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SÄTEILYTURVAKESKUS
Strålsäkerhetscentralen
Finnish Centre for Radiation and Nuclear Safety
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FINNISH CENTRE FOR RADIATION
AND NUCLEAR SAFETY
P.O.BOX 14 FIN-00881 HELSINKI
Finland
Tel. +358 0 759881

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ABSTRACT

ORIGEN2 is a computer code that calculates nuclide composition and other characteristics of nuclear fuel. The use of ORIGEN2 requires good knowledge in reactor physics. However, once the input has been defined for a particular reactor type, the calculations can be easily repeated for any burnup and decay time. This procedure produces large output files that are difficult to handle manually. A new computer code, known as OTUS, was designed to facilitate the postprocessing of the data. OTUS makes use of the inventory files precalculated with ORIGEN2 in a way that enables their versatile treatment for different safety analysis purposes. A data base is created containing a comprehensive set of ORIGEN2 calculations as a function of fuel burnup and decay time. OTUS is a reactor inventory management system for a microcomputer with WINDOWS interface. Four major data operations are available: 1) BUILD DATA modifies ORIGEN2 output data into a suitable format, 2) VIEW DATA enables flexible presentation of the data as such, 3) different CALCULATIONS, such as nuclide ratios and hot particle characteristics, can be performed for severe accident analyses, consequence analyses and research purposes, 4) SUMMARY FILES contain both burnup dependent and decay time dependent inventory information related to the nuclide and the reactor specified. These files can be used for safequards, radiation monitoring and safety assessment.

CONTENTS

1 INTRODUCTION

Radioactive material generated in the core of a nuclear reactor is a potential hazard that may manifest in a severe accident when the material behaves uncontrolled. Thus, it is of utmost importance to evaluate the characteristics of the radioactive material for estimating the radiological and technical hazards during the power operation of the plant, refuelling, disposal of the spent fuel, or during a hypothetical reactor accident. Different fuel characteristics are important in different cases. For example, the thermal load of long-lived radionuclides must be calculated when disposal of the spent fuel is considered whereas for a severe accident, the activity of released material is essential.

Radionuclides that are important vary in different applications. The amount of radioactive material, known qualitatively as 'reactor inventory', and its nuclide composition are needed for safety analyses. Quantification of nuclide-specific or element-specific inventories can be performed using quantities such as activity and mass concentration in the reactor fuel or specific thermal power.

Irradiated nuclear fuel contains many nuclides. The composition depends, for example, on the type of the reactor considered, enrichment of the fuel, the amount of energy taken out from the fuel, reactor operation history and the cooling time of the fuel. Because of complicated nuclear reactions during the reactor operation, the inventory calculations must be performed numerically.

Many computer codes are available for calculating the nuclide composition. Some of them are complex and sophisticated but they cannot take into account large amount of nuclides. These codes are typically used for fuel management and design purposes and also for heat transfer analysis. However, some of the codes are designed to give the inventory for a large number of radionuclides. These codes may be less accurate but they are good enough for many purposes.

ORIGEN2 (Croff 1983) is one of the most widely used computer codes for assessing the inventory of the radioactive material in the core of a nuclear reactor. ORIGEN2 computes time-dependent concentrations of a large number of nuclides and elements which are generated or depleted simultaneously through neutron induced transmutation, radioactive decay, fission, and input feed and removal rates of the radioactive material. ORIGEN2 produces large amount of output information but there are no inherent tools to reprocess this output data. Thus, the use of the code is rather tedious for user-specified purposes. In addition, the selection of input data, cross-sections in particular, requires deep knowledge of reactor physics. However, this analysis has to be performed only once for each reactor type.

Detailed nuclide-specific and element-specific concentrations of the reactor core give a possibility to build a data base that can be utilized in many applications in the field of nuclear safety. A data base management system, known as OTUS (ORIGEN TUlosten Suorasaanti), is developed in the Aerosol Laboratory of the Finnish Centre for Radiation and Nuclear Safety for different safety analysis purposes. OTUS together with a comprehensive inventory data base provides a useful tool for on-line core inventory analyses, deterministic severe accident analyses, (living-)PSA analyses and radiation monitoring purposes.

OTUS is an information, interface and presentation system. It can be used for research purposes and for operational calculations during an emergency. The code is designed in such a way that different data operations are simple, flexible and user-friendly. However, the use of the OTUS code is not possible without some knowledge of the inventory data base. Basic calculational operations can be performed following the examples of this report. More detailed code description and 'keyboard technique' are in the User's Guide (Lahtinen et al. 1995) and in the Technical Document (Ilander 1995).

2 REACTOR INVENTORY MANAGEMENT

2.1 ORIGEN2

ORIGEN2 is a reactor physics code for calculating the nuclide composition and other characteristics of the fuel. ORIGEN2 computes time-dependent concentrations of a large number of nuclides that are simultaneously generated or depleted through neutron induced transmutation, radioactive decay, and fission. Input feed rates and removal rates are also considered. Thus, the rate at which the amount of nuclide i changes as a function of time is (Croff 1983)

$$\frac{dX_i}{dt} = \sum_{j=1}^{N} l_{ij}\,\lambda_j\,X_j + \phi \sum_{k=1}^{N} f_{ik}\,\sigma_k\,X_k - (\lambda_i + \phi\sigma_i + r_i)X_i + F_i, \quad i = 1,. \tag{1}$$

where

X_i = atom density of nuclide i
N = number of nuclides
l_{ij} = fraction of disintegrations by other nuclides j which leads to formation of species i
λ_i = radioactive decay constant
ϕ = position- and energy-averaged neutron flux
f_{ik} = fraction of neutron absorption by other nuclides j which leads to formation of species i
σ_k = spectrum-averaged neutron absorption cross section of nuclide k
r_i = continuous removal rate of nuclide i from the system
F_i = continuous feed rate of nuclide i.

Coefficients of the equation 1 are stored in a large $N \times N$ matrix mainly filled with zeros. Indexing technique is used to store only the nonzero elements of the matrix. The system of simultaneous differential equations (one for each nuclide) represented by the coefficients in the transition matrix is solved using the matrix exponential technique. In the homogeneous case (without continuous material feed) the system of equations can be written as

$$\dot{X} = A\,X\,, \tag{2}$$

where

$\dot{X}$ = time derivative of the nuclide concentrations
A = transition matrix containing the transition rates
X = nuclide concentrations.

This equation has the solution

$$X(t) = X(0)\,\exp(At)\,, \tag{3}$$

where

$X(t)$ = concentrations of each nuclide at time t
$X(0)$ = initial nuclide concentrations
t = time at end of time step.

ORIGEN2 requires data base for radioactive decay, photon production, and cross section. The accuracy of the code depends strongly on these data libraries. A large number of cross-section libraries are constructed because one-group cross sections used by ORIGEN2 are sensitive to reactor and fuel types. Libraries are designed for a certain burnup of the reactor fuel but they can be used fairly well also for other burnups (Anttila 1993). Aggreement between ORIGEN2 results and analytical data is good (Liljenzin 1989).

Each data library is divided into three segments of nuclides: 130 actinides, 850 fission products, and 720 activation products. Similar structure is preserved in ORIGEN2 output structure consisting also reactivity and burnup data output and neutron and photon production tables. Mass concentration, activity and thermal power are produced for nuclide segments. Element-specific and various summary aggregations are also produced.

ORIGEN2 code has been applied to a wide variety of situations. The results of the code have been used as a design basis for fuel cycle facilities and operations. Heating load of the fuel pools, shipping casks, reprocessing plants, and waste repositories have been studied, too. The code can support nuclear power licensing and regulation activities. Risk analyses have also been performed to estimate the amount of the materials that could be released by a postulated accident sequence.

2.2 OTUS

ORIGEN2 calculates different characteristics of a large amount of nuclides and elements. Thus, the hierarchically organized output of the code is very large. The code itself does not include possibilities to treat all this information in a modern way; e.g. data plotting and linking to other codes are tedious. A tool for reactor inventory management is needed to utilize the results of ORIGEN2 effectively and user-friendly.

OTUS makes use of the reactor inventory files precalculated with ORIGEN2 program in a way that enables flexible treatment of the inventories in a microcomputer with WINDOWS user interface. The primary idea of OTUS is simple: an inventory data base is created (see section 2.3) contaning a comprehensive set of ORIGEN2 calculations as a function of fuel burnup and decay time for a reactor type specified. This large amount of data can be used for different applications. The amount of data needed in the data base depends on the application. Provided that the data base for the reactor type selected is comprehensive enough, there is no need to perform further ORIGEN2 calculations for user-specified problems. All that is needed is to pick up the appropriate data set, e.g. the results of one ORIGEN2 calculation, from the data base. If the data base is insufficient for the problem considered the data can be easily complemented performing new ORIGEN2 calculations whenever needed.

OTUS is constructed in such a way that different data base operations are flexible, fast and simple. Allowed data base operations are defined beforehand, i.e. only OTUS controls data base operations. The simplicity of use is achieved via WINDOWS interface. However, the inventory data without OTUS interface can be imported to spread sheet codes such as EXCEL. This enables data operations and calculations that are not considered in OTUS.

OTUS has versatile output possibilities. The data can be viewed as a table or as a plot on the screen. The files can be printed and nuclide-specific and element-specific ASCII files can be prepared, too. Nuclide ratios, particle properties and many other calculations can be performed in OTUS.

The user can create summary files for the nuclides chosen. Such a file contains the quantity chosen, activity e.g., as a function of fuel burnup and decay time. These files allow easy comparisons between different reactor types and radiation monitoring results can be linked to the information of the data base. Furthermore, they are an appropriate interface between the data base and other computer codes.

The MAIN window of OTUS contains three major selections (Fig. 1):
- the reactor type
- type of the data operation
- look/edit OTUS parameters.

Reactor type must be selected before the data operations are allowed (excluding SUMMARY FILES option). Data flow inside OTUS can be controlled using OTUS PARAMETERS option.

OTUS can manage four different reactor types, i.e. four sets of ORIGEN2 data. The number of data sets for each reactor type is not restricted. The practical limit is the capacity of mass storage (disc of the computer, CD-ROM etc.).

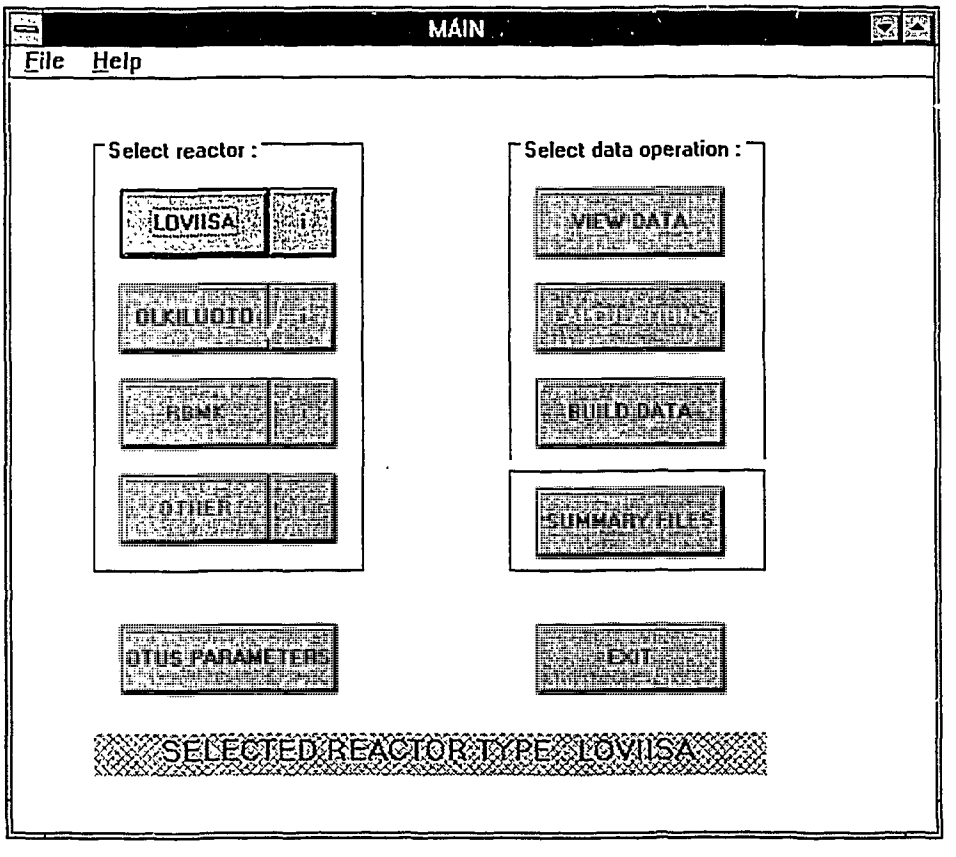

Figure 1. *MAIN window of OTUS. Here the reactor type LOVIISA (VVER-440) is selected for further treatment of inventories. Properties of each reactor type are found under the* i *buttons.*

Main data operations are:

- VIEW DATA enables presentation, i.e. viewing, plotting, and printing, of the inventory data.
- BUILD DATA modifies ORIGEN2 output data into a format used in OTUS.
- CALCULATIONS enable calculations of nuclide ratios, specific inventories, and particle properties, e.g.
- SUMMARY FILES can be created for every nuclide considered in ORIGEN2. Summary files contain inventories of one nuclide as a function of burnup and decay time. Summary files are major interface between OTUS and other codes.

Only one data set (reactor type) at a time can be used, except in the SUMMARY FILES option.

Viewing or plotting the inventory data can be tedious if all nuclides are selected at the same time. Radionuclides that are important in the application can be marked as important nuclides. To make data operations fast, only these nuclides can be viewed or used in the calculations. Different user-specified files for marked nuclides can be controlled by OTUS PARAMETERS.

OTUS is not only an inventory management system but an information system, too. Nuclide-specific and element-specific information (half-life, daughters, type of the decay and decay particle energies) are available. Because ORIGEN2 output contains hundreds of nuclides which are, perhaps, not so familiar to the user, this feature provides fast first-hand information of the nuclide selected. On-line help system that provides additional information of the use of the OTUS code is available for every window.

One of the main features of the OTUS code is that is is an interface between the ORIGEN2 data and other codes. This interface is carried out via different ASCII files or nuclide-specific SUMMARY FILES.

OTUS is a Visual Basic application. Minimum hardware configuration is an IBM compatible microcomputer with a central processing unit of 80386, internal storage of 4 megabytes (MB) and a printer. Size of the code itself and data needed during the OTUS execution is below 2 MB without the ORIGEN2 data base. Size of one data set is typically 1.5 MB. For creation of the data base, version 2.1 (8.1.1991) of the ORIGEN2 code must be used.

2.3 Data base

OTUS includes a preprocessor (BUILD DATA, see Fig. 1) that builds up a set of files from the ORIGEN2 output. The inventory data base is composed on these files. Every ORIGEN2 calculation must be performed in such a way that the files in the data base are inherently consistent. For example, the inventories must be calculated always for the same mass unit of the fuel considered (tons of UO_2). All nuclides and elements must be present in each calculation, i.e. no cutoff fractions in the ORIGEN2 output are allowed. Mass and activity concentration as well as specific thermal power output are selected for each calculation. The data base must be created in such a way that every ORIGEN2 calculation prints out maximum amount (12) of burnup or decay time values.

When the data base is created a principle 'as much data as possible' is obeyed, i.e. everything that is possible to print out during the ORIGEN2 execution is printed out. Thus, the amount of information in the data base used by OTUS is large. As an example, the steps to create the inventory data base are shown briefly for the Russian type pressurized light water reactor VVER-440, located in Loviisa at the southern coast of Finland.

Average discharge burnup of the fuel of VVER-440 is about 36000 MWd/tUO_2 and the mass of the fuel is 42.4 tUO_2. Fuel enrichment is 3.6 %. Fuel cycle period in the core is three years (irradiation of 312 days with fuel outage time of twenty days). The power density (32 MW/tUO_2) of the fuel is assumed to be constant during the power operation.

Because the inventories, calculated for a unit mass of the fuel of preselected reactor type, depend mainly on the irradiation time and decay time, one burnup dependent data set is created. Fourteen burnup values are selected for which the inventories as a function of decay time are calculated (Fig. 2). Each data set includes activity, mass and thermal power concentrations for nuclides and elements that belong to activation products, actinides and fission products. Reactor model PWRUS was used in ORIGEN2 calculations. Full description of creating the data base for selected reactor type can be found using the i button located beside each reactor type button (see Fig. 1). Input data for each ORIGEN2 execution is located under the Input info button (Fig. 2).

In practice, the data base for a specified reactor type is created as follows. To get more than 12 values of burnups or decay times, two consecutive output files are coupled side by side. For example, a burnup file (inventories as a function of burnup) with twelve values from 0 to 8000 MWd/tUO_2 are coupled to a file

including burnups between 9000 - 50000 MWd/tUO_2. Thus, the merged file contains the inventories for 24 burnups ranging from 0 to 50000 MWd/tUO_2.

Decay files (i.e. the inventories are calculated as a function of decay time for the fuel that is irradiated to a specified burnup) are constructed in the same way with 24 decay times ranging from 0 to 10 y. The inventory data is calculated for a fuel mass of 1 ton, not for the entire core. It is, of course, possible to create data files from a single ORIGEN2 execution.

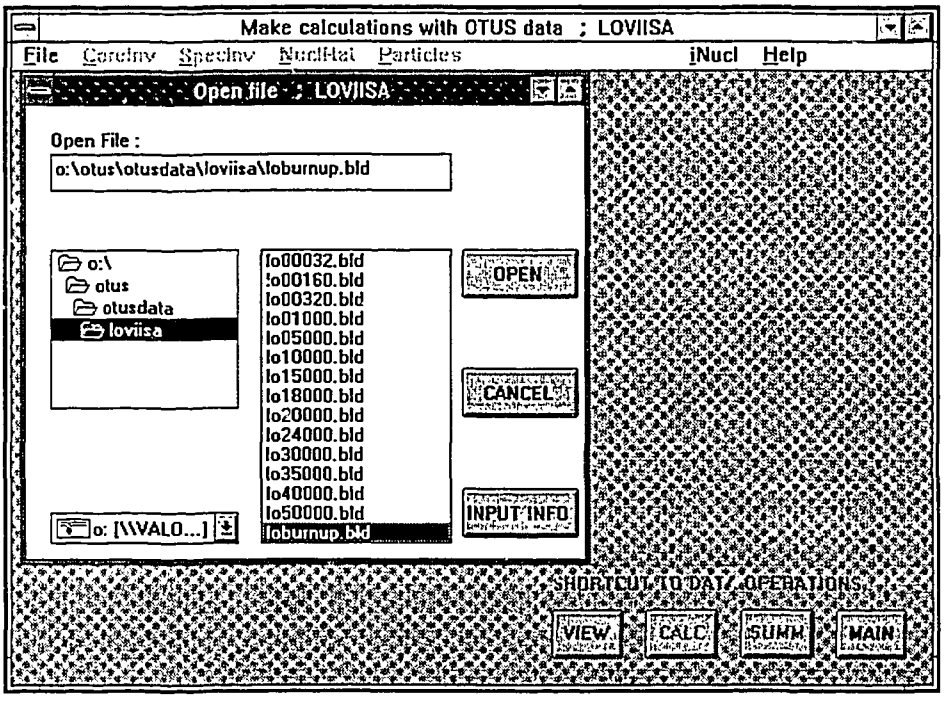

Figure 2. *Opening a burnup dependent inventory file (loburnup.bld) for a VVER-440 reactor located in the directory loviisa using* **File** *option in CALCULATIONS window. One burnup dependent inventory data set (known as burnup file) and fourteen data sets as a function of decay time (known as decay files) are in the data base. Decay files are calculated for a specified fuel burnup. For example, file lo01000.bld is an inventory data set as a function of decay time calculated for a fuel that is irradiated to a burnup of 1000 MWd/tUO_2. The four buttons at the bottom right corner of the screen are shortcut keys for fast transition between the VIEW DATA, CALCULATIONS, SUMMARY FILES and MAIN windows.*

The real file structure in the data base is hidden using WINDOWS interface. Selection of data is carried out using either pop-up menus (Fig. 3) or using special buttons defined for this purpose in CALCULATIONS and SUMMARY FILES windows (see later).

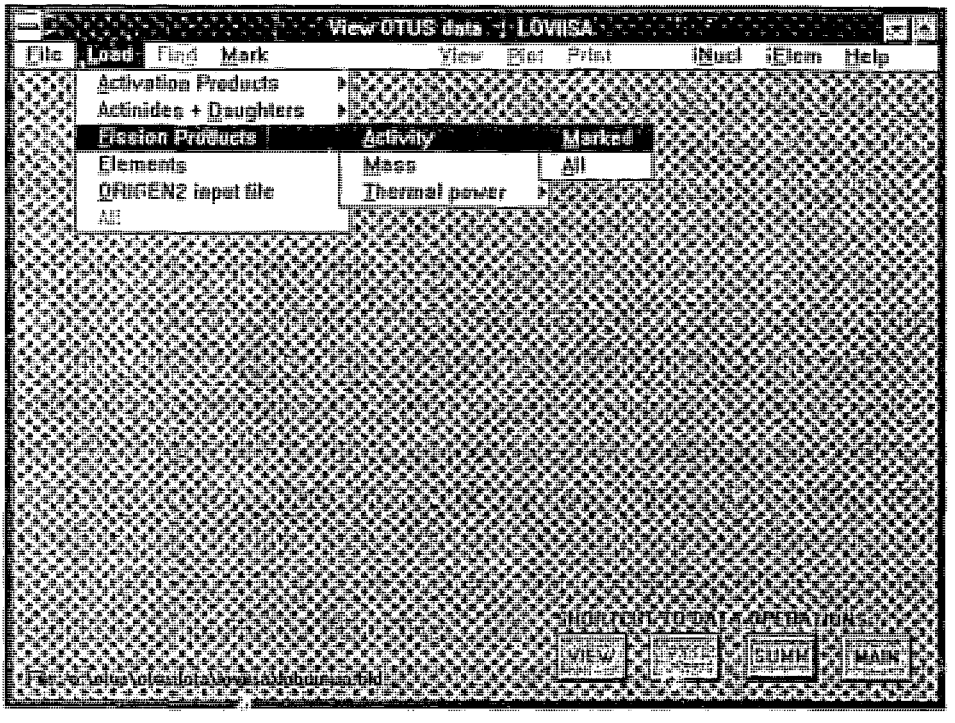

Figure 3. *Loading files for viewing. ORIGEN2 output structure is preserved. Nuclide-specific data is divided into three segments (***Activation products, Actinides** *and* **Fission products***).* **Element-***specific inventories can be loaded, too.* **ORIGEN2 input file** *contains an echo of ORIGEN2 input file. It is for the inventory file currently opened (file name in the bottom left corner of the screen). The user can load either* **Activity** *concentration,* **Mass** *concentration or specific* **Thermal power.** **All** *nuclides or only those that are* **Marked** *as important can be loaded.*

3 VIEW DATA - PRESENTATION OF INVENTORY

VIEW DATA window is a fast method for viewing inventory data files and associated nuclide-specific or element-specific information files. Neither calculations nor editing operations can be performed in this window.

The pop-up menu of the VIEW DATA window is divided in three parts (Fig. 4):

1. Operations concerning the inventory files (**File, Load**) and nuclides in these files (**Find, Mark**).
2. Selection of presentation type (**View, Plot, Print**).
3. Additional nuclide-specific or element-specific information (**iNucl, iElem**) and **Help** system.

3.1 Selection of files and nuclides

The data base operations **File** and **Load** were presented in section 2.3 (see Figs. 2 and 3). Presentation operations are allowed only after these two operations. **Find** operation can be used after choosing the **View** presentation.

The amount of nuclides in the data base is very large. Sometimes only a few nuclides are needed. The **Mark** operation gives a possibility to use only these important nuclides in the VIEW DATA and CALCULATIONS windows. Other nuclides are not shown on the screen.

Any nuclide can be marked as an important nuclide, denoted by an asterix after the nuclide name, e.g. nuclide ^{241}Am in the MARK window in Fig. 4. A list of the marked nuclides is stored in a file. For different user-specified purposes, it is possible to make several such files. The user can then select any of these files using the OTUS PARAMETERS button in the MAIN window (see Fig. 1).

The **Find** operation (Fig. 4), used after the **View** operation, gives a possibility to locate a specified nuclide in the large inventory tables (see Fig 5).

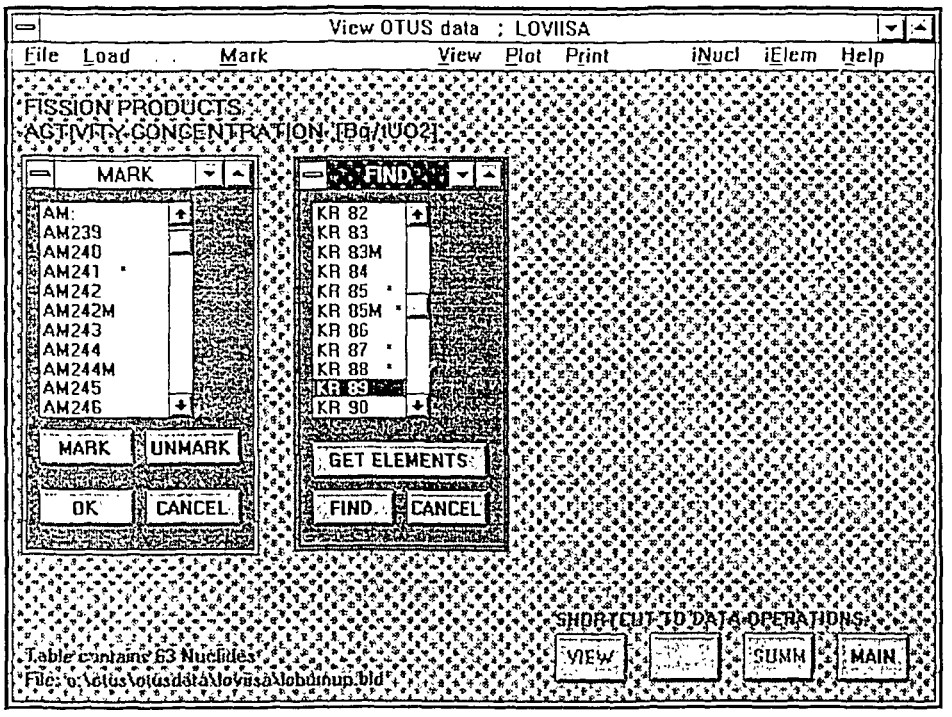

Figure 4. *MARK and FIND windows in the VIEW DATA window. A burnup-dependent fission product file containing activity concentrations (see heading at the top) has been loaded for Loviisa reactor (63 nuclides in this file, see left corner at the bottom). Under the* **Mark** *operation a nuclide can be marked by first selecting the nuclide name and then clicking the* MARK *button.* UNMARK *removes the nuclide from the list of important nuclides.* OK *button accepts marking operations. A specified nuclide in the large inventory tables can be found using the* **Find** *operation. First, element in the list must be selected; then pressing the* GET NUCLIDES *button makes a list of the isotopes of that element appear (in this case* ^{89}Kr *is selected; another nuclide that belongs to another element is selected by using the* GET ELEMENTS *button). Finally, the* FIND *button brings the selected nuclide at the top of the view grid (see Fig. 5).*

3.2 Presentation

When the inventories are loaded into the computer memory they can be presented as a table (**View** option) or as a figure (**Plot** option). With the **Print** command the inventories can be printed to a printer or to an ASCII file for further treatment. Activity concentration of some fission products as a function of fuel burnup are presented in Fig. 5. Mass concentration or specific thermal power for the same burnup file can be viewed after a new **Load** operation. The above mentioned quantities can be displayed as a function of decay time, provided that the **Open** and **Load** operations for the decay file in question have been performed.

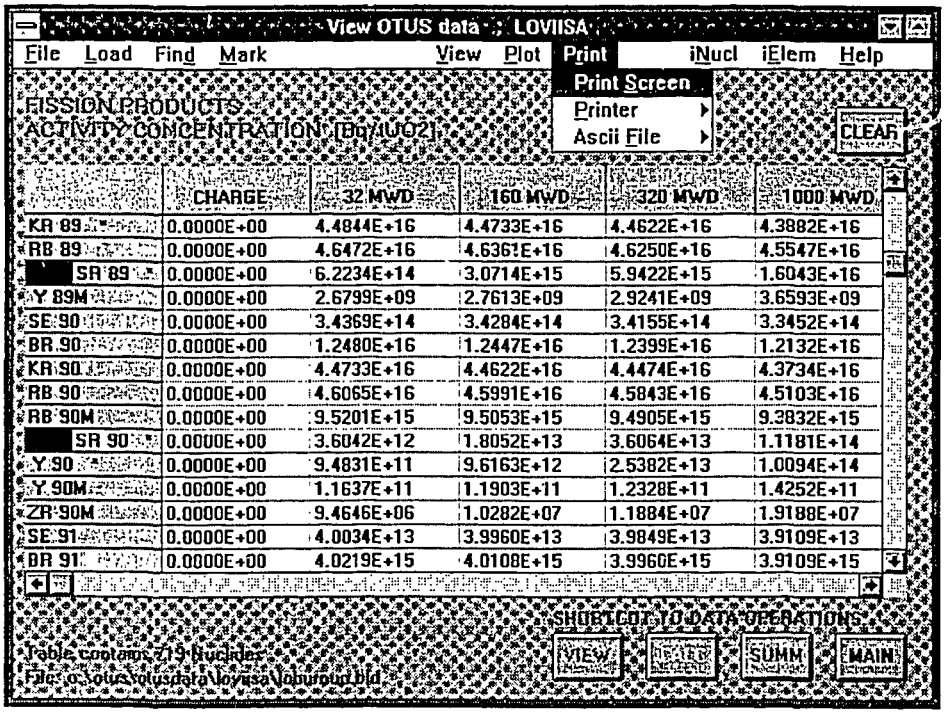

Figure 5. *Activity concentration in the fuel (Bq/tUO_2) as a function of burnup (MWd/tUO_2) for 719 fission products in the* **view** *grid. All nuclides (including the marked ones, see Fig. 3) have been selected in the table. Nuclides can be* **plot**ted *by pressing the ctrl key of the keypad and selecting a nuclide from the list with the left mouse button. A red bar appears in the field of the nuclide name, e.g. for nuclides ^{89}Sr and ^{90}Sr.* CLEAR *button at the top right corner of the screen clears all choices. If nuclides are not selected before the* **plot** *operation, a list of marked nuclides will be displayed on the screen.* **Print** *options at the top of the screen are shown here, too.*

Nuclides or elements to be plotted can be selected either from the **view** grid or from a separate list (SELECT button in Fig. 6). As an example, mass concentration (g/tUO_2) of some important actinides in the fuel is shown in Fig. 6 as a function of fuel burnup. Fig. 7 shows the activity concentration (Bq/tUO_2) of some fission products as a function of fuel burnup. Finally, activity concentration for the same fission products as a function of decay time is presented in Fig. 8. Figures 5 - 8 are examples of the output forms in OTUS.

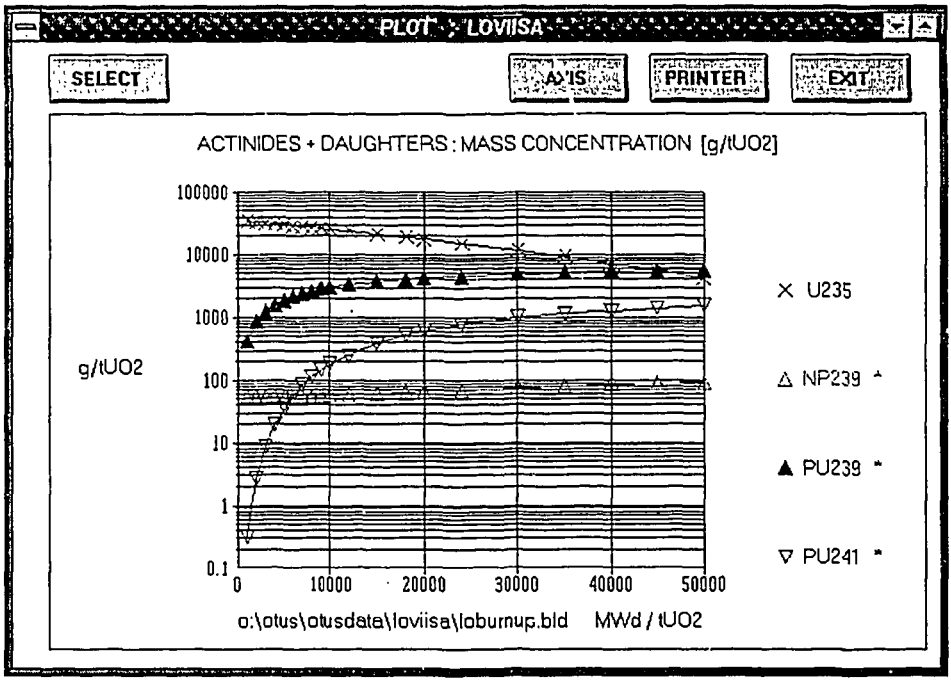

Figure 6. *Mass concentration (g/tUO_2) of ^{235}U, ^{239}Np, ^{239}Pu and ^{241}Pu in the fuel as a function of fuel burnup (MWd/tUO_2). Note that ^{239}Pu concentration is higher than ^{235}U concentration when the burnup is larger than about 45000 MWd/tUO_2. Nuclides to be plotted can be selected with SELECT button, too. Y-axis scale, limits of x-axis and line-type can be changed with AXIS button.*

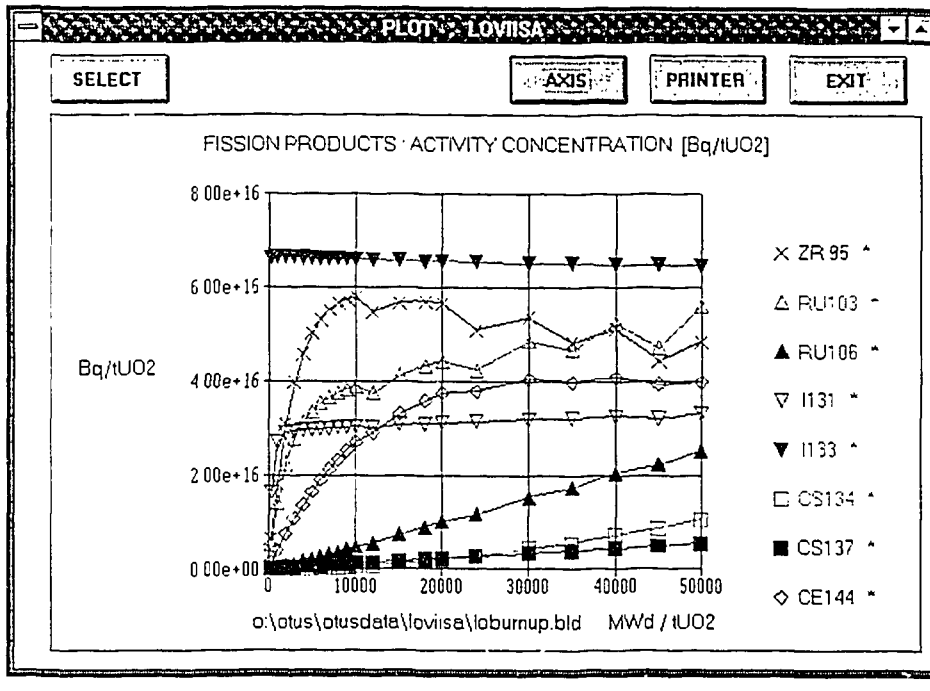

Figure 7. *Activity concentration (Bq/tUO$_2$) of ^{95}Zr, ^{103}Ru, ^{106}Ru, ^{131}I, ^{133}I, ^{134}Cs, ^{137}Cs and ^{144}Ce in the fuel as a function of fuel burnup(MWd/tUO$_2$). For short-lived nuclides (^{133}I) the activity concentration is directly proportional to the thermal power of the reactor whereas for long-lived nuclides (^{137}Cs) it is proportional to the burnup of the fuel. The concentration of ^{133}I rises rapidly from zero to 6.6*10 Bq/tUO$_2$. The irregular behaviour of ^{95}Zr and ^{103}Ru (half-lives of the order of a few months) is explained by the fuel outage time of twenty days thet is included in the burnups of 10000, 20000, and 30000 MWd/tUO$_2$. Activity concentration of ^{95}Zr decreases at burnups larger than about 10000 MWd/tUO$_2$ because the cross section for thermal-neutron fission is lower for ^{239}Pu than for ^{235}U (see also Fig. 6).*

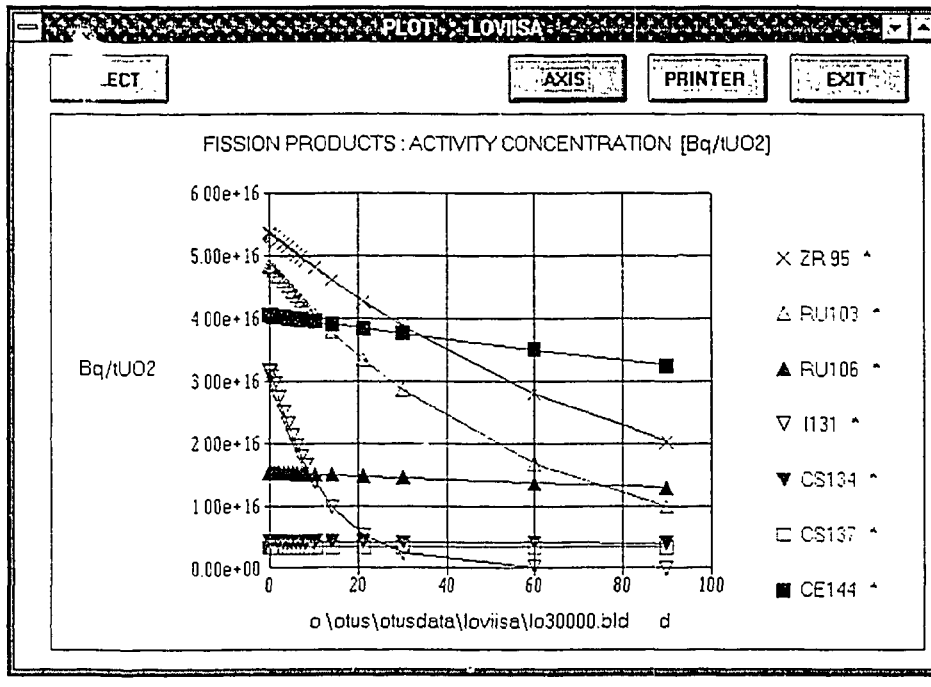

Figure 8. *Activity concentration (Bq/tUO$_2$) of ^{95}Zr, ^{103}Ru, ^{106}Ru, ^{131}I, ^{134}Cs, ^{137}Cs and ^{144}Ce in the fuel as a function of decay time (d). The fuel of the Loviisa reactor has been irradiated to the burnup of 30000 MWd/tUO$_2$. Concentration of ^{134}Cs and ^{137}Cs remain unchanged because of the relatively short time interval (90 days) shown in the figure.*

3.3 Nuclide-specific and element-specific data

Hundred elements and 1700 nuclides are included in ORIGEN2 calculations. To facilitate the management and utilization of the nuclide-specific properties, the ORNL data base (Kocher 1981) has been implemented in OTUS. The same data is used in RADDECAY computer code (Negin and Worku, 1991), too. Half-life, daughters, decay modes and decay particle energies of the selected nuclide can be shown by the **iNucl** operation (Fig. 9). Some element-specific (or compound-specific) data is available through the **iElem** option.

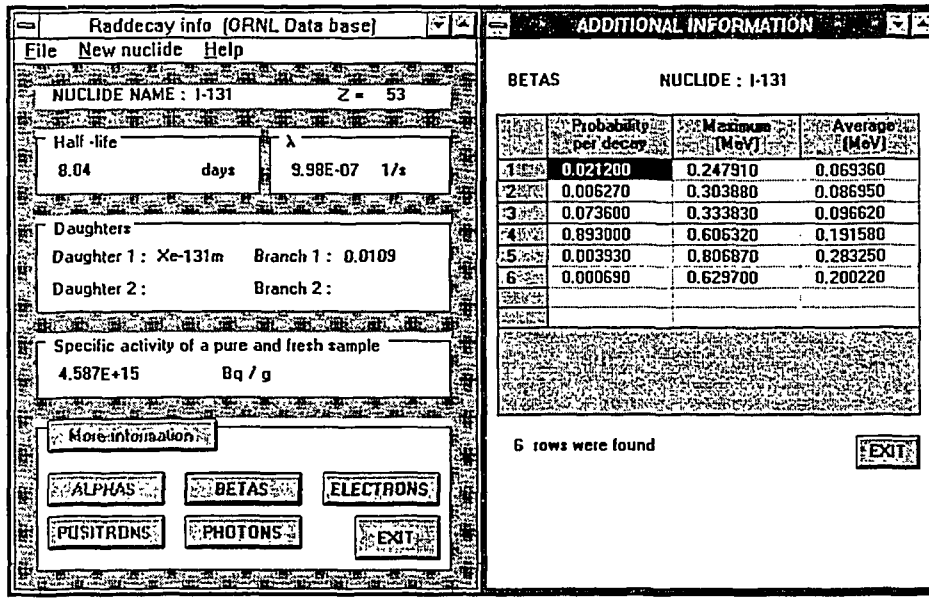

Figure 9. *Information from ORNL data base for ^{131}I. By clicking the* **iNucl** *option in the VIEW DATA window a screen presented at the left appears. Through* More information *button additional information (yield and particle energies) is available (emitted betas, electrons and photons). Beta particle data is shown in the table on the right.*

4 CALCULATIONS - DATA SOURCE FOR SAFETY ANALYSES

OTUS system can be used in various applications (see section 2.1). However, a modern interface provides novel possibilities for utilizing the data base for other purposes, too. So far, total core inventory, specific inventory, nuclide ratio and particle property calculations can be performed in the CALCULATIONS window. A few examples of the use of OTUS for the needs of emergency preparedness, deterministic severe accident analyses and probabilistic safety analyses are given below. The reactor type considered is VVER-440 (see section 2.3).

4.1 Total core inventory

The specific thermal power of the fuel and the activity and mass concentrations in the fuel are considered in ORIGEN2 to represent an average value of the unit mass of the reactor fuel. The inventory data base has been calculated for the initial UO_2 loading of one ton. Core inventory depends mainly on the operation history of the reactor, i.e. on burnup and decay time of the fuel (see Figs. 6, 7, and 8).

Total nuclide-specific activity of the core is needed for estimating the radiation consequences of a hypothetical severe nuclear accident. This information is valuable for emergency preparedness or for probabilistic safety analyses. Off-site doses are calculated by several consequence analysis codes from the release fractions of the activity inventory of the core. These fractions multiplied by the inventory give the total release. Total thermal power generation as a function of decay time is an other quantity that is often needed in deterministic severe accident analyses, e.g.

4.1.1 Discharge inventory

For the purposes of emergency preparedness, it is useful to estimate maximum inventory, i.e. the total activity of the core at the end of the fuel cycle period. For VVER-440 the discharge inventory I_{tot} can be calculated by dividing the fuel into three different burnup regimes. Then

$$I_{tot} = \frac{m_{fuel}}{3} * [I(bu_1) + I(bu_2) + I(bu_3)] , \quad (4)$$

where $I(bu_1)$, $I(bu_2)$, and $I(bu_3)$ are the nuclide-specific concentrations per ton of one, two and three years old fuel (fuel has been irradiated in the reactor for one, two and three years, respectively) in the end of the fuel recharge cycle (see Wilson et al 1988). m_{fuel} is the total mass of the fuel (tons). In practice, after the selection of the calculation method (see pop-up menu in Fig. 2) the discharge inventory calculations are performed as shown in Fig. 10.

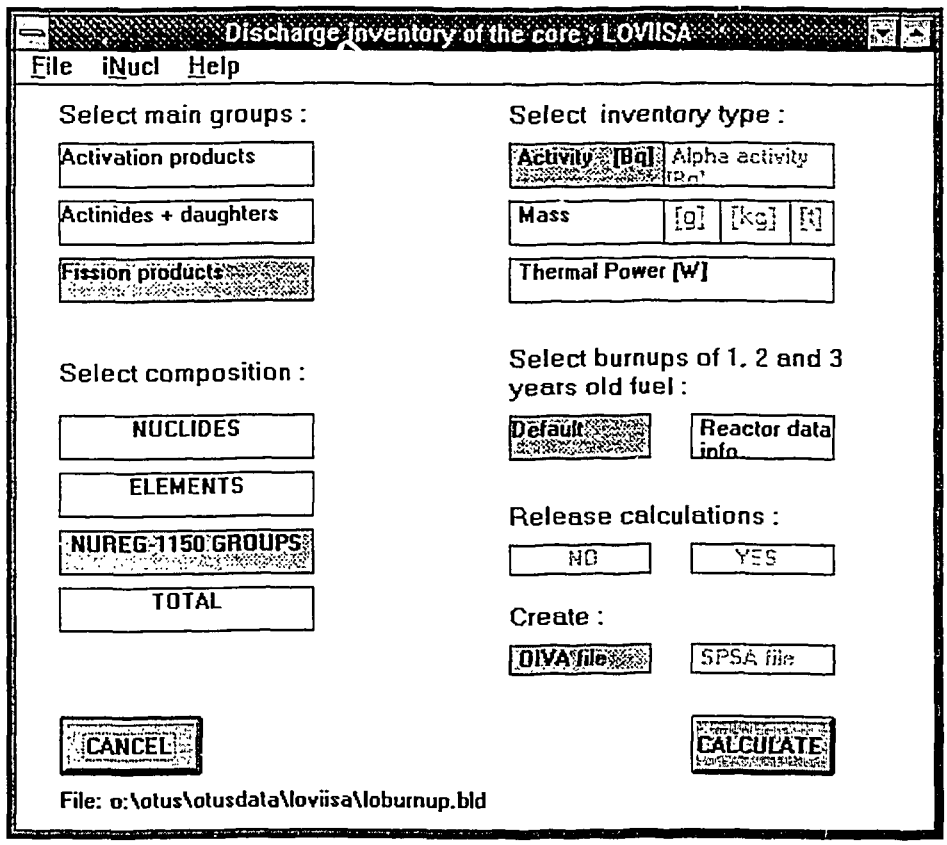

Figure 10. *Calculation of discharge inventory. Main group and inventory type must be selected first. Discharge inventory can be calculated either for* NUCLIDES, ELEMENTS *or* NUREG-1150 GROUPS. *The burnups of 1, 2 and 3 y old fuel are either the* Default *values (from* Reactor data info, *Fig. 1) or they can be specified by editing the data in the reactor data info. Input files for OIVA code (Lahtinen and Blomqvist 1988) or SPSA code (Okkonen 1995) can be created,* too.

At least one of the main groups (activation products, actinides, fission products) must be selected before the selection of the appropriate inventory type (activity, mass, thermal power). If two or three main groups are chosen, the total inventories are calculated by summing up the inventories of the chosen groups (some nuclides and elements belong in two groups). Nuclides, elements or groups are selected under the select composition option. Nuclides belonging to a specified group can be defined with the NUREG-1150 GROUPS button (Figs. 10 and 11).

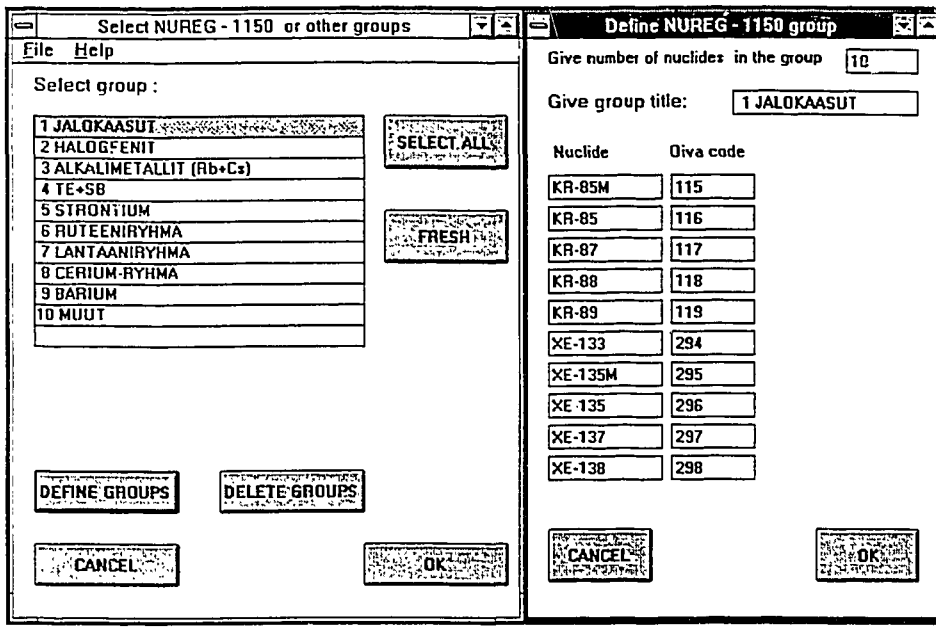

Figure 11. *NUREG-1150 groups (shown at the left). New groups can be defined or deleted by using* Define groups *and* Delete groups *buttons, respectively. A group can be selected by clicking one of the groups in the list or by using* Select all button. Fresh *button clears all choices. The define groups window for noble gases is presented at the right. OIVA code number beside the nuclide name is optional (see text below).*

Discharge inventory for some fission products is presented in Fig 12. The inventories are close to the values that are reported in final safety analysis report (LOFSAR 1993) of the Loviisa reactor. These values can be transferred via ASCII files to other computer codes. OIVA (Lahtinen and Blomqvist 1988) is a code for real-time off-site dose estimation in a nuclear accident. OTUS can supply nuclide-specific activities to OIVA in a straightforward way (not shown in the figure). SPSA (Okkonen 1995) is a probabilistic safety analysis code developed at STUK for level 1 and level 2 PSA analyses. An interface for SPSA level 2 analyses may be given, too.

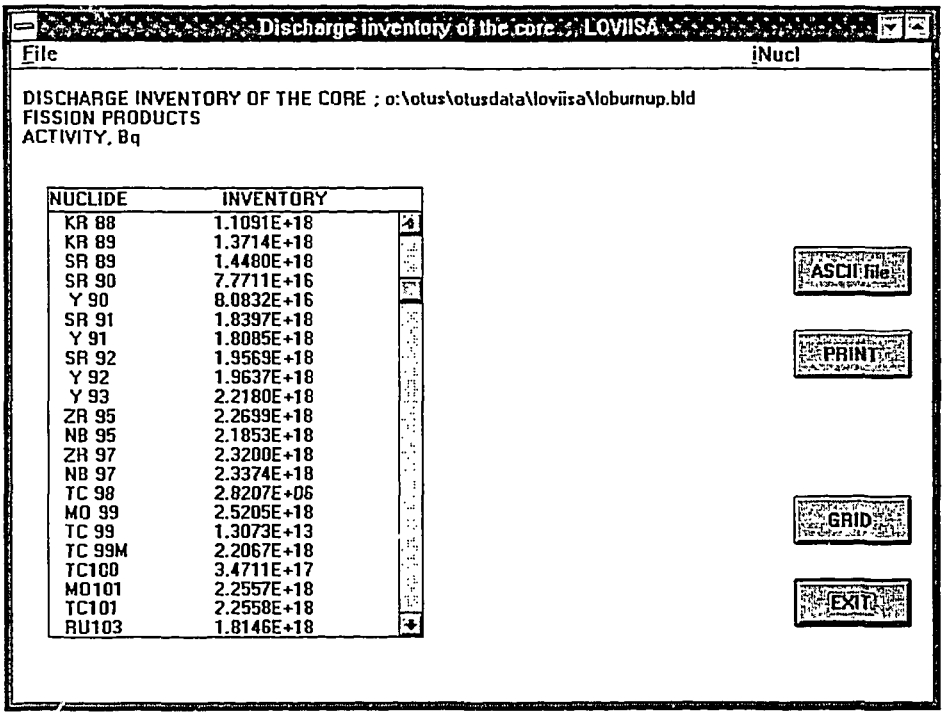

Figure 12. *Discharge inventory of some fission products for Loviisa reactor. The inventory file can be sent to a* PRINTer *or to an* ASCII file. *Nuclide-specific information for the selected nuclide can be accessed under the* **iNucl** *option.*

4.1.2 Total core inventory based on average burnup

In reactors which operate in continuous refueling mode, RBMK reactor e.g., the total inventory can be estimated from the average burnup bu_{avg} of the core and the decay time (cooling time):

$$I_{tot} = I\ (bu_{avg},\ decay\ time)\ *\ m_{fuel} \qquad (5)$$

This information is taken from the reactor data info. Linear interpolation is used if bu_{avg} is between the precalculated burnup values. Equation 5 can be used also for the VVER-440 reactor, provided that the average core burnup is known. Total core inventory calculations based on the average fuel burnup are performed in a window similar to Fig. 10.

4.1.3 Current inventory

Discharge inventory in equation 4 is a maximum inventory at the end of the fuel cycle period. Sometimes, during an emergency e.g., it is useful to estimate on-line inventory (current inventory) of the core. This information can be used in level 2 living-PSA analyses or in consequence analysis codes. Current inventory can be calculated from the average fuel burnup of the core.

If fuel charging is carried out periodically the estimation of average burnup may be tedious. However, the date of the last fuel discharge is known. One third of the fuel is less than 1 year old, one third less than 2 years old and the rest less than 3 years. Let bu_1 and bu_2 be the burnups of one and two years old fuel, respectively. Current inventory is calculated by assuming that there are d days passed from the last fuel discharge:

$$I_{tot} = \frac{m_{fuel}}{3} * [\ I(d*P) + I(bu_1+d*P) + I(bu_2+d*P) \qquad (6)$$

where P is the specific power (MW/tUO_2) of the fuel, assumed to be constant during the plant operation. Equation 6 is valid only for a power history described in section 2.3, i.e. reactor power must be constant between the recharging outages. Inventory calculations, based on the knowledge of fuel outage times, are performed in a window that resembles Fig. 10.

4.2 Specific inventory

Here, the generic term 'specific inventory' is defined either as an activity concentration or specific thermal power of the selected species (nuclides or elements) divided by the elemental mass concentration. Specific inventories can be calculated for masses of one g, kg, and t. Calculations are performed as presented in Fig. 10. For each case the appropriate composition, i.e. the species considered in the unit mass, must be defined beforehand (Fig. 13).

An example visualizing the use of specific inventories is given below. The knowledge of specific thermal power provides a possibility to estimate thermal load onto the tubes of primary circuit in a core melt accident.

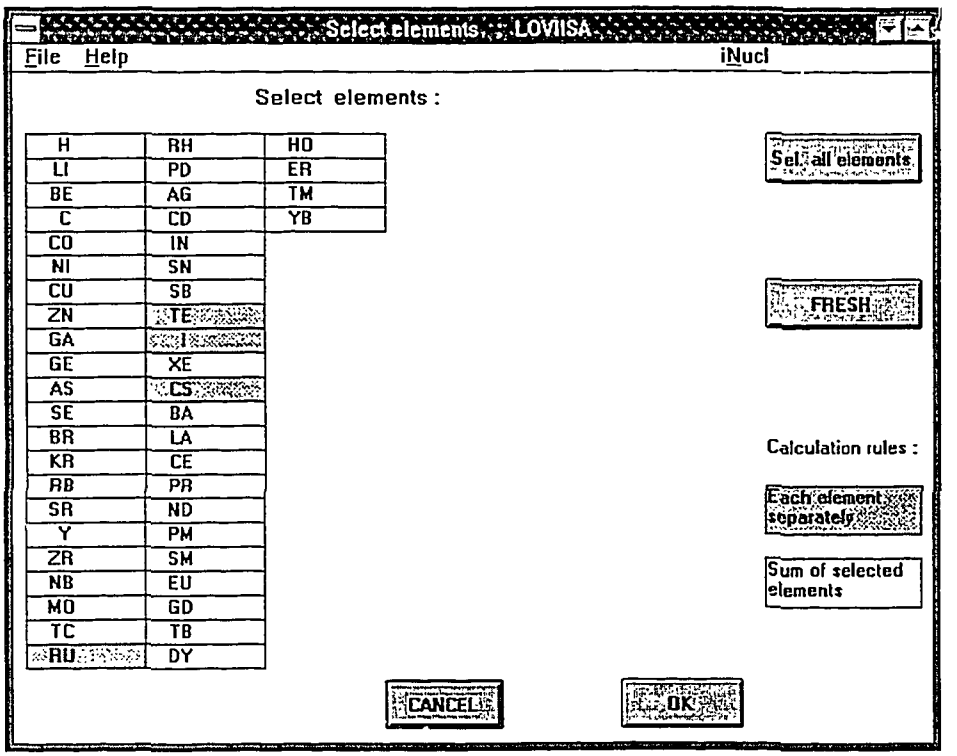

Figure 13. *Selection of elements (Ru, Te, I and Cs) for specific inventory calculation. Specific inventory for all elements can be calculated with* Sel. all elements *button.* FRESH *button clears all choices. Rules of calculation (see equations 7- 9) are selected through buttons* Each element separately *or* Sum of selected elements.

In a severe reactor accident, the highly radioactive material deposited on the surfaces of the reactor coolant system (RCS) may have an essential influence on the thermal hydraulics of the system, its integrity and, hence, the overall safety of the plant. The temperature increase of the structures of RCS has an incluence on the material deposition rate onto the surfaces and re-vaporization of the deposited material. The integrity of RCS ensures that the radionuclides are not released uncontrolled from the plant. Radioactive material released from the fuel and deposited on the primary ciruit, on the pipes of steam generators e.g., may melt or weaken the structures which, in turn, could lead to the breakdown of the consecutive safety barriers?

In principle there are two main approaches in estimating the effects of decay heat. Computer codes, such as VICTORIA (Heames at al. 1990) or TRAP-MELT (Kuhlman et al. 1986), have been designed to calculate thermal hydraulics and

radionuclide transport during a nuclear accident. In these codes thermal loads are estimated from the amount of radioactive material released from the fuel, transported in the RCS and finally deposited on the surfaces of RCS. However, the physics and chemistry related to highly radioactive material in high temperatures and pressures are rather uncertain. Considerable difficulties may arise because of the complex phenomena lying behind the calculations of thermal hydraulics and radionuclide behaviour.

There is another approach for estimating the amount of radioactive material sufficient to melt or break the structures. Firstly, the amount of heat, generated in a small surface area of a structure and sufficient to cause essential structural damages to the surface, is estimated. Secondly, the amount and type (elemental composition) of radioactive material producing this heat is evaluated. Thirdly, utilizing aerosol physics, the possibility of this material deposition must be estimated.

Here, specific thermal power of nuclide N (defined as the power per unit mass of fuel generated by nuclide N divided by the mass concentration of the corresponding element in the fuel) is a quantity that has no practical importance. The mechanism of the release of radioactive material is an element-specific process, not a nuclide-specific phenomenon. In other words, during a nuclear accident the escape of radioactive material is dominated by the elemental properties (physical or chemical properties of the elements or compounds) of the material.

The specific thermal power of a single element E (W/kg of element E) is defined here as

$$P_{spec,E} = P_E / M_E , \qquad (7)$$

where P_E is power of element E in the fuel (W/tUO$_2$) for a given burnup and decay-time and M_E is the corresponding mass concentration of element E in the fuel (kg/tUO$_2$). Specific power defined in this way is useful when the deposited material is monoelemental.

Fig. 14 visualizes the behaviour of specific thermal power for elements Ru, Te, I and Cs as a function of fuel burnup. Elements are assumed to be in a monoelemental form. For low burnups the specific thermal power for Te, I and Cs is of the order of tens of kW's per gram of the element considered.

Often the radioactive material released from the core is in the compound form rather than in the elemental form. In that case the amount of elements in a unit mass of the compound must be calculated. The present version of OTUS does not calculate the molecular weight of radioactive compounds (it differs from the corresponding stable

isotopes, because the isotopic composition of an element in the reactor is different from that in the nature). However, when the atomic weights of the elements in the compound are almost equal, the following approximation can be used for the total specific power of the compound C

$$P_{spec,C} = \sum_{E=1}^{e} P_E \Big/ \sum_{E=1}^{e} M_E \,, \tag{8}$$

where the summation of the power density and mass concentration is over the elements in the compound. Similarly, the specific thermal power of a single element E in the compound C is

$$P_{spec,E(C)} = P_E \Big/ \sum_{E=1}^{e} M_E \,. \tag{9}$$

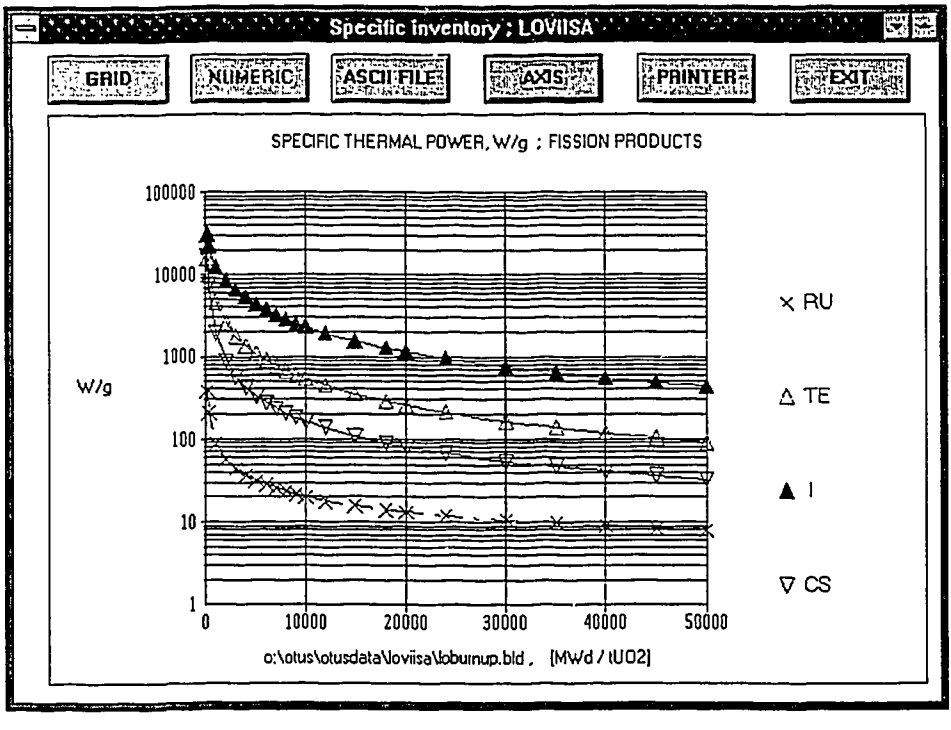

Figure 14. *Specific thermal power (W per g of element considered) of Ru, Te, I, and Cs as a function of fuel burnup (MWd/tUO$_2$) for* Each element separately, *see Fig. 13.*

High values of the specific thermal power at low burnups are explained by the low amount of stable material. At high burnups larger amounts of stable elements are present (Fig. 15), leading to a lower specific power. Does this phenomenon affect the RCS integrity in the reactor accident?

Let us assume that one gram of iodine is released from the reactor and deposited at a point on the surface of a primary circuit tube. The thermal load is then tens of kW's at this point (and surrounding structures) for the fuel of low burnup (see Fig. 14). If the fuel is near its exhaust burnup the thermal load is below one kW. But the conclusion that low-burnup fuel would cause larger risks to the integrity of this particular point of the tube is too straightforward, because iodine's mass concentration in the fuel is low (Fig. 15). In other words, the low burnup fuel does not contain, perhaps, sufficient amounts of such material that could damage the integrity of the RCS. These results are worth for further thermal hydraulic examination, but such a study is beyond the scope of this report.

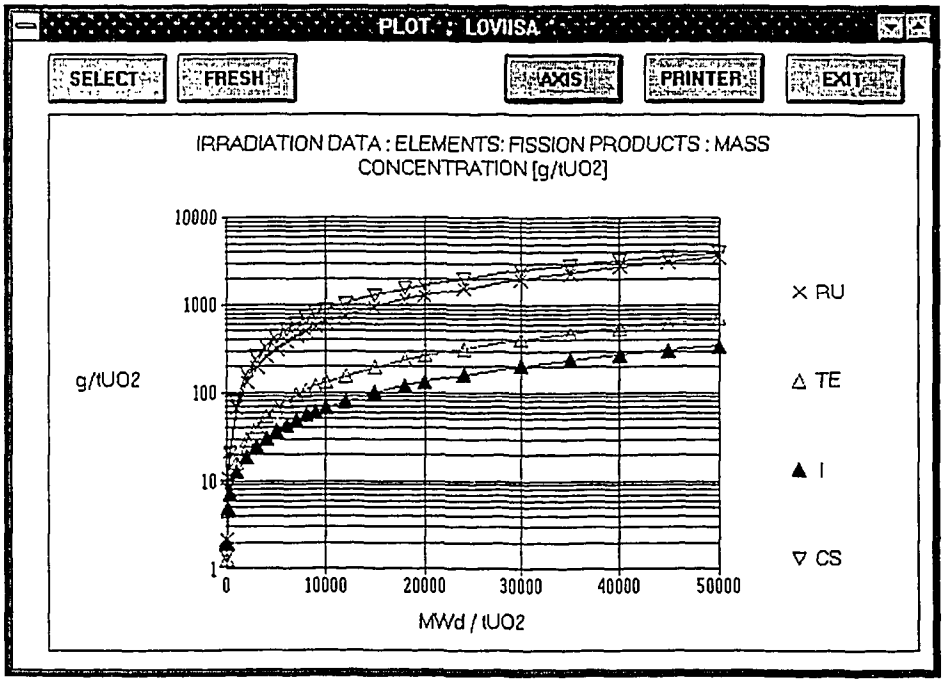

Figure 15. *Mass concentration (g/tUO_2) of Ru, Te, I and Cs in the fuel as a function of fuel burnup (MWd/tUO_2).*

4.3 Ratios of nuclide-specific quantities

Ratios of nuclide-specific quantities, i.e. activity concentration, mass concentration or specific thermal power of a nuclide divided by the corresponding quantity of an other nuclide, can be used for a wide variety of applications. For the use of these ratios in radiation monitoring see chapter 6.

The present analysis is limited to activity ratios although OTUS can calculate thermal power and mass concentration ratios, too. Activity ratios can be calculated as a function of fuel burnup or decay time for all nuclides considered in ORIGEN2. Appropriate burnup or decay dependent file must be **opened** before calculations, which are performed using a window presented in Fig. 16.

Activity ratios depend often strongly dependent on burnup and decay time of the fuel. If airborne radioactive material of artificial origin is detected, these relationships can be used, for example, for estimating the properties of the material at the time of reactor shutdown or at the time of release.

Activity ratios can provide information on the behaviour of the elements during an accident. For example, radionuclide fractionation in hot particles is widely studied using activity ratios for pairs of isotopes of the same element (Jaracz et al. 1990). Fractionation of non-chemical origin can then be revealed. An example of activity ratios is given in Fig. 17.

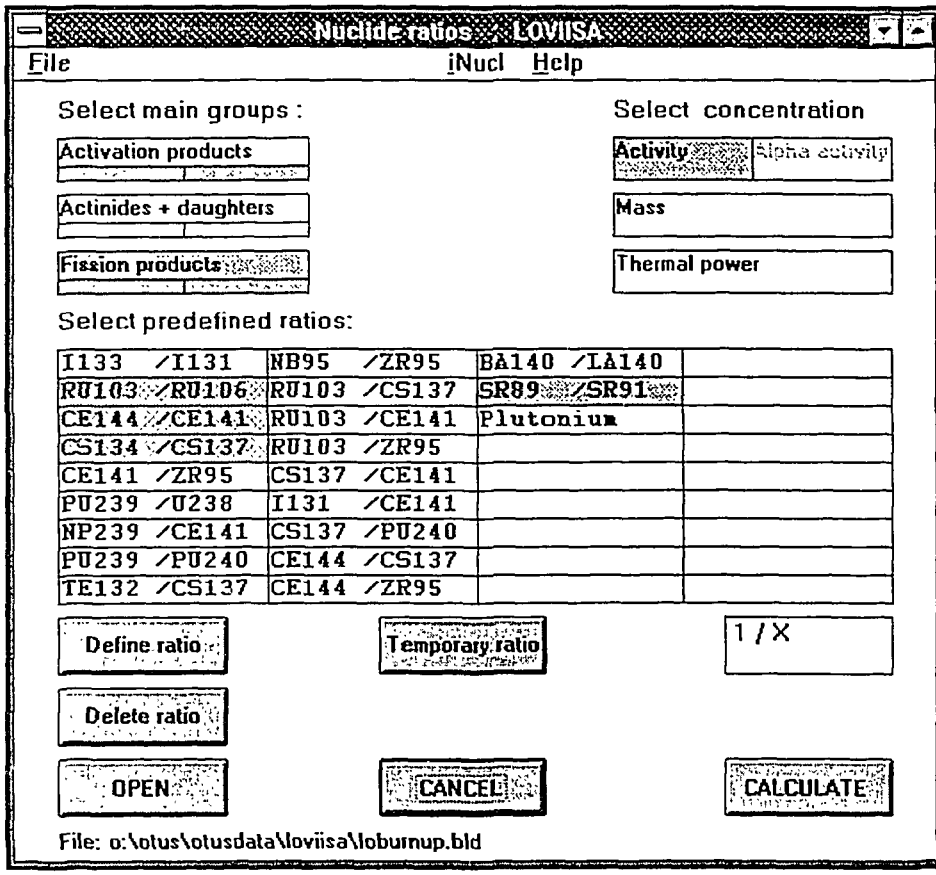

Figure 16. *Activity ratio calculations as a function of fuel burnup. Predefined nuclide ratio(s) must be selected before the selection of main group and ratio type. For the selected ratios, a coloured bar appears below each main group provided that the group includes the nuclides specified in the ratio (the left bar is for the nuclide in the numerator and the right bar is for the nuclide in the denominator). Predefined (most important) ratios are permanent whereas temporary ratios disappear when the program is closed. Permanent ratios can be (re)defined with the* Define ratio button. *The* Temporary ratio *button creates provisional ratios.* 1/X *button inverts a ratio. By clicking the* OPEN *button a new inventory file (either burnup dependent or decay time dependent file) can be loaded.*

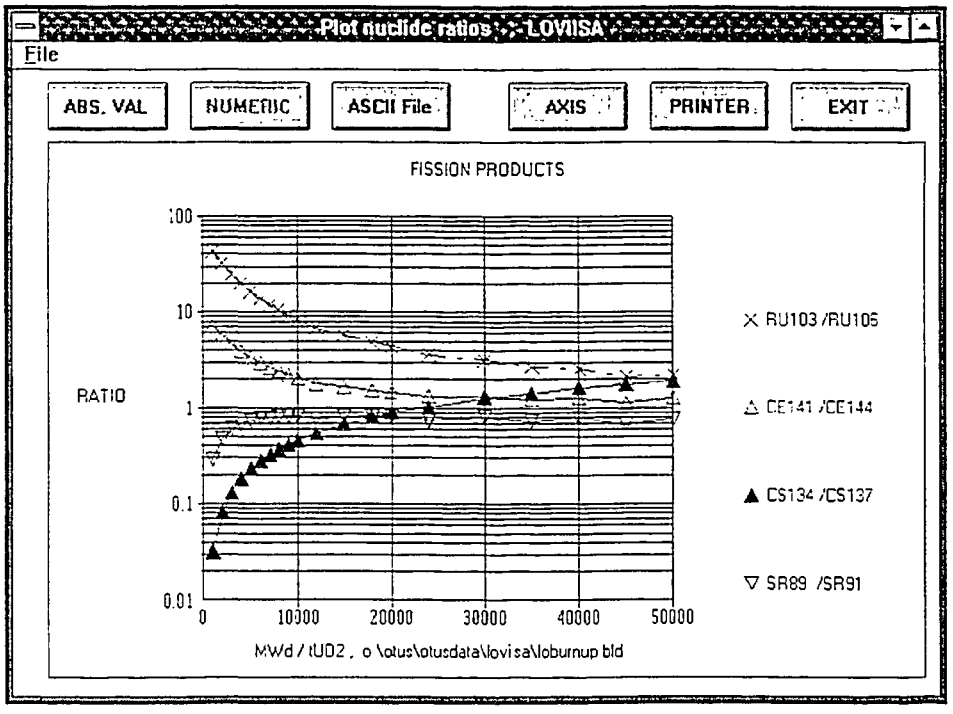

Figure 17. *Activity ratios as a function of fuel burnup (MWd/tUO2). Ratios shown in the figure can be presented in a numerical form (*NUMERIC *button). Absolute values for each nuclide (e.g. activity concentration in the fuel, Bq/tUO$_2$) can be displayed with the* ABS.VAL *button.*

4.4 Properties of hot particles

Nuclide-specific or element-specific activity, mass or thermal power of a particle as a function of fuel burnup, decay time or particle size can be estimated by choosing the **Particles** option in the CALCULATION window (see Fig. 2). The calculations can be performed for mononuclide, monoelemental or uranium fuel particles.

A code for estimating the transport range of particles, TROP (Pöllänen et al. 1995), can be executed using the option **Transport range**. TROP calculates the transport range of particles of predetermined sizes in various atmospheric conditions. Beta dose caused by a radioactive particle deposited on the skin can be calculated using the PSS model (Pöllänen and Toivonen 1994) under the **Skin beta dose** option. Before the execution a separate installation is needed for TROP and PSS codes.

4.4.1 Mononuclide particles

A mononuclide particle is composed of a single radioactive nuclide. Activity of a mononuclide particle as a function of particle size can be estimated from the equation

$$A_d = \frac{\pi}{6} \frac{N_A \lambda \rho d^3}{W}, \qquad (10)$$

where N_A = Avogadro constant,
λ = decay constant,
ρ = particle density,
d = particle diameter and
W = atomic weight.

ORIGEN2 data base is, thus, not needed. Calculations are performed in a window that resembles Fig. 18.

4.4.2 Monoelemental particles

A monoelemental particle is composed of nuclides that have the same atomic number, i.e. stable and unstable isotopes of a specific element are present. During a severe accident monoelemental particles may be released. These particles are mainly composed of volatile elements, such as I and Cs, or semi-volatile elements. Ru and Mo are examples of semivolatile elements.

In the Chernobyl accident nearly monoelemental carrier-free ruthenium particles were released (e.g. Sandalls et al. 1993). Activity of these particles was up to 300 kBq (Broda 1987). Ruthenium particles constitute a potential health hazard because of their high specific activity. Moreover, they can be transported hundreds of kilometres away from the plant. Activity of particles of different sizes must be estimated in order to evaluate their radiological consequences, i.e. transport range, skin dose, inhalation dose etc.

Nuclide-specific activity of a monoelemental ruthenium particle can be calculated by dividing the nuclide-specific activity concentration in the fuel with the elemental concentration of the corresponding element. A property P_d (activity or thermal power) of a monoelemental particle of diameter d is defined as

$$P_d = P_{spec} \frac{\pi}{6} \rho \, d^3 \,, \qquad (11)$$

where P_{spec} is nuclide-specific or element-specific quantity (activity concentration (Bq per ton of UO_2) or specific thermal power (W per ton of UO_2)) divided by the corresponding mass concentration (g per ton of UO_2) of the element considered.

Calculations for a monoelemental particle can be performed as a function of fuel burnup/decay time or particle size (Fig. 18). Main group, property and composition must be choosed before the calculations. Density of a particle as well as fuel burnup must be given, too.

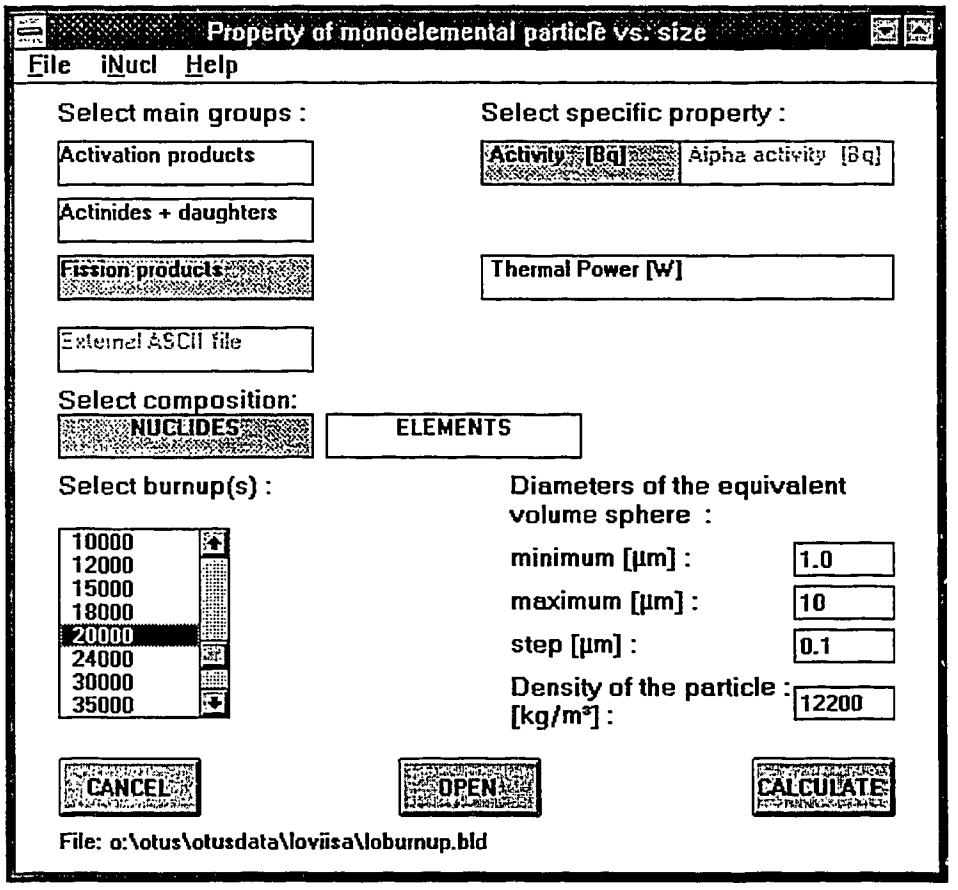

Figure 18. *Calculation of nuclide-specific activity for a monoelemental particle as a function of particle size (1 - 10 µm).*

The examination of the Chernobyl particles revealed that mixing of fission products produced in different parts of the reactor core was not strong (Jaracz et al. 1990). In other words, local properties of the fuel, fuel burnup e.g., have an essential influence on the specific properties of the particles. Therefore, estimation of particle properties as a function of fuel burnup or decay time is highly useful.

The burnup dependency of activity of a ruthenium particle, presented in Fig. 19, shows that the risks associated to these particles may arise from the fuel of low burnup. The total activity of a Ru-particle of diameter 1 μm may be nearly 10000 Bq for fresh fuel, whereas for the fuel of high burnup the total activity is smaller by two orders of magnitude. Although the total amount of ruthenium in the reactor fuel is small for low burnups (see Fig. 15), the high activity of Ru-particles suggests re-estimation of the significance of these particles in a severe reactor accident.

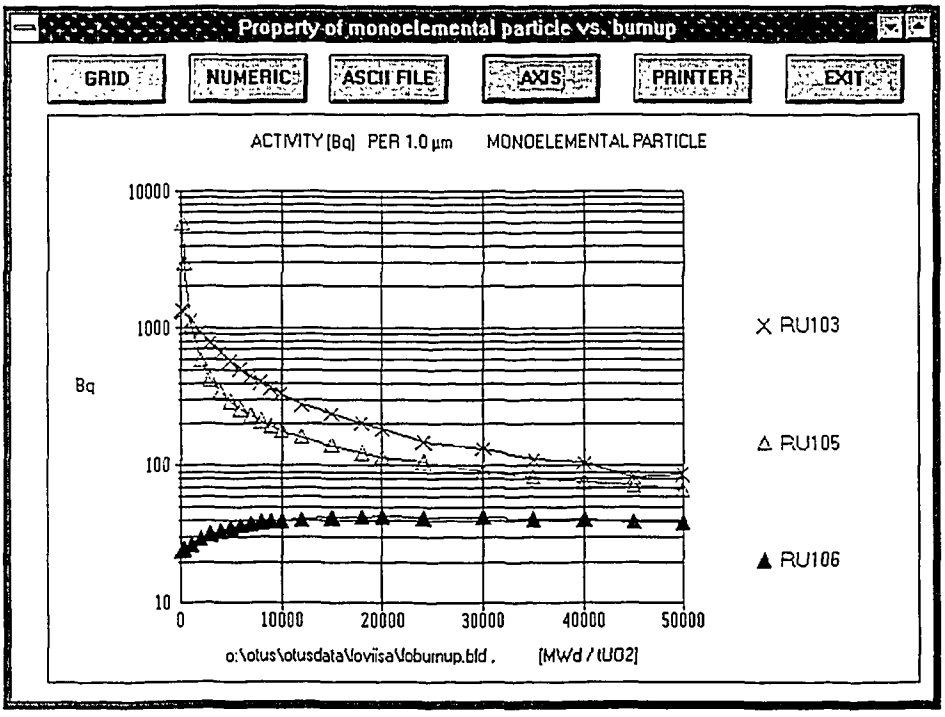

Figure 19. *Activity (Bq) of ^{103}Ru, ^{105}Ru and ^{106}Ru in a ruthenium particle of diameter 1 μm as a function of fuel burnup (MWd/tUO2). Particle density is 12200 kg m^{-3}. The calculation is performed for the Loviisa reactor.*

4.4.3 Uranium fuel particles

Uranium fuel particles are fragments of uranium oxide fuel containing a range of fission products and actinides present in the fuel. In practice, noble gases are missing and volatile or semi-volatile elements are often depleted. Uranium fuel particles were found in the Northern and Eastern Europe after the Chernobyl accident (Sandalls et al. 1993). High-resolution gamma-ray spectrometry showed the presence of fission products such as ^{95}Zr, ^{95}Nb, ^{140}La, ^{141}Ce, ^{144}Ce. Isotopes of Cm and Pu were found in alphaspectrometric analyses. Particles with activity up to tens of kBq's were found in many European countries.

A property P_d (activity, mass or thermal power) of a nuclide or an element in a single uranium fuel particle of diameter d is obtained from

$$P_d = C_p \frac{\pi}{6} \rho \, d^3 , \qquad (12)$$

where ρ is density of the particle and C_p is concentration of property P_d in uranium fuel (Bq or W per ton of UO_2). Note that the concentration C_p is different than P_{spec} in equation 11. C_p includes all elements in the fuel while P_{spec} is only for one specified element.

Properties of uranium fuel particles can be calculated as a function of fuel burnup/decay time or as a function of particle size. Activity as a function of particle size for ^{89}Sr, ^{90}Sr, ^{106}Ru and ^{141}Ce is shown in Fig. 20.

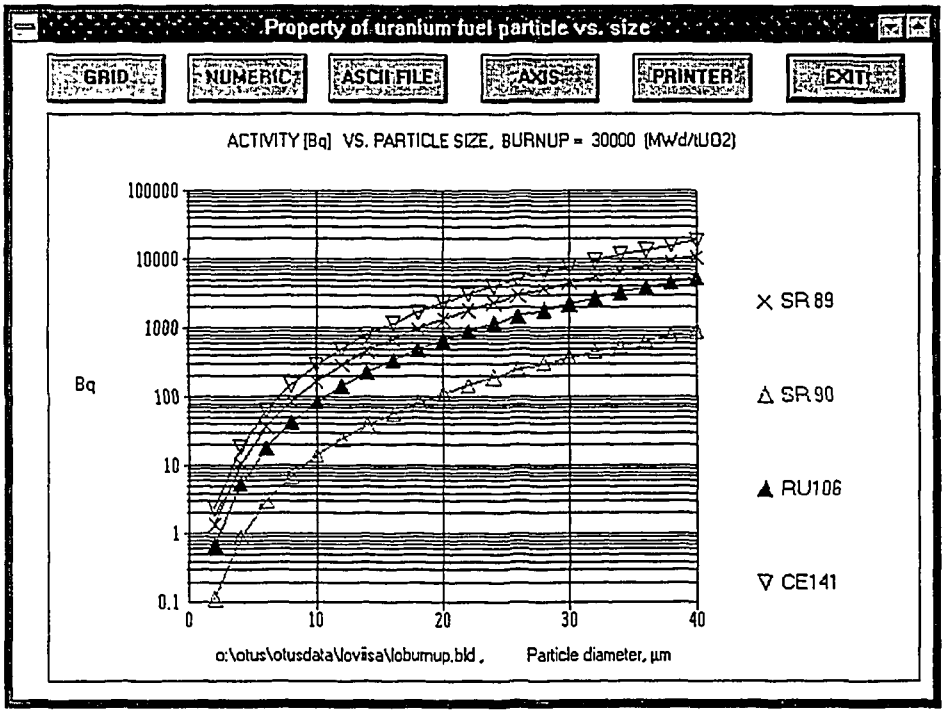

Figure 20. *Activity (Bq) of ^{89}Sr, ^{90}Sr, ^{106}Ru and ^{141}Ce in a uranium fuel particle as a function of particle size (µm). Particles are assumed to represent the Loviisa fuel irradiated to a burnup of 30000 MWd/tUO_2. Density of the particle is 10500 kg m^{-3} (nominal density of the fuel).*

5 SUMMARY FILES - INTERFACE TO OTHER APPLICATIONS

ORIGEN2 can handle 1700 nuclides. Every nuclide is present in each calculation, i.e. in a burnup dependent file and in all decay time dependent files, see Fig. 2. Let us assume that the user needs an overall view (information from all inventory files) of the behaviour of a certain important nuclide. If the methods presented in the VIEW DATA window are applied here, processing of large inventory files would be time-consuming due to consecutive opening, closing and searching procedures. An other approach, creation of a summary file, is therefore needed.

The basic idea of summary files is that all burnup dependent and decay time dependent information, related to the nuclide specified, is gathered into one file. This procedure is performed only once. The computer disc quota needed for summary files is small because the number of important nuclides in user-specified applications is limited. An example of a summary file is shown in Fig. 21.

All summary file operations are performed in the SUMMARY FILES window. Summary files are created by using **Create** option in the pop-up menu. Files can be presented as a table by choosing **View** option or as a figure by using **Plot** operation. **RatioFit** enables calculation of the ratio of nuclides that are in different summary files. This ratio can be used in operational applications (estimation of the fuel burnup or the time of accident).

Summary files are in ASCII format which makes their further use simple for other codes. Other ASCII files that are created in OTUS can be exported, too, but the information density for the specified nuclide is relatively low (i.e. the information is typically only for one burnup and decay time, not for all burnups and decay times).

LOCS134.ACT : Activity vs decay time and burnup

File Help

MWd/tU02 / Bq / tU02 | FILE INFO | PRINT | PLOT | EXIT | CLE

CS134	00032	00160	00320	01000	05000
0.00	3.6341E+08	1.8075E+10	1.5581E+11	3.8147E+12	1.3738E+14
0.25	3.9627E+08	1.8230E+10	1.5636E+11	3.8147E+12	1.3738E+14
0.50	4.0404E+08	1.8263E+10	1.5647E+11	3.8147E+12	1.3734E+14
1.00	4.0589E+08	1.8267E+10	1.5644E+11	3.8147E+12	1.3727E+14
2.00	4.0589E+08	1.8252E+10	1.5629E+11	3.8110E+12	1.3716E+14
3.00	4.0552E+08	1.8234E+10	1.5614E+11	3.8073E+12	1.3701E+14
4.00	4.0515E+08	1.8219E+10	1.5599E+11	3.8036E+12	1.3690E+14
5.00	4.0478E+08	1.8200E+10	1.5584E+11	3.7999E+12	1.3679E+14
6.00	4.0441E+08	1.8186E+10	1.5570E+11	3.7962E+12	1.3664E+14
7.00	4.0404E+08	1.8167E+10	1.5555E+11	3.7925E+12	1.3653E+14
8.00	4.0367E+08	1.8152E+10	1.5544E+11	3.7888E+12	1.3638E+14
10.00	4.0293E+08	1.8119E+10	1.5514E+11	3.7814E+12	1.3616E+14
14.00	4.0145E+08	1.8052E+10	1.5455E+11	3.7703E+12	1.3564E+14
21.00	3.9886E+08	1.7934E+10	1.5359E+11	3.7444E+12	1.3479E+14
30.00	3.9553E+08	1.7786E+10	1.5229E+11	3.7148E+12	1.3368E+14
60.00	3.8480E+08	1.7301E+10	1.4815E+11	3.6131E+12	1.3002E+14
90.00	3.7407E+08	1.6831E+10	1.4412E+11	3.5146E+12	1.2647E+14
182.63	3.4366E+08	1.5455E+10	1.3235E+11	3.2271E+12	1.1614E+14
365.25	2.9049E+08	1.3065E+10	1.1189E+11	2.7280E+12	9.8161E+13
730.50	2.0753E+08	9.3351E+09	7.9920E+10	1.9492E+12	7.0152E+13
1095.75	1.4830E+08	6.6711E+09	5.7128E+10	1.3927E+12	5.0135E+13

Figure 21. *A summary file of ^{134}Cs (Bq/tUO_2) presented using* **View** *operation (see also Fig 23). Decay times (days) are at the left and fuel burnups (MWd/tUO_2) on the top. Concentrations can be presented as a figure by pressing the ctrl key of the keypad and selecting eiher decay times (rows) or burnups (columns). A red bar appears in the field of decay time or in the field of burnup (in the present figure for burnups 320 and 5000 MWd/tUO_2).* PLOT *button produces the graphical output.* CLEAR *button removes the choices.* FILE INFO *button shows the names of decay files included in this summary file (see later).*

5.1 Creation of summary files

At the beginning of each decay file (decay files are calculated for a burnup specified in the file name, see Fig. 2) is the inventory at the zero decay time. This value is the same as in the burnup dependent file for the burnup considered. For example, first decay value in file lo00032.bld represents the zero decay time which is the same value as in file loburnup.bld for the burnup of 32 MWd/tUO_2. First line of a summary file refers to the zero decay time for all burnups considered. Subsequent lines are for other decay times.

When a summary file is created the decay data (inventory vs. decay time) for the specified nuclide is collected from every decay files (Fig. 22). Provided that the data base is comprehensive enough, summary files give extended possibilities to utilize concentration information for various purposes. The size of a summary file is small (at present a 24*14 matrix, 24 decay values and 14 burnup values). This enables fast handling of information concerning one nuclide.

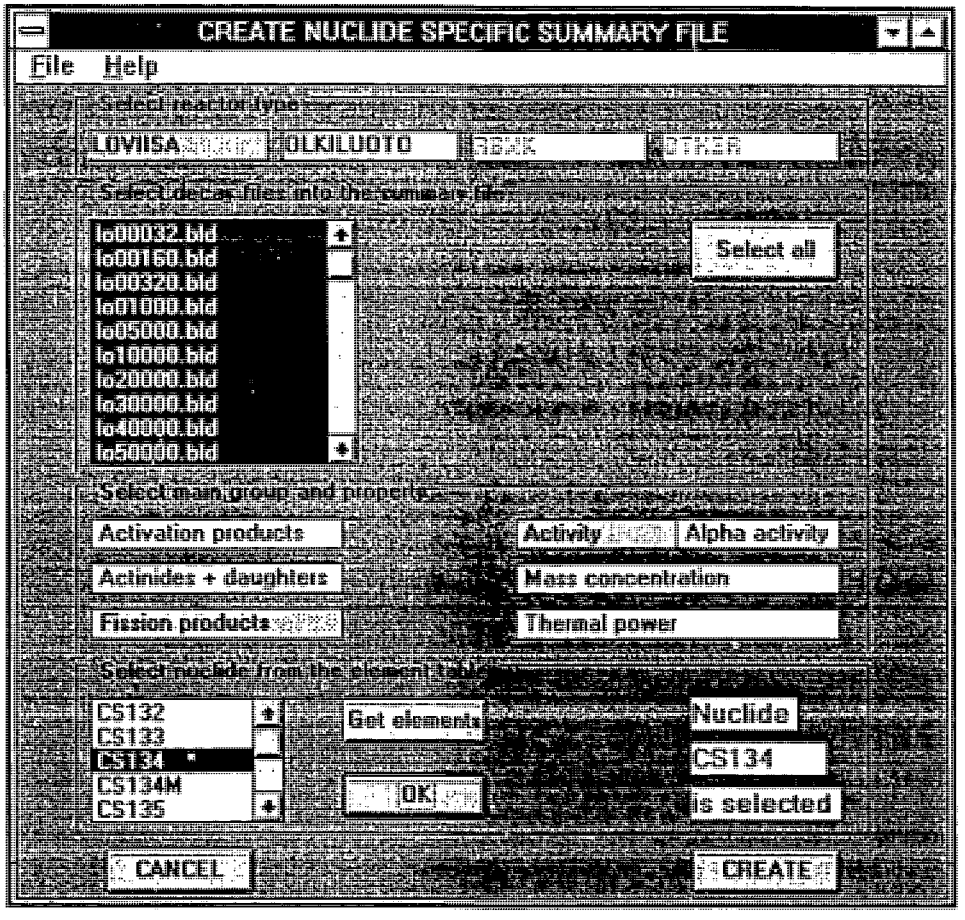

Figure 22. *Creation of a summary file for ^{134}Cs. Reactor type, here* LOVIISA, *must be selected first. Only decay files can be selected when creating a summary file. All decay files can be selected by using* Select all *button. Thereafter, main group (some nuclides belong to two groups) and type of the summary file must be selected. Summary files are nuclide-specific files. The element, in this case Cs, must be choosed before the selection of the particular nuclide (*Get elements *and* Get nuclides *button; in the figure the element list is hidden under the nuclide list). Finally,* CREATE *button creates the summary file.*

At the beginning of each summary file there are lines showing the names of the decay files included. Selected main groups are also shown. These lines are for informative purposes and they can be seen by using FILE INFO button in Fig. 21. A similar button is also in the VIEW, PLOT, and RATIOFIT windows.

Summary files are saved in the appropriate subdirectory determined by the reactor selected. OTUS PARAMETERS in the MAIN window control treatment of summary files. Files are named according to the reactor and nuclide name. The file name extension comes from the selected property (quantity). For example, the file locs134.act is an activity summary file for reactor loviisa and nuclide ^{134}Cs. Extensions *alp*, *mas*, and *pow* refer to *alp*ha activity concentration, *mas*s concentration and specific thermal *pow*er, respectively.

5.2 Presentation of summary files

Summary files can be presented as a table (**View**) or as a figure (**Plot**). In the **View** procedure only one summary file in turn can be shown whereas in the **Plot** option several summary files (one for each reactor type) can be considered. The latter feature is useful e.g. for comparison purposes. Because of the small size of these ASCII files they can also be viewed using standard editors.

5.2.1 Viewing summary files

Reactor type and file type, i.e. the concentration type for which the summary file is calculated, must be selected first in the VIEW operation (Fig 23). Files representing the selected type are shown in the list. FILE INFO button (see above) and GRID button appear on the screen after the selection of a summary file.

The GRID button brings the selected summary file onto the screen (Fig. 21). When rows (decay times) are selected, the concentrations are plotted as a function of fuel burnup. When columns (fuel burnups) are selected, the concentrations vs. decay time are displayed.

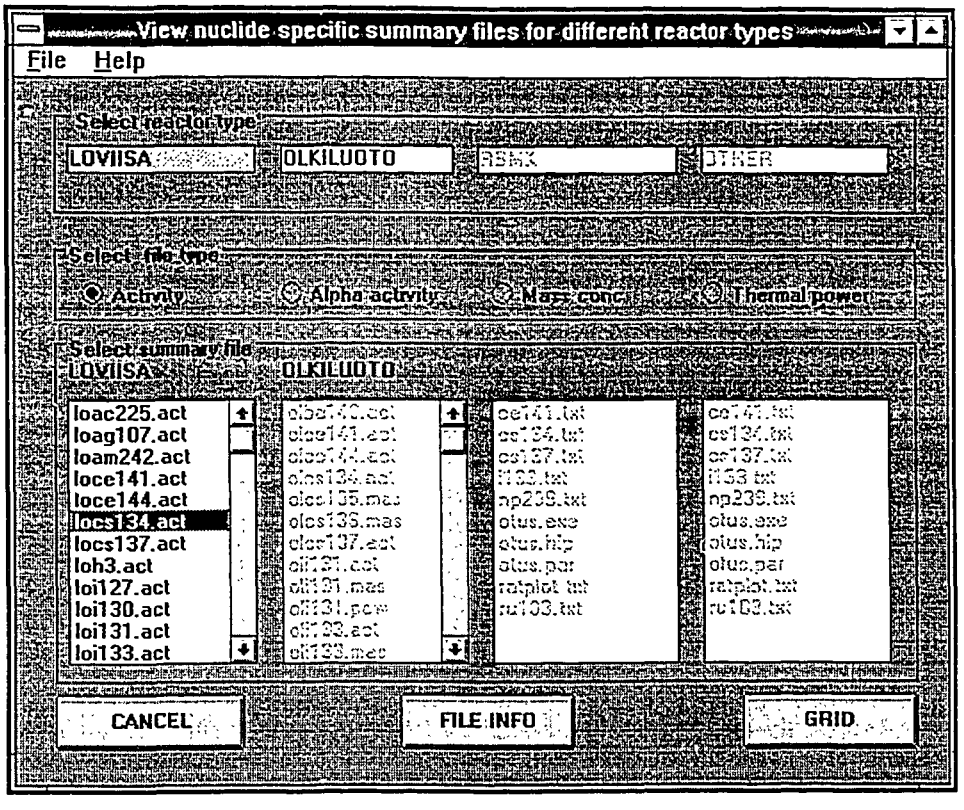

Figure 23. *Selection of summary file* locs134.act *(see also Fig.21).*

5.2.2 Plotting summary files

Plot operation enables, for example, comparison of inventories of different reactor types. The files are selected in the PLOT window presented in Fig. 24. One or more reactor types, as well as summary files, can be selected. Activity concentration, alpha activity concentration, mass concentration or specific thermal power can be plotted as a function of burnup or decay time. Appropriate decay times (burnups) must be selected if concentrations are plotted versus burnup (decay time). An example for ^{131}I in the Loviisa fuel is shown in Fig. 25 a). The activity concentration in Loviisa, Olkiluoto (Swedish type BWR) and RBMK (Chernobyl) fuel for ^{144}Ce is shown in Fig. 25 b).

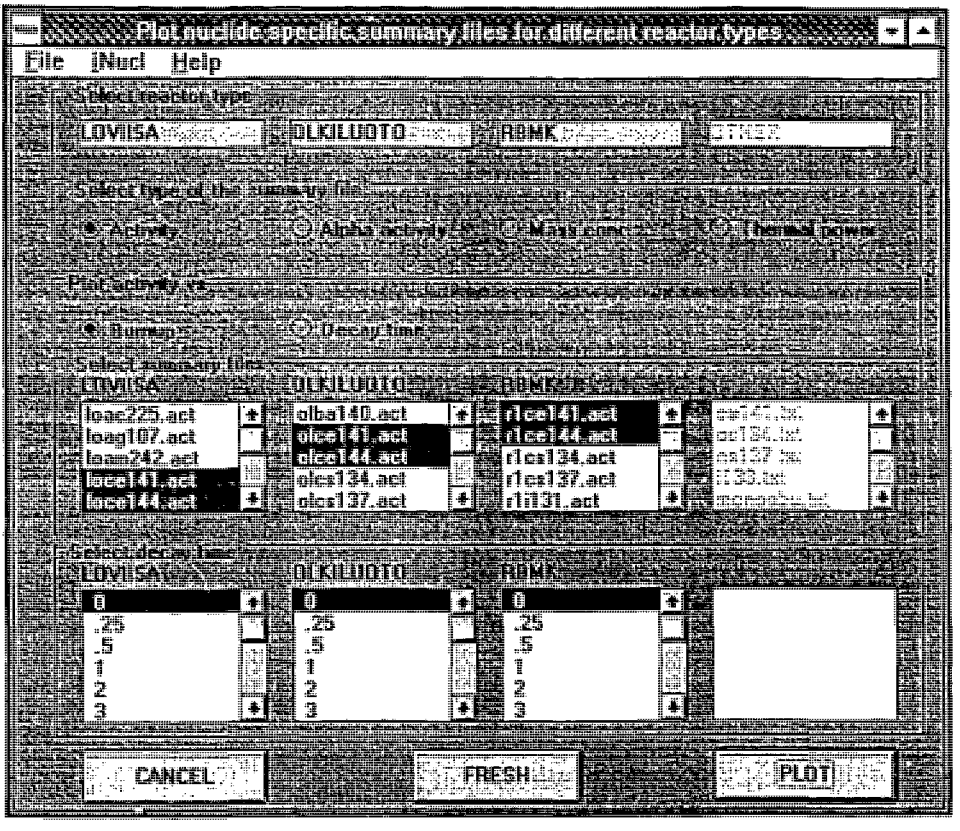

Figure 24. *Plotting summary files for ^{141}Ce and ^{144}Ce in Loviisa, Olkiluoto and RBMK reactors (the chosen cooling time is zero in each file).*

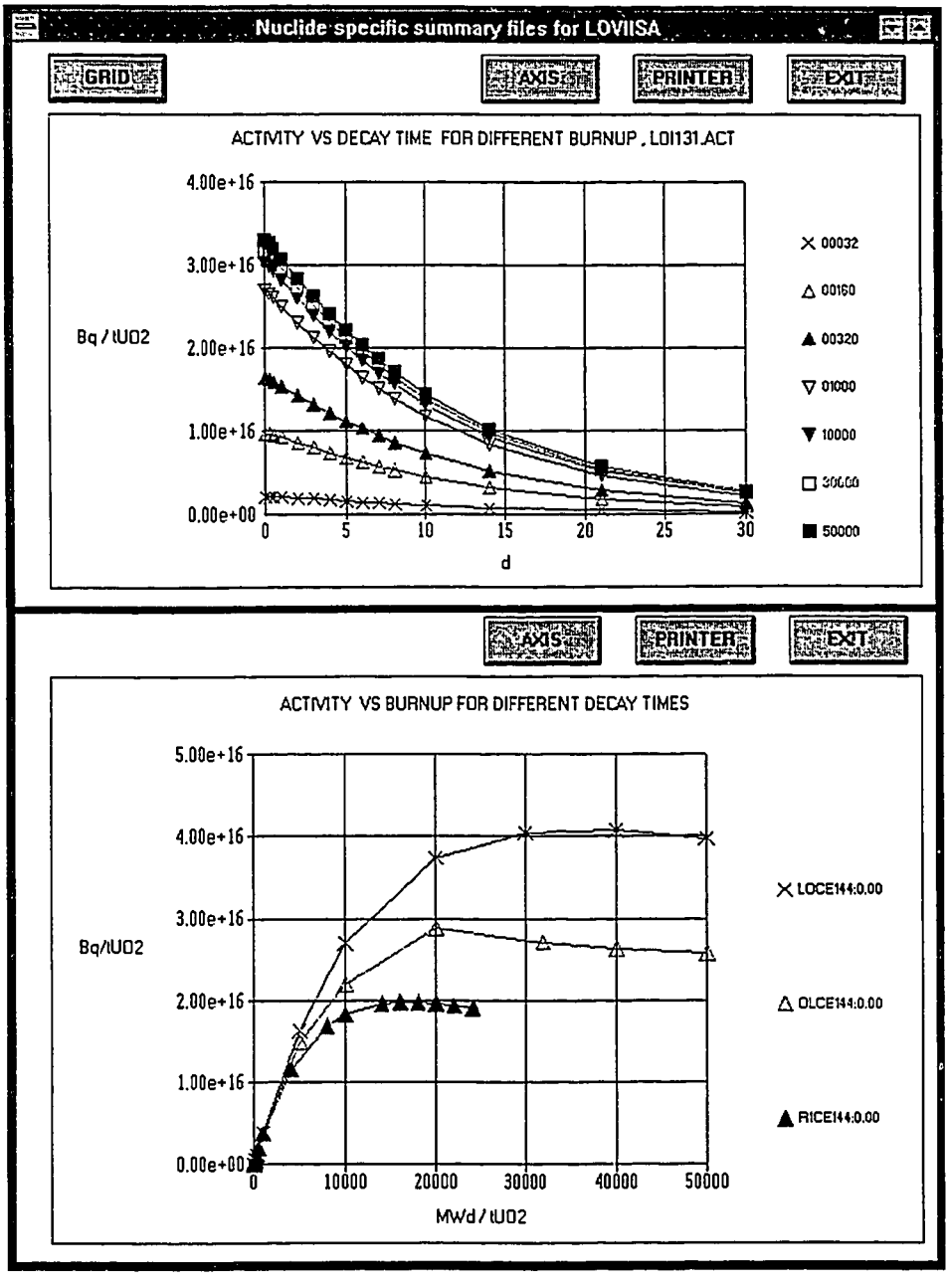

Figure 25. *a) Activity concentration (Bq/tUO_2) of ^{131}I in the Loviisa fuel as a function of decay time (d). Labels on the right show the burnup (MWd/tUO_2) of the fuel. b) Activity concentration of ^{144}Ce for Loviisa, Olkiluoto and RBMK fuel as a function of fuel burnup (zero cooling time).*

6 SUMMARY FILES IN OPERATIONAL USE

Activity ratios depend often strongly on burnup and cooling time of the fuel. If airborne radioactive material of artificial origin is detected, these dependencies can be used for estimating the properties (e.g. burnup) of the material from which the nuclides were released. The time interval between the shutdown of the reactor and the detection time can also be estimated.

6.1 Estimation of fuel burnup

Detected activity ratios compared with the calculations give a possibility to characterize the properties of the irradiated nuclear fuel. This analysis can provide useful information about the progression of the accident/incident and fuel characteristics. The following reasoning is valid for nuclides that are not produced continuously through decay of other nuclides (parents).

The effective decay time of an activity ratio is

$$t_{eff} = \ln 2 \; / \; \lambda_{eff} \, , \qquad (13)$$

where the effective decay constant, λ_{eff}, is the difference between the individual decay constants λ_1 and λ_2 for nuclides 1 and 2

$$\lambda_{eff} = \lambda_1 - \lambda_2 \, . \qquad (14)$$

Estimation of fuel burnup is based on the time interval between the reference time and the time of reactor shutdown and on the isotopic activity ratio at the reference time. Let us assume that the measured activity ratio at the reference time (at the middle of the sampling time) is R_{ref} (nuclide with longer half life in the denominator). Let the difference between the time of reactor shutdown and the reference time be t. The activity ratio at the beginning of the accident, R_0, is then

$$R_0 = R_{ref} \exp(\lambda_{eff} \, t) \, . \qquad (15)$$

The activity ratio $^{134}Cs/^{137}Cs$ is used for the estimation of fuel burnup of spent fuel pins (Cheng Si Tsao and Lung Kwang Pan 1993). The effective decay time for this ratio is about two years. Activity concentrations of ^{134}Cs and ^{137}Cs in the fuel depend almost linearly on the fuel burnup (see Figs. 7 and 17). This enables estimation of fuel burnup for a wide range (Fig. 26). The caesium isotope ratio can be used for the estimation of the average fuel burnup during a nuclear accident, too. Caesium is a volatile element that can easily be released from the degraded fuel.

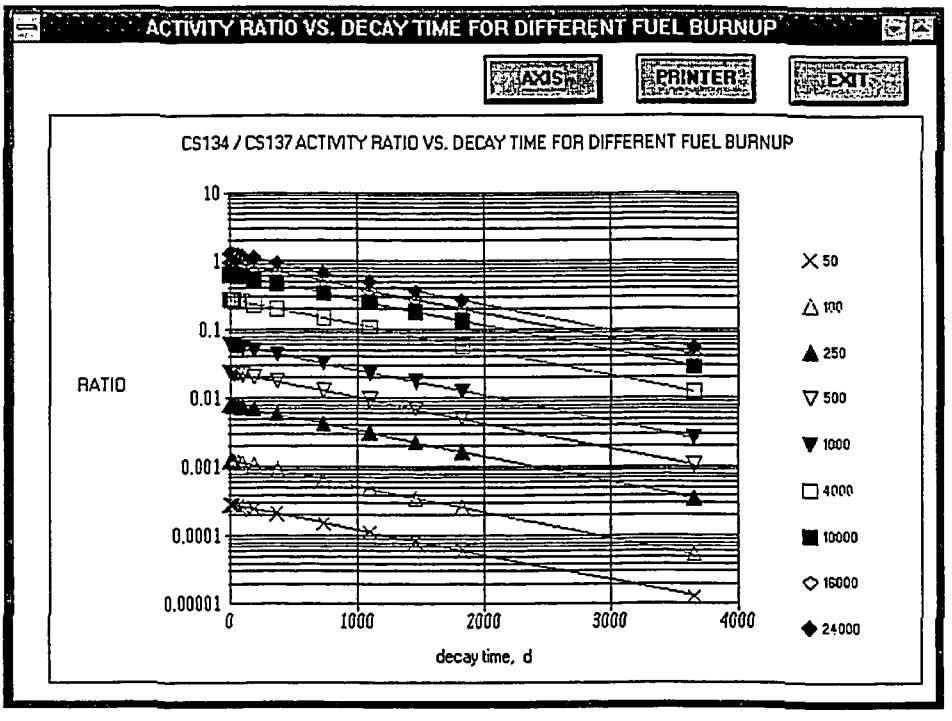

Figure 26. *Activity ratio for nuclides ^{134}Cs and ^{137}Cs as a function of decay time (d). The Loviisa fuel is irradiated to a different burnup (MWd/tUO_2) shown at the right.*

Fuel burnup estimation is performed in the SUMMARY FILES window under the **RatioFit** option. Results of the measurements of the ratio $^{134}Cs/^{137}Cs$, carried out in Loviisa, Kotka, and Helsinki during the Sosnovyy bor incident (Toivonen et al. 1992), are used as an example (Fig. 27). The reactor type assumed is an RBMK with fuel enrichment of 1.8 % (Chernobyl inventory).

OTUS calculates first the nuclide ratios with the corresponding error estimate at the reference time. Then, the values of R_0 are computed on the basis of equation 15. These R_o values are compared to precalculated values of R_0 (the value in the y-axis in Fig. 26, e.g.). The fuel burnup corresponding to this specific value is estimated with linear interpolation between the precalculated burnup values. Results will be shown in a separate window (Fig. 28) for each measurement and as an average value. The error estimate of the average value is weighted by the square of the individual measurement errors.

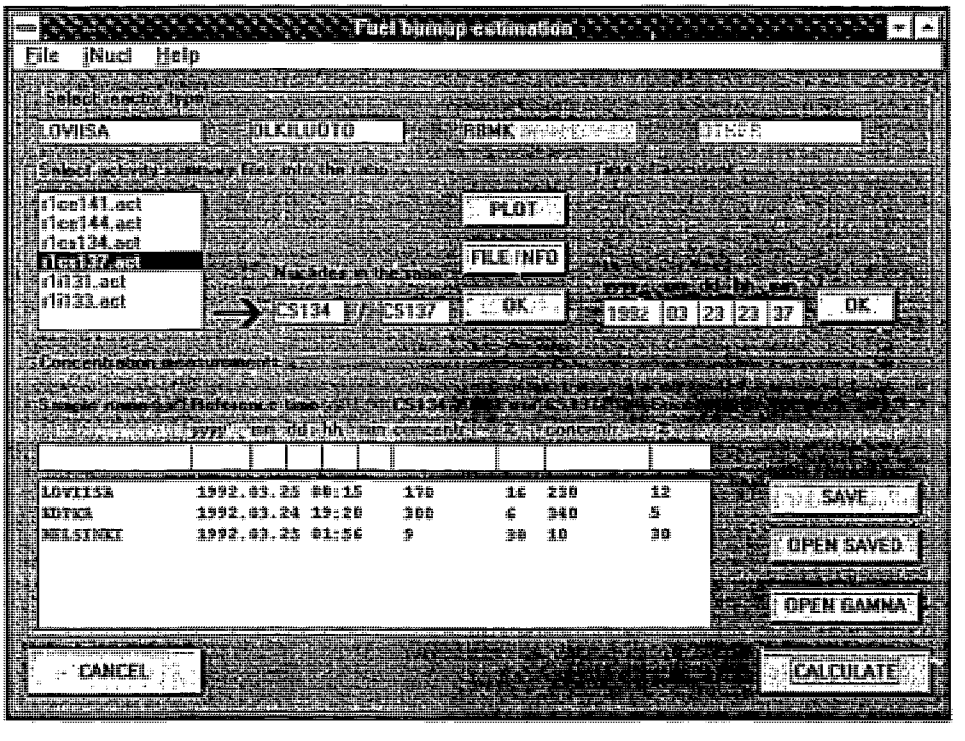

Figure 27. *Input window for the estimation of fuel burnup. Reactor type, nuclides in the ratio (i.e. activity summary files) and estimated time of accident (or time of reactor shutdown) must be selected first. Results of activity measurements can be given manually or using previously saved measurement files with* OPEN SAVED *and* OPEN GAMMA *(see text later) buttons.*

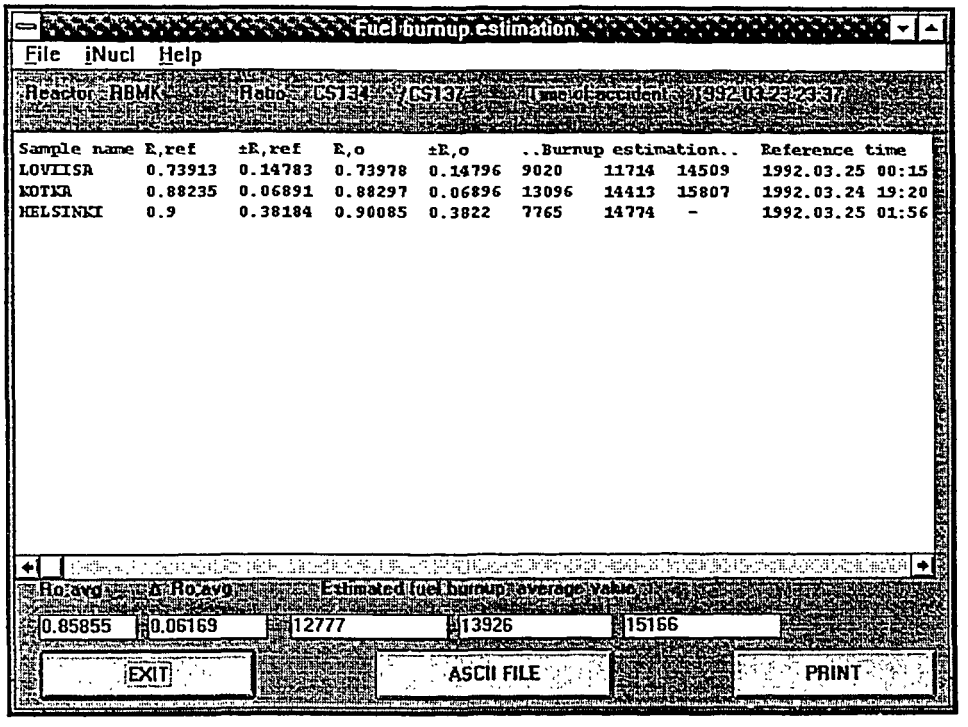

Figure 28. *Fuel burnup estimation from the ratio $^{134}Cs/^{137}Cs$. Time of accident (reactor shutdown) refers to the Sosnovyy Bor incident (Toivonen et al.1992). The three values for burnup refer to the estimates based on the reference values with the error estimates $R_{ref} - \Delta R_{ref}$, R_{ref} and $R_{ref} + \Delta R_{ref}$, respectively.*

Measured activity concentrations in air can be given either manually in the input window or transferred within the computer network of the Finnish Centre for Radiation and Nuclear Safety. STUK has a continuous programme for the monitoring of airborne radioactive material. The samples from the nationwide monitoring network are analyzed in the laboratory with the GAMMA computer code (Sinkko and Aaltonen 1985). Output of this code can given directly to OTUS.

6.2 Estimation of time of accident

Estimation of the time of reactor shutdown is based on the measured nuclide-specific ratio, R_{ref}, at the reference time and on the known average burnup of the fuel from which the radioactive material has been released (i.e. known nuclide ratio, R_0, at the time of reactor shutdown). Provided that the nuclides considered are not produced through the decay of other nuclides (parents) the time interval, t, between the accident and the reference time is given by

$$t = - \frac{\ln(\frac{R_{ref}}{R_0})}{\lambda_{eff}} . \qquad (16)$$

The measuring results of the continuous air surveillance programme of STUK are automatically stored in a data base that can be utilized by OTUS. Traces of ^{134}Cs and ^{137}Cs from the Chernobyl accident are often detected in the air samples. In the following analysis we assume, that the time point of Chernobyl accident is unknown.

Let us assume, that the fuel from which the caesium isotopes were released was irradiated to a burnup of 10000 MWd/tUO_2 (close to the average burnup of the Chernobyl reactor). For this burnup the ratio R_0 is 0.65. ^{134}Cs and ^{137}Cs concentrations, detected at the end of 1994 in Kotka, are given to OTUS by using the OPEN GAMMA button in Fig. 29 a. These are real measurements published quarterly by STUK. R_{ref} for each sample can be calculated easily, and using equation 16, the time difference between the reference time and the occurrence of the Chernobyl accident is calculated (Fig. 29 b). Within the errors, the time estimates calculated for each sample are in good agreement with the real time point, April 26 in 1986.

This, of course, is only an example but it manifests that the timing of an unknown reactor accident can be estimated fairly well, provided that properties (burnup) of the fuel are known. Nuclides in the ratio must be identified before the calculations. In addition, the effective decay time of the ratio (equation 13) must not be considerably longer than the expected time difference between the accident and sampling.

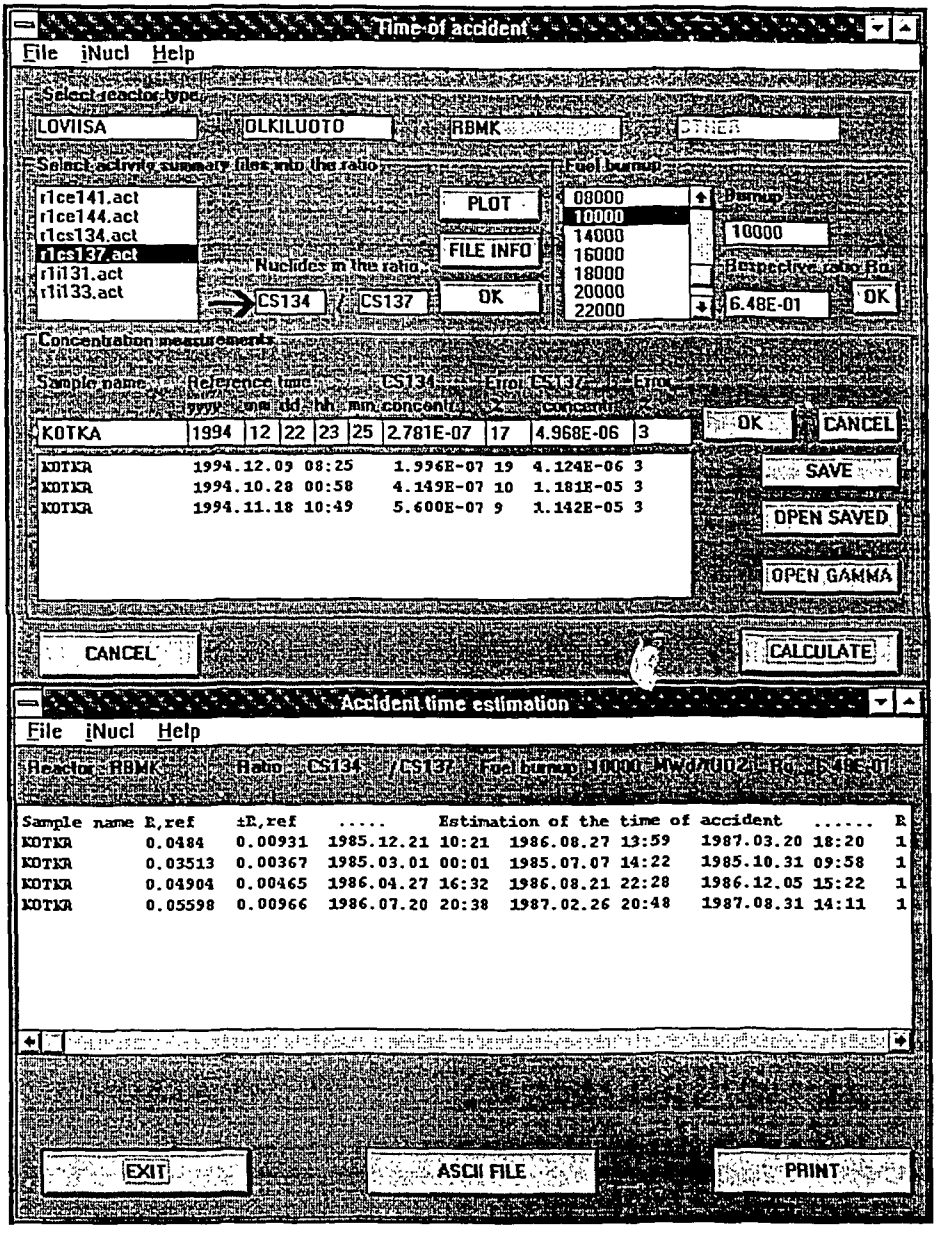

Figure 29. a) *Input window and b) results window for the estimation of time of the accident. Activity concentrations are directly given using* OPEN GAMMA *button. Fuel burnup and the respective R_0 value are shown on the top of the results window. Three values of timing refers to the estimate based on the reference values and their error estimates $R_{ref} - \Delta R_{ref}$, R_{ref} and $R_{ref} + \Delta R_{ref}$, respectively.*

7 DISCUSSION

Large number of radionuclides can be released during a severe nuclear accident. Most of them have relatively unimportant environmental consequences mainly because of the short half-live or small concentration in the reactor fuel. However, nearly hundred nuclides may cause potential radiation hazard at least during the early stages of the accident. Thus, there is a need for a tool that can give their properties and their concentration in the fuel as a function of fuel burnup or decay time. OTUS is designed to be an information, interface and presentation system that can be used for operational applications or for different research purposes.

The need of radiation monitoring data in a nuclear accident is of utmost importance. Sometimes nuclide-specific data is needed to make correct decisions for counter-measures. Unfortunately, some nuclides can be detected only using tedious and time-consuming sample preparation procedures. For example, ^{89}Sr and ^{90}Sr as well as many actinides are difficult to detect. However, ^{91}Sr can be easily detected using gamma-ray spectrometric methods. This gives a possibility to get a rapid first-hand estimate for all isotopes of strontium at the early stage of the accident. All relevant calculations can be easily performed in OTUS.

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Finland
Tel. +358 0 759 881

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