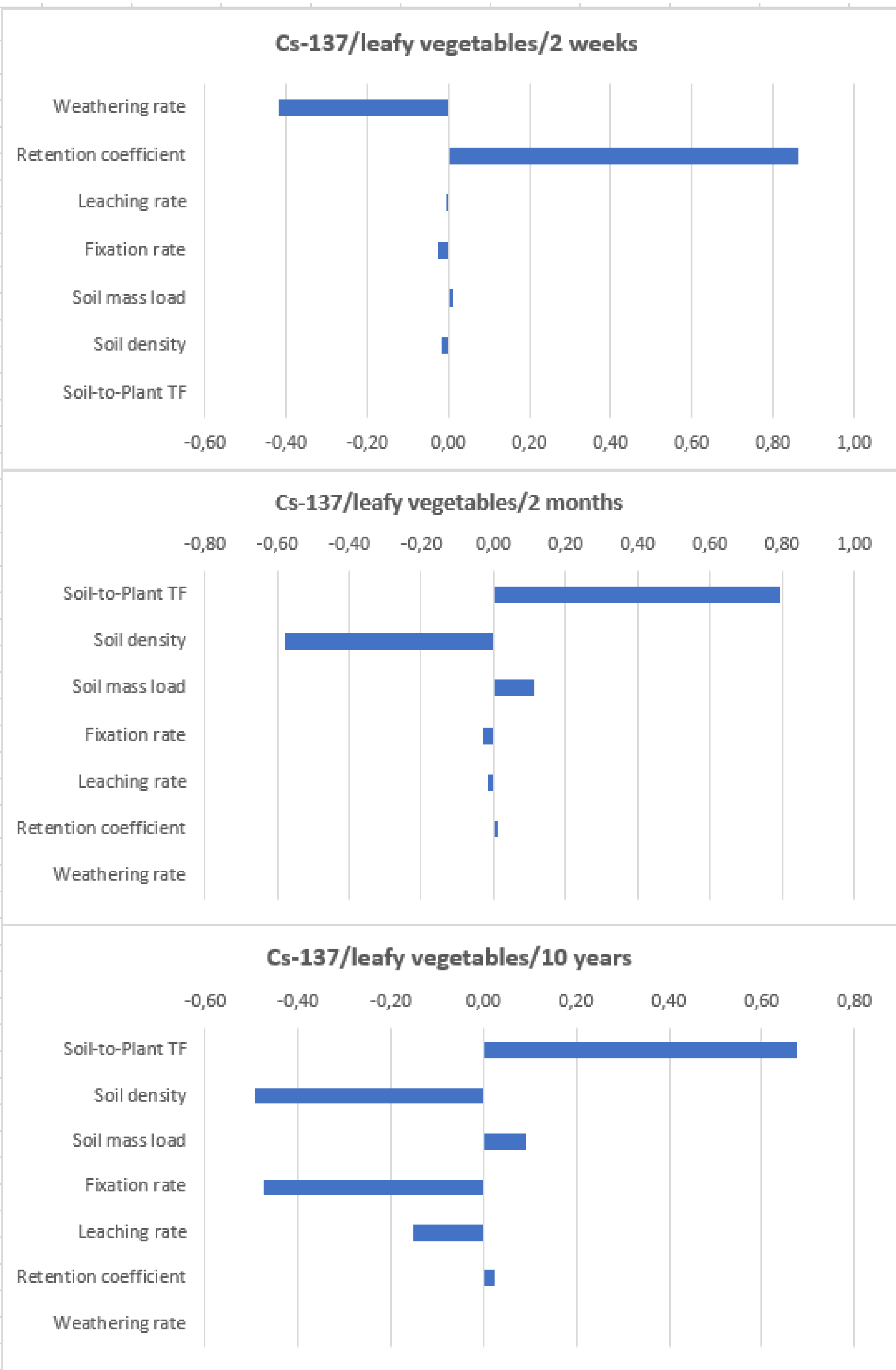


Fig. 9 Cs-137 leafy vegetables: Spearman rank correlation coefficients between parameters and output, for various time points. Note that the order of parameters on the vertical axis changes between the first and second plots.

The information provided from the Spearman rank correlation coefficients illustrate that, whereas the retention coefficient has a positive correlation with the assessment endpoint, the correlation with weathering rate is an inverse one (i.e. an increase in weathering rate will lead to a decrease in the simulated levels of Cs-137 in leafy vegetables). From a period of 2 months and extending in time up to the end of the simulation at 25 years, the soil to plant transfer factor (i.e. concentration ratio, *Fv,*) becomes an important factor.

To avoid over-interpretation of the results from the sensitivity analysis conducted in this study, the following should be noted. In particular, we lack insight into the model sensitivity to those parameters which have been defined by look-up tables, as noted earlier in the text. Of course, a sensitivity analysis could be conducted to consider the influence of these parameters without using look-up tables, but this was considered beyond the scope of our demonstration and has in any case been looked at elsewhere [58]. In this particular instance, we strongly suspect that LAI for leafy vegetables would have been defined as sensitive, at least in the initial phase post deposition, had there been a means of characterising variability in this parameter. Furthermore, the timing of events such as the start of the harvesting period and the time interval between the deposition event and the harvest are likely to confound any extrapolation of these findings to a generic situation. Although this can be partly accounted for by considering numerous scenarios/cases, the regional aspects of farming practices relevant for model parameterisation are still likely to exert a great, and currently largely unquantifiable, influence on (some of the conclusions that might be drawn from) the sensitivity analyses.

4. Concluding remarks

Improving decision support systems used to manage risks in an emergency situation through quantification and reduction of uncertainties in underlying models has been identified as being important but has not yet satisfactory addressed [21]. To address this and in order to make FDMT fit for purpose, the model has been implemented into the flexible ECOLEGO modelling platform. This transformation has yielded new functionality and a great degree of freedom with regards to developmental work needed to improve the model further and to make it more user friendly.

The focus of this work has been to demonstrate what could be improved within the FDMT implementation in the ARGOS and RODOS decision support systems and to create a platform to identify future model development needs. However, there is no foreseeable hindrance to including the revised model/implementation into the decision support systems.

FDMT can now be run probabilistically and the new platform allows for a sensitivity analysis to be conducted. By including the uncertainties of the underlying parameters through assignment of PDFs we can now acquire insight regrading uncertainties in predictions and also evaluate the relative importance of various parameters as a function of time for selected endpoints through making use of the sensitivity analysis functionality.

There is a clear requirement for further testing of the probabilistic model outputs. There are suitable datasets that have been collated following the Chernobyl accident (for example BIOMOVS datasets [59]) and these could provide a good start for model testing. An initial check may be to see whether the empirical data measurements fall within given percentiles (e.g. 5^{th} and 95^{th}) of the model outputs.

In addition to having the possibility of employing numerical solvers to more challenging model configurations, implementation of FDMT within the ECOLEGO modelling platform opens up the potential for investigation of various model components either in isolation or in combinations which reflect more specific settings. In other words, the new model offers flexibility in working with the model components such that these can be tested, modified or replaced. The latter option has encouraged, following the implementation and testing described in this paper, the introduction of a library structure. To achieve this, the overall model has been first disaggregated into its components/sub-models, such that each unit can be treated standalone and be applied independently. The advantage of organizing the model in this way is that the user can select specifically any component they are interested in for any given model run without invoking the entire FDMT model. This in turn, allows for getting better insight into underlying operations and increases the traceability and transparency.

Deposition and interception models in FDMT should be revised in order to take into account important factors such as chemical form of radionuclides as well as surface characteristics of vegetation. This requires moving from the possibility to just change/revise parameters to the consideration of new models which are more complex in terms of considering underlying mechanisms and processes to a greater extent. For example, there are other models that can be used to consider dry and wet deposition to those used as default in FDMT (e.g. [59, 60]) and future plans involve exploring the efficacy of using such alternative models.

The new design paves the way towards a more process-based modelling [32] approach and allows for evaluation of different models of varying complexities. This possibility provides a platform for considering case/region specific issues and to make predictions which are of more relevance and of better use with regards to decision making and management of risk.

Currently process based models would have applicability in making long term predictions of soil-plant transfer after a deposition event (see [2,6,32]) in order to better identify areas where resources need to be focused and countermeasures potentially applied. However, they could also be developed to better define processes identified as being important through sensitivity analyses (e.g. to better model radionuclide concentrations following direct deposition on crops.However, even though the new design of FDMT provides novel opportunities, the extent to which we are able to take advantage of these is limited for the moment. For instance, FDMT can now be run probabilistically or a sensitivity analysis can be conducted, but lack of relevant statistical data, which is necessary to characterise uncertainties related to some model parameters, limits the use of these new features. To overcome these shortcomings some progress has been made, but there is a need to expand the statistical data collation to parameters not originally covered (i.e., non-radioecological, agricultural parameters) and to consolidate the information for those parameters that have been considered.

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Author Declarations

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Conflicts of interests - There are no conflicts of interest.

Competing interests - not applicable

Availability of data and materials - not applicable

Code availability - not applicable

Authors' contributions - AH coordinated the activities in the study and is the main author of the work. AH Collated parameter datasets and conducted simulations using the newly developed software. RA was responsible for the development and implementation of the software/programme code used in the study. NB was coordinator of the project under which this work was performed (i.e. CONFIDENCE work-package Leader) and was instrumental in directing this work. NB was a co-author and involved in drafting of the manuscript and collated parameter datasets. JB is a co-supervisor of AH's PhD and as such was involved in the planning and direction of the study. He was heavily involved in assisting to draft and structure the manuscript, collated parameter datasets and conducted simulations using the newly developed software. DO is the main supervisor of AH's PhD and as such was involved in the planning and direction of the study. DO was involved in prior-to-submission review of the manuscript.

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7. Appendix

Soil to plant transfer factors (TF , unitless) for caesium, strontium and iodine (new values from IAEA [29]).

Element	Plant	New default (old default)	Distribution*	
			Mean	STD
Cs	Beet_leaves	5.6E-3 (3.0E-2)	1.1E-2	1.9E-2
	Leafy_vegetables	6.0E-3 (2.0E-2)	1.7E-2	2.1E-2
	Maize	1.8E-2 (2.0E-2)	3.0E-2	2.8E-2
	Beet	6.7E-3 (1.0E-2)	1.2E-2	1.8E-2
	Corncobs	6.3E-3 (1.0E-2)	1.1E-2	1.1E-2
	Fruit	8.7E-4 (2.0E-2)	2.3E-3	3.3E-3
	Oats	2.5E-2 (2.0E-2)	6.6E-2	1.3E-1
	Potatoes	1.2E-2 (1.0E-2)	2.1E-2	2.5E-2
	Rye	2.5E-2 (2.0E-2)	6.6E-2	1.3E-1
	Spring_barley	2.5E-2 (2.0E-2)	6.6E-2	1.3E-1
	Spring_wheat	2.6E-2 (2.0E-2)	6.7E-2	1.3E-1
	Winter_barley	2.5E-2 (2.0E-2)	6.6E-2	1.3E-1
	Winter_wheat	2.6E-2 (2.0E-2)	6.7E-2	1.3E-1
	Berries	1.5E-3 (2.0E-2)	2.9E-3	3.3E-3
	Fruit_vegetables	1.1E-3 (1.0E-2)	3.5E-3	7.5E-3
	Root_vegetables	6.7E-3 (1.0E-2)	1.2E-2	1.8E-2
	Grass (Intensive)	5.5E-2 (5.0E-2)	1.2E-1	1.8E-1
	Grass (Extensive)	1.7E-1 (1.0E0)	2.4E-2	2.6E-2
Sr	Beet_leaves	1.2E-1 (8.0E-1)	2.4E-1	2.2E-1
	Leafy_vegetables	7.6E-2 (4.0E-1)	1.9E-1	1.8E-1
	Maize	1.8E-1 (3.0E-1)	2.5E-1	1.9E-1
	Beet	1.2E-1 (4.0E-1)	2.4E-1	2.2E-1
	Corn_cobs	6.1E-2 (2.0E-1)	1.1E-1	1.2E-2
	Fruit	2.6E-3 (1.0E-1)	3.8E-3	2.9E-3
	Oats	9.6E-2 (2.0E-1)	1.6E-1	1.7E-1
	Potatoes	3.4E-2 (5.0E-2)	5.0E-2	4.6E-2
	Rye	9.6E-2 (2.0E-1)	1.6E-1	1.7E-1
	Spring_barley	9.6E-2 (2.0E-1)	1.6E-1	1.7E-1
	Spring_wheat	9.7E-2 (2.0E-1)	1.6E-1	1.7E-1
	Winter_barley	9.6E-2 (2.0E-1)	1.6E-1	1.7E-1
	Winter_wheat	9.7E-2 (2.0E-1)	1.6E-1	1.7E-1
	Berries	3.3E-2 (1.0E-1)	5.5E-2	6.9E-2
	Fruit_vegetables	1.8E-2 (2.0E-1)	4.9E-2	9.0E-2
	Root_vegetables	1.2E-1 (3.0E-1)	2.4E-1	2.2E-1
	Grass (Intensive)	2.9E-1 (5.0E-1)	3.74E-1	2.6E-1
	Grass (Extensive)	2.9E-1 (1.0E0)	3.74E-1	2.6E-1
I	Beet_leaves	1.2E-3 (1.0E-1)	2.1E-3	1.9E-3
	Leafy_vegetables	6.5E-4 (1.0E-1)	1.6E-3	2.9E-3
	Maize	1.3E-2 (1.0E-1)	2.8E-2**	4.5E-2**
	Beet	1.2E-3 (1.0E-1)	2.1E-3	19E-3
	Corn_cobs	1.2E-4 (1.0E-1)	2.7E-4	5.3E-4
	Fruit	9.5E-4 (1.0E-1)	1.8E-3	1.8E-3

	Oats	5.5E-4 (1.0E-1)	1.3E-4	2.4E-3
	Potatoes	2.1E-2 (1.0E-1)***		
	Rye	5.5E-4 (1.0E-1)	1.2E-4	2.4E-3
	Spring_barley	5.5E-4 (1.0E-1)	1.2E-4	2.4E-3
	Spring_wheat	5.5E-4 (1.0E-1)	1.2E-4	2.5E-3
	Winter_barley	5.5E-4 (1.0E-1)	1.2E-4	2.4E-3
	Winter_wheat	5.5E-4 (1.0E-1)	1.2E-4	2.5E-3
	Berries	1.5E-2 (1.0E-1)***		
	Fruit_vegetables	5.0E-3 (1.0E-1)***		
	Root_vegetables	1.2E-3 (1.0E-1)	2.1E-3	1.9E-3
	Grass (Intensive)	8.1E-4 (1.0E-1)	9.9E-2	3.1E-2
	Grass (Extensive)	8.1E-4 (1.0E-1)	9.9E-2	3.1E-2

*Untruncated Lognormal distribution; **for cereal stem and shoots; ***No distribution, based on one value.