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GENERIC UNCERTAINTY MODEL FOR DETRA FOR ENVIRONMENTAL CONSEQUENCE ANALYSES

Application and sample outputs

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ABSTRACT

Computer model DETRA applies a dynamic compartment modelling approach. The compartment structure of each considered application can be tailored individually. This flexible modelling method makes it possible that the transfer of radionuclides can be considered in various cases: aquatic environment and related food chains, terrestrial environment, food chains in general and food stuffs, body burden analyses of humans, etc.

In the former study on this subject, modernization of the user interface of DETRA code was carried out. This new interface works in Windows environment and the usability of the code has been improved.

The objective of this study has been to further develop and diversify the user interface so that also probabilistic uncertainty analyses can be performed by DETRA. The most common probability distributions are available: uniform, truncated Gaussian and triangular. The corresponding logarithmic distributions are also available. All input data related to a considered case can be varied, although this option is seldomly needed. The calculated output values can be selected as monitored values at certain simulation time points defined by the user. The results of a sensitivity run are immediately available after simulation as graphical presentations. These outcomes are distributions generated for varied parameters, density functions of monitored parameters and complementary cumulative density functions (CCDF).

An application considered in connection with this work was the estimation of contamination of milk caused by radioactive deposition of Cs (10 kBq(Cs-137)/m^2). The multi-sequence calculation model applied consisted of a pasture modelling part and a dormant season modelling part. These two sequences were linked periodically simulating the realistic practice of care taking of domestic animals in Finland. The most important parameters were varied in this exercise.

The performed diversifying of the user interface of DETRA code seems to provide an easily applicable tool for uncertainty analyses and for localisation of the input parameters having the greatest contribution to uncertainty obtained in result values.

TIIVISTELMÄ

Tietokonemalli DETRA on kompartmenttimalli, jonka kompartmenttirakenne voidaan laatia kulloisenkin laskentatapauksen vaatimusten mukaisesti. Tämä mahdollistaa, että mallin avulla voidaan tarkastella radionuklidien kulkeutumisen aikariippuvuutta erityyppisissä tilanteissa: vesistöt ja vesiympäristön ravintoketjut, maaperä, ravintoketjut yleensä ja elintarvikkeet, radionuklidien kulkeutuminen ihmiseen, jne.

Edellisessä tämän aihepiirin toimeksiannossa malliin kehitettiin verraten laaja graafinen käyttöliittymä Windows-ympäristöön soveltuvaksi. Tämän ansiosta mallin käyttö tuli aiempaa helpommaksi ja nopeammaksi.

Tässä työssä mallin käyttöliittymää on edelleen laajennettu siten, että myös todennäköisyyspohjaiset epävarmuusanalyysit ovat mahdollisia. Varioitaville lähtötiedoille voidaan antaa yleisimmät jakaumat tunnuslukuineen: tasainen jakauma, typistetty normaalijakauma ja kolmiojakauma. Vastaavat logaritmiset jakaumat ovat myös käytettävissä. Kaikkia tarkasteltavan tapauksen lähtötietoja voidaan varioida, mihin ei yleensä kuitenkaan ole tarvetta. Laskettavat tulossuureet voidaan valita monitoroitaviksi parametreiksi käyttäjän valitsemilla simuloinnin ajanhetkillä. Epävarmuusanalyysin tulokset ovat välittömästi simuloinnin jälkeen katsottavissa graafisista esityksistä. Tuloskuvia ovat lähtötiedoille generoidut jakaumat sekä monitoroitavien parametrien tiheysfunktiot sekä komplementaariset kumulatiiviset tiheysfunktiot (CCDF).

Sovellustapauksena työssä on tarkasteltu maidon saastumista radioaktiivisen Cs-laskeuman seurauksena (10 kBq(Cs-137)/m²). Laskentamallina on käytetty ns. monijaksomallia, jossa laidunkautta sekä sisäruokintakautta kuvaavat mallit vuorottelevat jäljitellen todenmukaista tilannetta. Sovelluksessa varioitiin tärkeimpiä laidunmallin lähtötietoja esimerkinomaisesti.

Nyt kehitetty DETRA-mallin käyttöympäristön laajennus näyttää tarjoavan useissa analyyseissä käyttökelpoisen työkalun epävarmuustekijöiden selvittämistä varten ja antaa mahdollisuuden paikallistaa kuhunkin tapaukseen liittyvät suurinta epävarmuutta aiheuttavat lähtötiedot.

CONTENTS

FOREWORD

This contracted study related to the further development and diversifying of the user interface of the biospheric transfer and dose prediction model DETRA was financed by the Radiation and Nuclear Safety Authority (STUK). The developed software will replace the software version which has been earlier assigned by VTT to STUK. This work has been carried out in the Nuclear Energy research field at VTT Energy as contracted STUK. The contact persons have been senior inspector Riitta Hänninen and head of laboratory Aino Rantavaara (STUK) and research scientist Vesa Suolanen (VTT Energy).

1 INTRODUCTION

The compartment model DETRA has been utilized at VTT Energy for several years in applications of safety analyses of nuclear waste disposal and environmental consequences of nuclear power plants, particularly in prediction of transfer of radionuclides in terrestrial or aquatic environments.

Quite recently the user interface of DETRA has been modernized and the usability of the model was thus improved. The new interface works in Windows environment. In the scope of this work the calculation properties of the model have been developed and the interface has been diversified so that also sensitivity analysis runs are now possible.

2 DESCRIPTION OF THE DEVELOPED UNCERTAINTY MODEL

The calculation method of the DETRA code is a dynamic type compartment model based on first order kinetics. Essential benefit of the model is that its compartment structure can flexibly be tailored corresponding to a considered application.

In connection with an earlier study performed by VTT Energy, a new user interface was developed for DETRA. After that development phase the use and applicability of the model became easier. This earlier developed version of the model, with new user interface, is described in detail in ref. [1].

The calculation properties of DETRA have by this work been extended so that also sensitivity analyses can now be carried out. This added feature makes it possible to study the effect of variation of input data on the uncertainty of the output (monitored values). Programming of the new version has been carried out in Microsoft Visual C++ environment.

In order to perform a sensitivity run the user opens the *sensitivity* menu (Fig. 1) from the main window of DETRA interface. After that the user specifies distributions of input parameters (*Input distribution*-option) and the output parameters to be monitored (*Select monitored values*-option). The user can also open an earlier saved sensitivity file by activating the *Open*-option from the menu. The
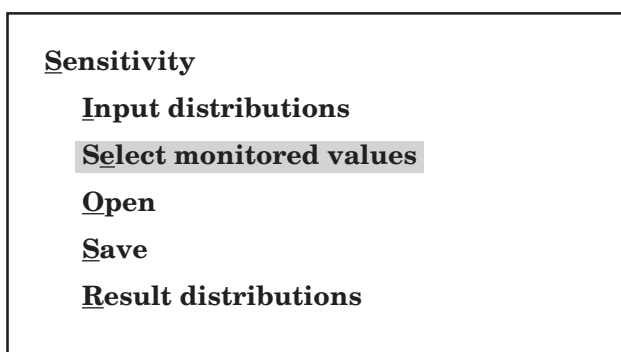
results of a sensitivity run are available under *Result distributions*-option of the menu.

After selecting the 'Input distributions' option, the user has access to the distribution specifications window (Fig. 4). The leftmost column is merely a running line number, and the user can scroll the table by clicking on the two small buttons on the left. The next column is for the codes of the varied parameters. Their form (v1, v2, ...) is exactly the same as in the actual input windows where arbitrary input parameters can be marked as 'varied parameters'. The order of the codes in this column has no significance.

The third column specifies the type of probability distribution to be used for the corresponding varied parameter. The English name of the desired distribution can be chosen from the dropdown list or typed by hand. Currently available are four basic distributions and their logarithmic counterparts ('logarithmic' means in each case that the base-10 logarithm of the value has the specified distribution):

uniform	log uniform
triangular	log triangular
normal (Gaussian)	log normal
truncated Gaussian	log truncated Gaussian

After specifying a certain distribution, the user sees the names of its parameters appear as column headings above the corresponding row. For uniform distribution, the parameters are the minimum and maximum occurring values. Each value between them is equally likely to be generated.

Likewise, the triangular distribution has minimum and maximum, but also a peak value, which has to be between minimum and maximum. Now the probability density function (pdf) is piecewise linear, being zero at minimum and maximum, and showing a maximum probability density at the peak location value.

Sensitivity

  Input distributions

  Select monitored values

  Open

  Save

  Result distributions

Fig. 1. *Preparation of a sensitivity run.*

A normal distribution is completely specified by its mean and standard deviation. Any value that can be expressed as floating point may be generated, the extremes being quite unlikely of course. Note that when the truncated form is used, mean and standard deviation refer to the corresponding untruncated distribution, and two additional parameters, minimum and maximum, have to be specified.

For all distributions, a generated value will be the point where the integral of the pdf equals the value generated by a uniform 0…1 interval random number generator. In the cases of uniform and triangular distributions, this point can be solved analytically in a straightforward fashion, but the other, Gaussian-based distributions, call for a built-in numerical integration of the Gaussian pdf. The CPU time used for the numerical integration is negligible when compared with the total running time.

The random number generator is automatically reseeded each time when a sensitivity analysis run is started. So the same sequence of random numbers will not be produced, and the results can be added to an existing result file (use the 'append' option), thus providing a bigger set of independent cases.

3 A SAMPLE APPLICATION

3.1 Case specification

In order to demonstrate the applicability of the developed uncertainty model, a deposition episode causing contamination of pasture and in the later phase also the final product milk, was selected for a closer consideration [1].

The considered calculation case concerns milk contamination model chain. Selected input parameters of the model were varied. The calculation model is of multi-sequence type and basically consists of two parts: the pasture season part (Fig. 2) and the dormant season part (Fig. 3). These two sequences follow each other periodically during the simulation. Total deposition of 10 kBq(Cs-137)/m^2 on the pasture within a short period of time, in few hours, was expected to happen. The considered radioactive deposition was assumed to take place on the 1st of May.

There are many transfer mechanisms of radio-nuclides related to the pasture model and to the cow's metabolic model. Such transfer mechanisms are wash-off from the grass surface onto the ground, resuspension from the ground to grass surface, concentration of radionuclides from soil into the grass and sorption in the soil. Absorption factors of the metabolic model affect the concentrations observed in milk. Uncertainties related to the pasture model parameters are broadly studied and comprehensive sets of measurements have been performed during the past years.
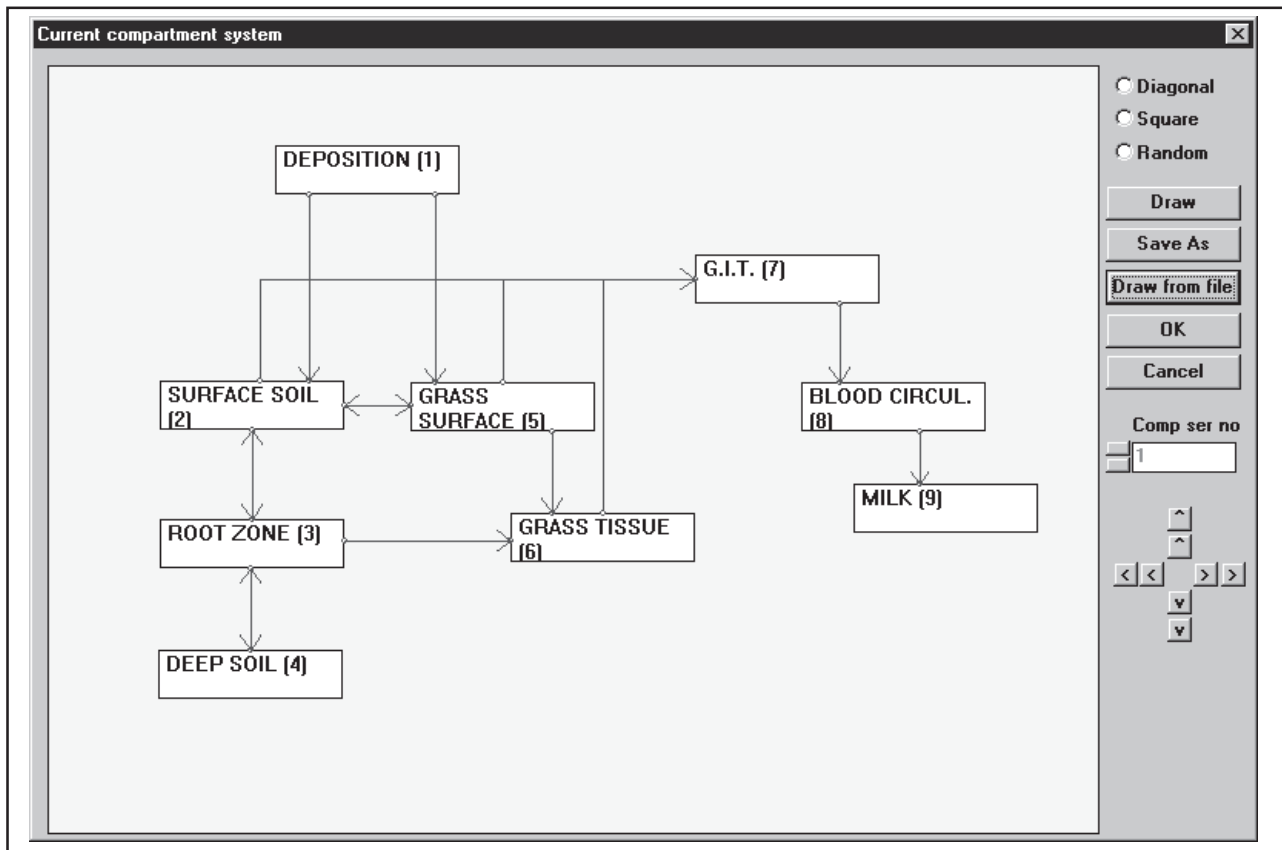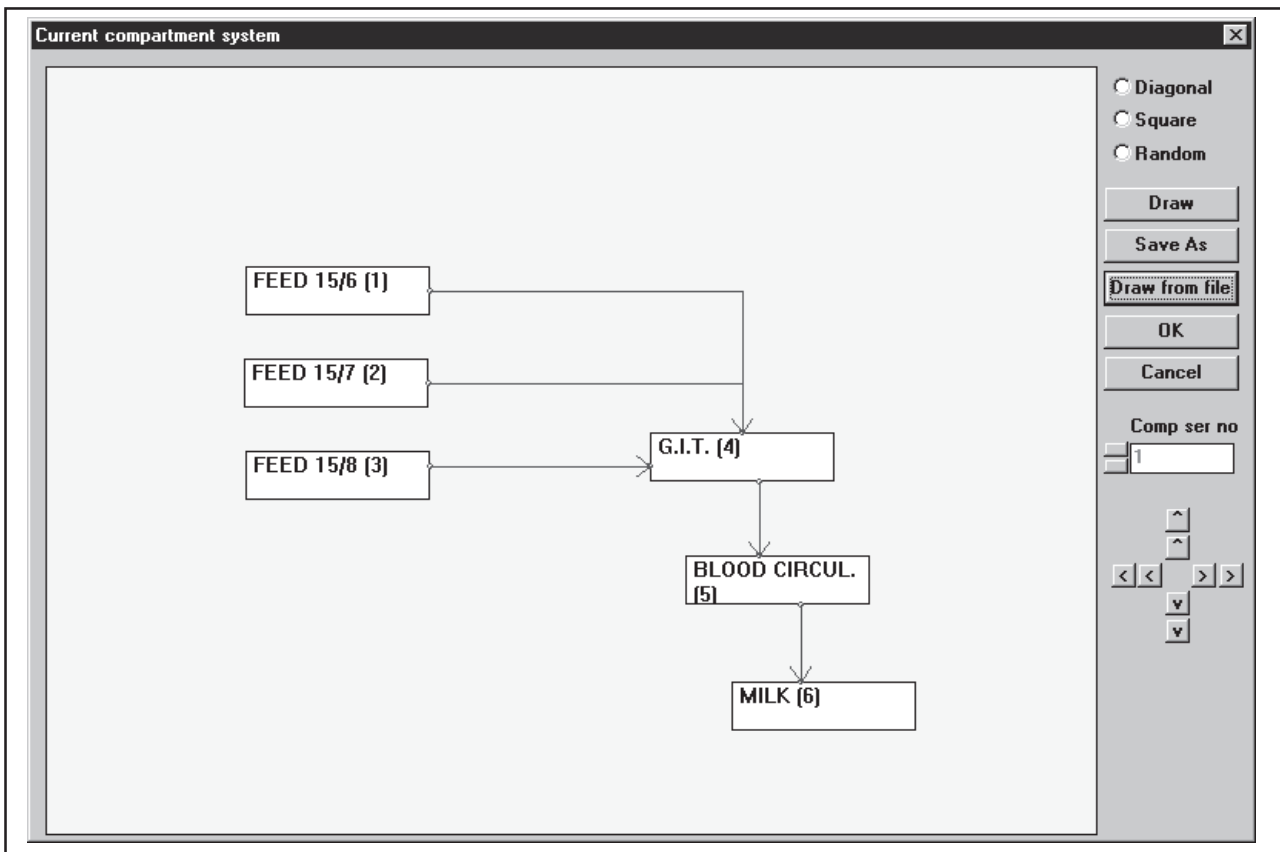

Fig. 2. *The pasture season model.*

Fig. 3. *The dormant season model.*

3.2 Varied parameters

At a random moment when a radioactive deposition occurs there might exist many kinds of circumstances in the pasture environment. The point of time during the growing season varies affecting changes to the biomass content of pasture. The weather circumstances vary affecting changes to the transfer rates of radionuclides from grass leaves to the ground surface. In case of rainy weather the transfer rates of nuclides are higher than in the case of dry weather type. The velocity of wind causes changes to resuspension activity from the soil surface. The adsorption properties of various elements in soil are related to the soil type and this generates wide variability to sorption factors of elements.

In the consideration of uncertainties related to milk contamination after radioactive deposition, it is worth restricting the number of varied parameters—in order to limit the simulation time needed to solve the problem. The developed model provides the possibility to vary all used input parameters, although this option is seldomly really needed. Generally, sensitivity of the results can

be estimated by sampling from given distributions of certain key parameters of a model.

Many international research projects, co-ordinated e.g. by IAEA (International Atomic Energy Agency) or OECD (Organisation for Economic Co-operation and Development), have studied uncertainties related to environmental consequence assessment models.

This report gives a demonstration on how the developed model can be utilized as an uncertainty analysis tool. Three input parameters of the model were selected to be varied (Table I). Relevant probability distributions and bounds were attached to them (Table II). The specified *input distributions*, saved as DETRA interface format, are presented in Fig. 4. Considering the migration and leaching of radionuclides in soil, the solid-liquid distribution coefficient (K_d) could have the largest degree of variability [2]. This is due to the large amount of various soil types i.e. various retardation properties of radionuclides. Based on these facts it was expected that an asymmetric distribution, like the logarithmic truncated Gaussian, probably describes the actual distribution of K_d values in a relevant way.

Table I. Varied parameters and confidence intervals of relevant values [2, 3].

Varied parameter	Unit	90% confidence interval		
		lower value	upper value	default /peak
liquid–solid distribution coefficient (K_d)	$(Bq/kg_s)/(Bq/litre_w)$	200	60000	1000
concentration factor (CF)	$(Bq/kg_{f.w.})/(Bq/kg_s)$	0.001	0.3	0.02
removal factor from grass surface (λ_w)	(1/year)	7.0	63.2	10.1

Table II. Distributions and characteristic values of varied parameters as they are input in DETRA.

Varied parameter	Distribution	mean 1)	std_dev 1)	min	max	peak
K_d	log trunc. Gaussian	3.00	0.54	2.30	4.78	
CF	log trunc. Gaussian	−1.7	0.4	−3.0	−0.52	
λ_w	triangular			7.0	63.2	10.1

1) Of the untruncated distribution.

Soil-to-grass concentration factors are measured extensively and their responses in different soil types for at least most important elements are quite well known. Although the most probable value could be estimated, there exist bound values which might differ from the default value by orders of magnitude. The logarithmic truncated Gaussian distribution was also selected for the CF parameter.

The removal factors from grass surface (λ_w) have been experimentally studied to some extent and the results have been reported [4]. It is obvious that the removal factor value is exceptionally important when considering the permanency of the deposited nuclides on the grass surface. The triangular distribution was expected to describe sufficiently well the actual distribution obtained in natural conditions.

3.3 Monitored parameters

The developed model allows for the user to study the uncertainty of any of the model output parameters. In this application, milk concentration was selected to be the monitored parameter. Milk concentration was followed and considered at different time points after the deposition episode:

- 1st pasture season (= 1st calculation sequence)
- 1st dormant season (= 2nd calculation sequence)

Fig. 4. Specified input distributions of the case.

- 2nd pasture season   (= 3rd calculation sequence)
- 2nd dormant season (= 4th calculation sequence)
- 3rd pasture season   (= 5th calculation sequence).

The total length of the time period from the beginning of simulation to the 3rd pasture season control time point is two years. By following milk concentration results at different time points it is possible to estimate sensitivity levels of the results against the varied parameter values applied. The sensitivity simulation was in fact extended up to ten calculation sequences, but the results are presented graphically in this report only for five sequences, showing the tendency of uncertainty development during the simulation case. The specified monitored values are presented in Fig. 5.

3.4 Sample outputs

After starting the simulation of a case the code generates the distributions of varied parameters to be used. In the considered application those varied parameters are K_d, CF and λ_w, marked by V1, V2 and V3 symbols. The generated varied parameters distributions are available in graphs (Fig. 6, 7 and 8) also displaying the number of simulation rounds. For K_d and CF the selected distribution was logarithmic truncated Gaussian and for λ_w triangular type. Generally, as the number of rounds increases sufficiently, the varied parameter distributions should converge to the originally selected distribution type. The graphs of distributions can, of course, be presented also with some other programme tools (like Excel) by just using the numeric output file of distributions generated originally by the DETRA code.

During simulation the code automatically generates a real-time output distribution of a selected monitored parameter. This output graph (Fig. 9) can be seen from the '*Start Calculation*'-window and provides the user a possibility to real-time follow-up of the formation of the monitored parameter final distribution. Generation of milk concentration (Bq/litre) distribution at a selected time point of calculation sequence number 1 is presented in this case (Fig. 9).

Probably the most illustrative are the calculated complementary cumulative distribution functions (CCDFs) which are always rapidly available after simulation of a certain case. The following graphs (Fig. 10, 11, 12, 13 and 14) give an outlook on the development of the uncertainty related to the contaminated milk concentrations at various time points after the deposition episode of ^{137}Cs nuclide. From the figures it can be noticed that remarkable uncertainty is related to the first sequences, but in the later phases of the simulation the different uncertainty factors will compensate each other to some extent.

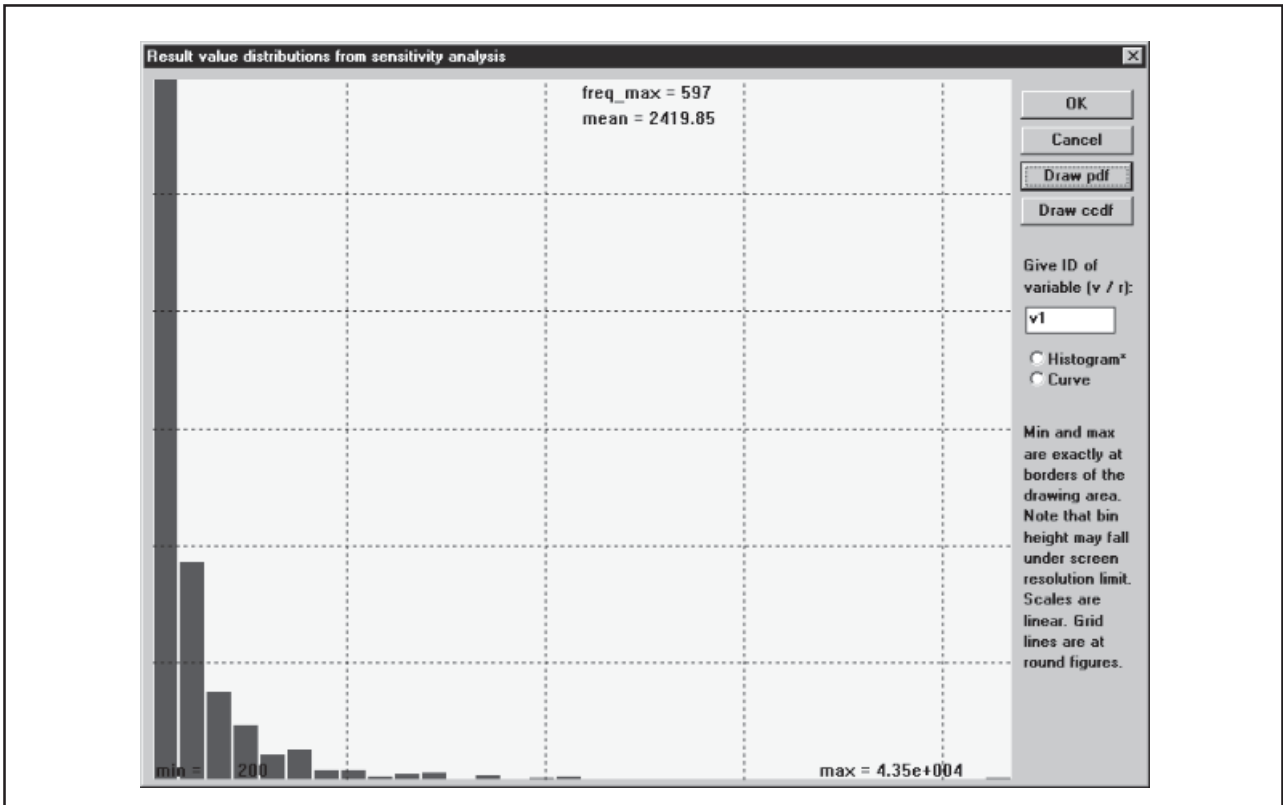*Fig. 5.* *Selected monitored values of the case*

Fig. 6. *Distribution of the varied parameter V1 (K_d (Bq/kg_s)/(Bq/$litre_w$)) after 999 rounds of simulation.*
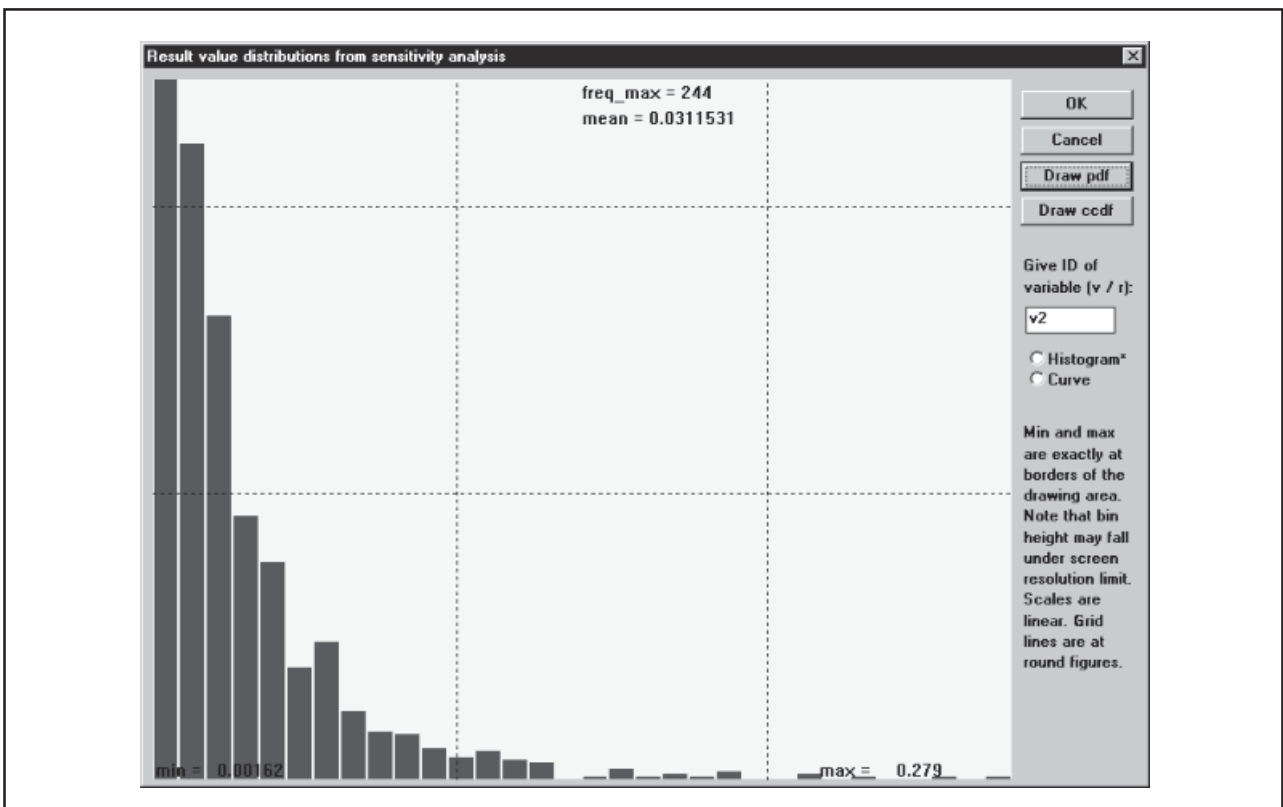

Fig. 7. *Distribution of the varied parameter V2 (CF (Bq/$kg_{f.w.}$)/(Bq/kg_s)) after 999 rounds of simulation.*
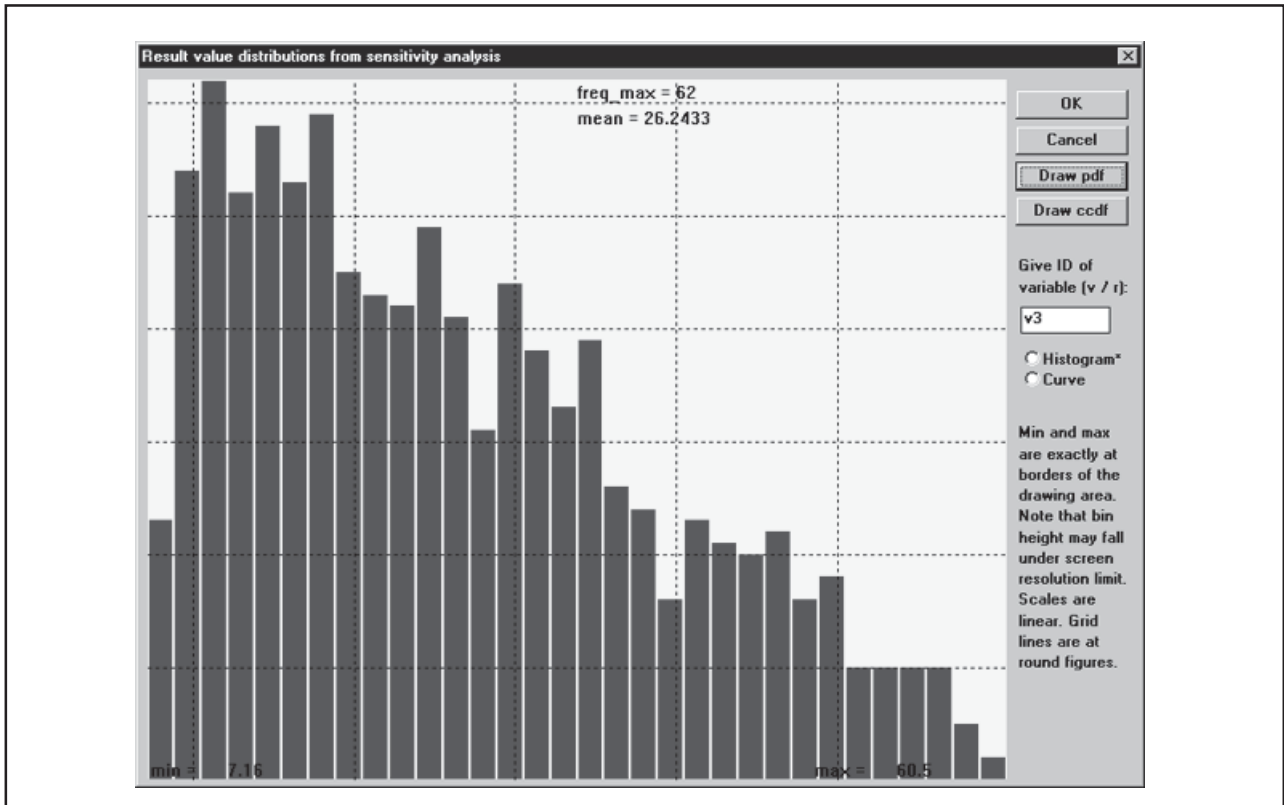
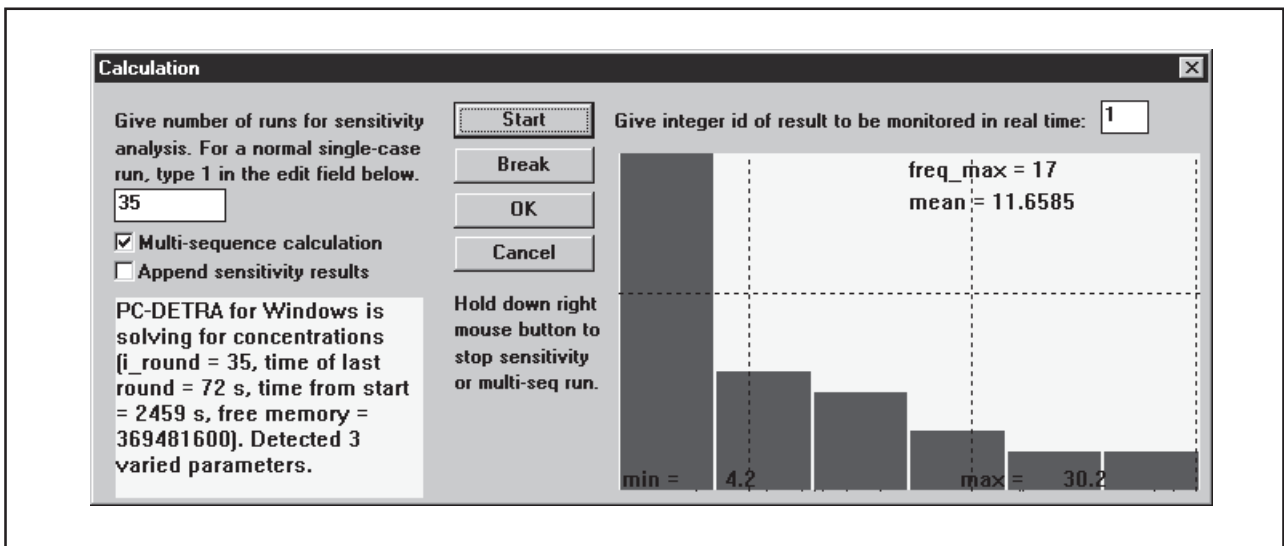**Fig. 8.** *Distribution of the varied parameter V3 (λ_w (1/year)) after 999 rounds of simulation.*

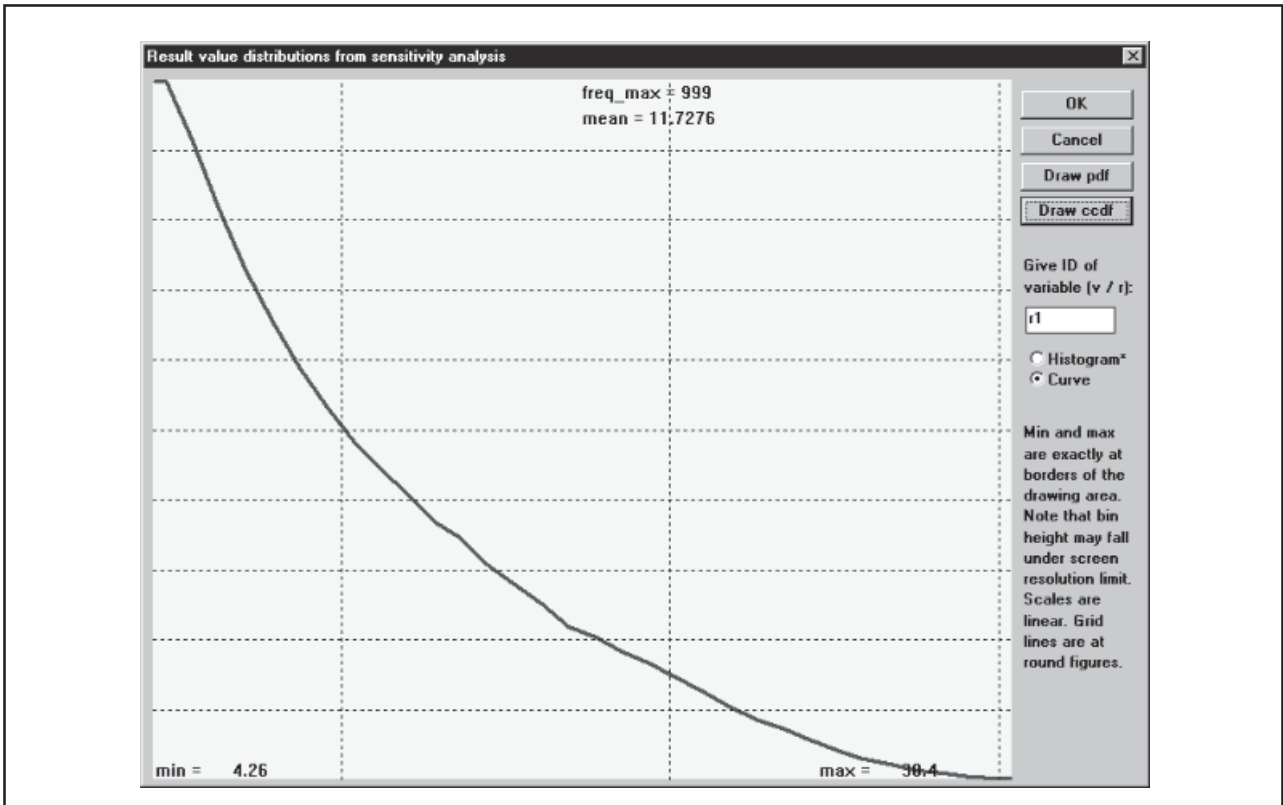**Fig. 9.** *A real-time sample output of the monitored parameter distribution.*

Fig 10. CCDF for the monitored parameter (C_{milk} (Bq / litre)) at 1st calculation sequence.

Fig 11. CCDF for the monitored parameter (C_{milk} (Bq / litre)) at 2nd calculation sequence.
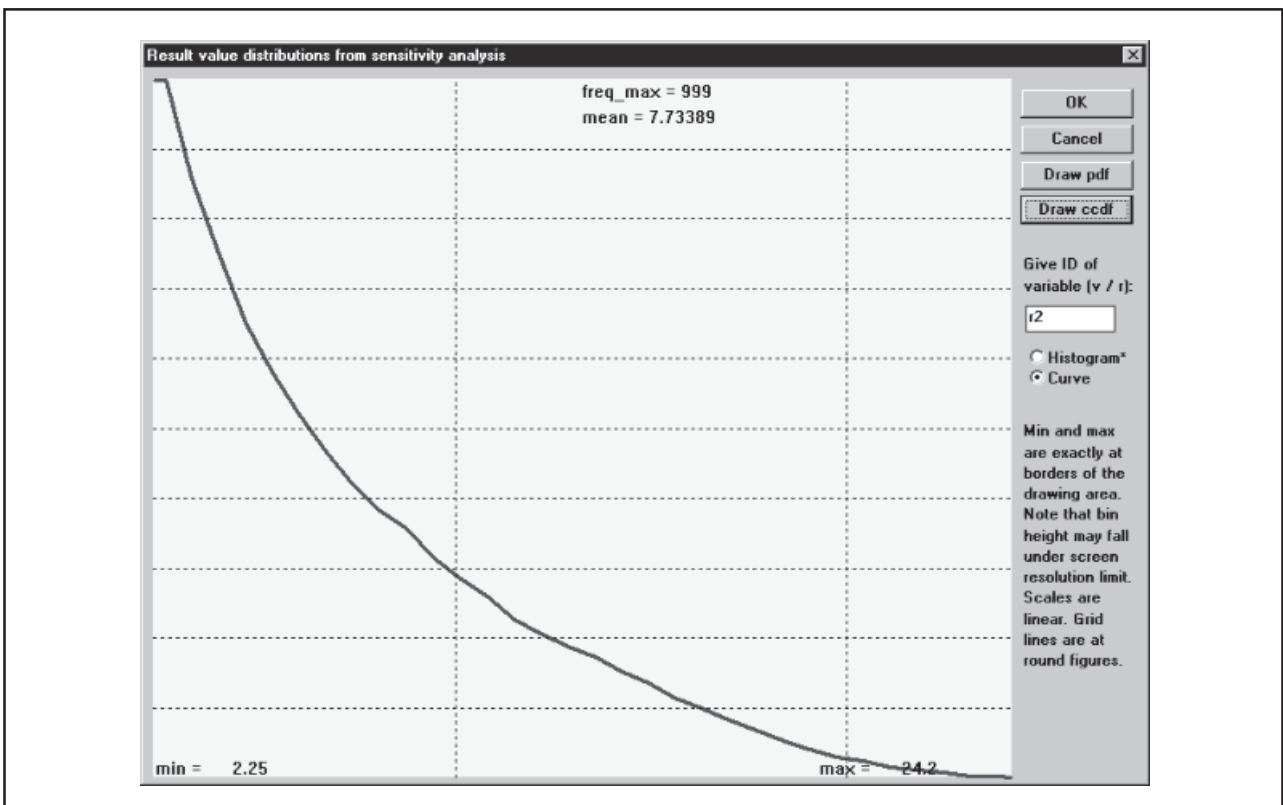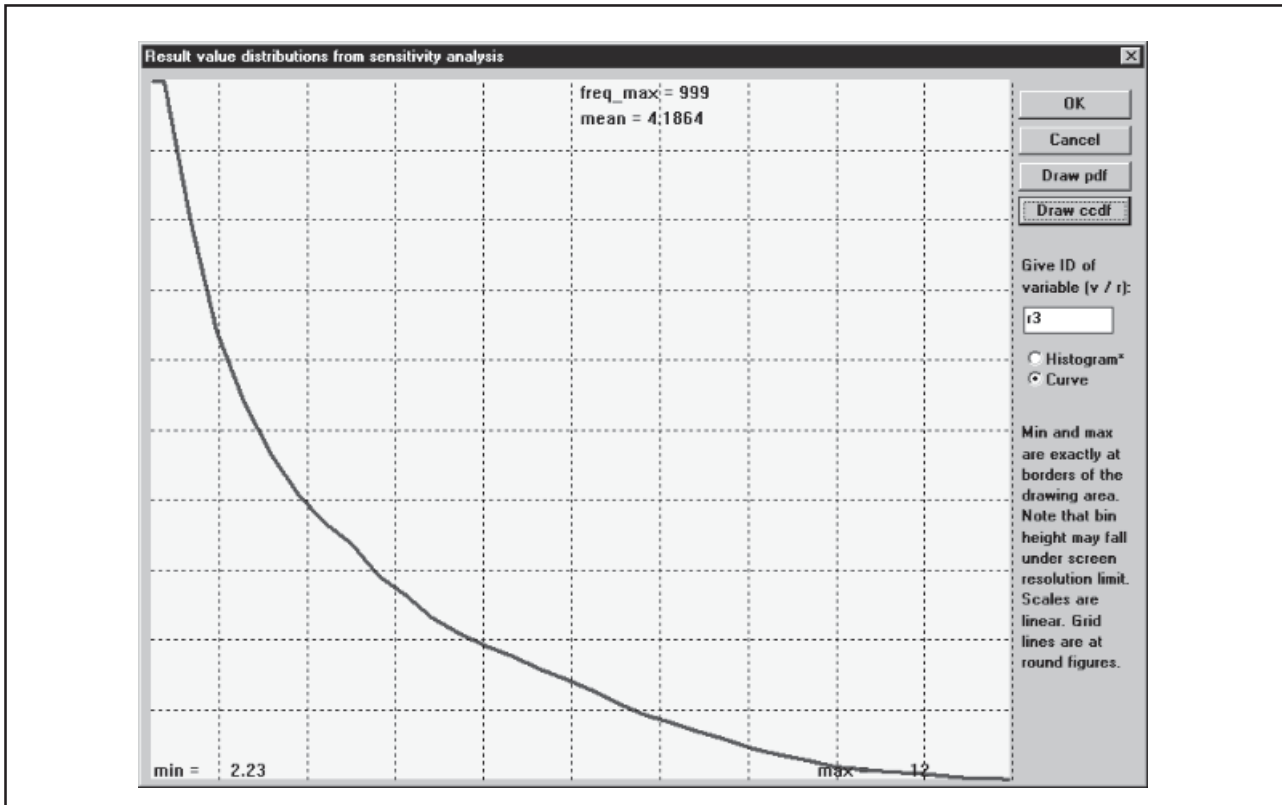
Fig 12. CCDF for the monitored parameter (C_{milk} (Bq/litre)) at 3rd calculation sequence.
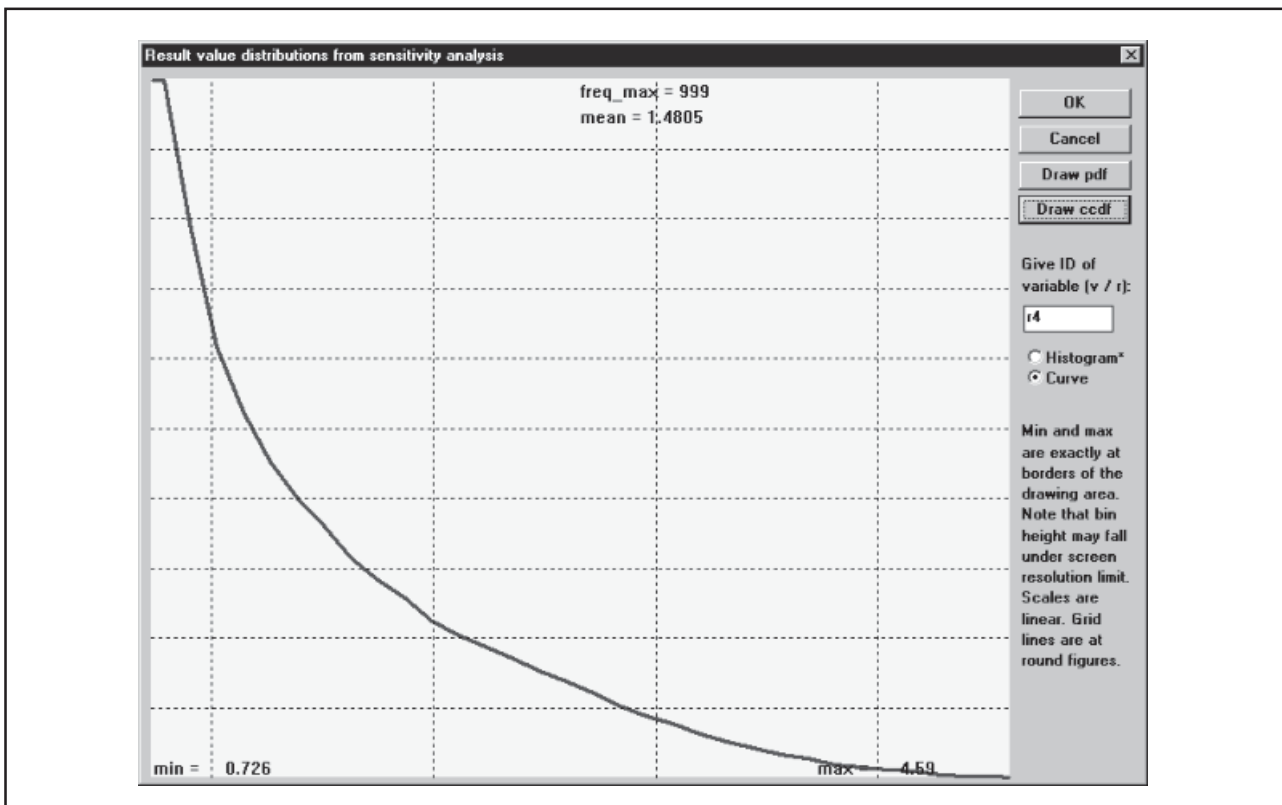

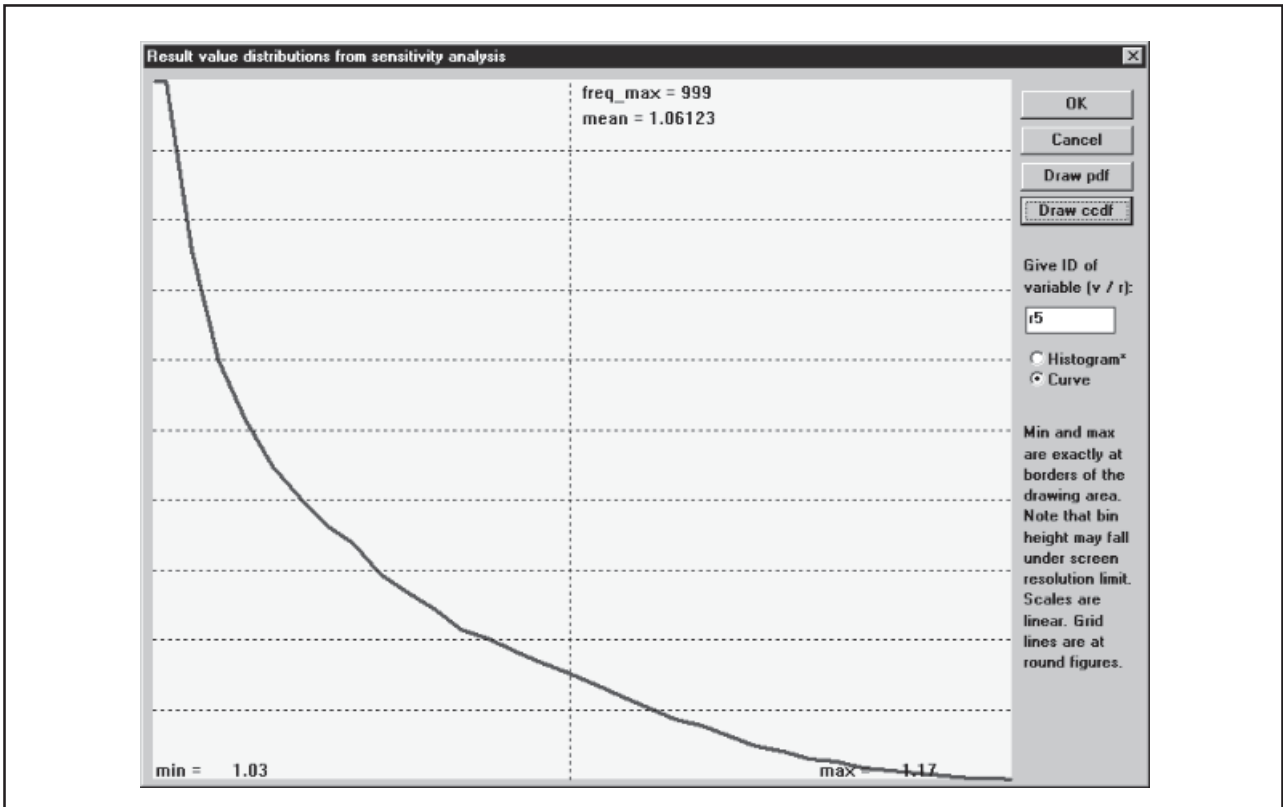Fig. 13. CCDF for the monitored parameter (C_{milk} (Bq/litre)) at 4th calculation sequence.

Fig. 14. *CCDF for the monitored parameter (C_{milk} (Bq/litre)) at 5th calculation sequence.*

4 SUMMARY

The scope and object of this study was to further develop and diversify the user interface of DETRA code. The renovated interface now fullfills those expectations, and the necessary features of performing uncertainty analyses are installed in DETRA calculation properties.

The modelling principle of DETRA is based on the compartmental approach, by tailoring the compartment structure in each considered case individually. In the earlier study on this subject the user interface of DETRA was fully modernized to be compatible with Windows environment. In this work the user interface has been further developed and diversified so that parametric uncertainty analyses are also possible with the code. The generic features of the code allow now that all input parameters of a considered case can be varied with given distributions.

The developed new version of DETRA was tested by carrying out an excercise related to milk contamination analysis after a radioactive caesium deposition episode, taking place during a pasture season. The most important parameters were varied and sensitivity runs of hunreds of simulation rounds were succesfully performed with the code. The monitored parameter distributions were available as numeric as well as graphical presentations. The typical output of sensitivity runs are probability density functions (PDFs) and complementary cumulative density functions (CCDFs).

According to this rather condensed test phase so far, the new uncertainty options of DETRA seem to work reliably. Based on these experiences, the code could be applicable also in certain future analyses. The uncertainty calculation properties are especially beneficial by linking and utilizing the earlier produced ready input templates of various environmental analyses with sensitivity runs.

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