ChainSolver code for calculations of transmutations

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http://snow.prohosting.com/roeug/index.htm or http://www.websamba.com/roeug/default.htm (May, 2003)

Program ChainSolver is intended for carrying out the concrete calculations at the final stage before an irradiation or before delivery of received isotopes to the customer. The depression of a thermal neutrons flux, resonance self-shielding of isotopes during an irradiation, and the irradiation schedule (the schedule of the reactor work and rearrangement of an irradiated target in various positions) are taken into account. These calculations are extremely tedious because of at each stage of an irradiation the specific neutron fluxes, cross-sections of reactions, time of an irradiation, and structure of initial products should be taken into consideration [1]. Such calculations allow to define more precisely the chosen mode of an irradiation and to calculate the expected outputs for both products and inevitable impurities. The approximation used at calculation of transmutations is the assumption that the influence of changes in the irradiated material structure on characteristics of reactor operation modes (a reactor as a neutron source) is insignificant.

The interface of ChainSolver program is constructed on the basis of Delphi visual component that displays several pages in the main form. Each page is intended for the definition of some group of the tasks necessary for calculation of accumulation and/or derived quantities.

The 'Chain' page Fig.1 allows user to create, change structure and to edit the transmutation chain. Editing here is understood as a change in characteristics of the chain states and/or the chain links (a link is a connection between two nuclides or two isotope states, possibly of the same nuclide). There exist a lot of ways for a chain creation: the chain earlier kept in a file may be loaded into ChainSolver program by means of 'Load' button. The chain file may be either created earlier by the program ('Save' button) or generated by ChainFinder code. The chain also may be created by means of nuclide state additions (additions into an empty chain are possible). To add a nuclide state the user should type its

name (the format is U-235 or U-235g, U-235m or U-235m1, Hf-177m2) in the edit window of 'States' panel (above the 'Add' button) and press the button. Also where it is necessary to input a lot of nuclide names; it is possible to take advantage of the edit window expansion button ('···'). Links between isotopes that already are in the chain and ones to be added are automatically constructed at the moment of nuclides addition. For automatic construction of links it is necessary to check 'Build Links' check-box and to choose taken into account types of links: 'Decay' - radioactive decays, 'Capture' - captures of thermal and resonance neutrons, 'Fission' – neutron induced fission, 'Threshold' - threshold neutron reactions for fast neutrons. Any link between isotopes is constructed on the basis of the information available in ORIP_XXI software suite data file (the default file name is ORIP_XXI.oob). The data should be loaded in program ChainSolver by 'Load DB' button. The whole data set is not loaded automatically because of the data are not required for earlier kept chains. If the data file is not loaded and a state is added to the chain under edition, then the program gives out a warning query for the data loading.

Channels of disintegration/reception of the isotopes, caused by spontaneous fissions of heavy elements nuclei are not taken into account at nuclide state addition into the chain. Generally, spontaneous fission contributions to the speeds of accumulation are small in comparison with speeds of neutron reactions (the yield for spontaneous fission is very small in comparison with other channels because of usually huge time of a parent isotope half-life). If necessary to take into account accumulation of an isotope as the spontaneous fission product, then it is possible to add the corresponding link or to edit available one, which was constructed for reaction of neutron-induced fission. "Branching" for radioactive decays and for neutron capture is considered (for example, at beta-decay of Zr-95 the child isotope Nb-95 is formed both in ground and metastable states with specific probabilities).
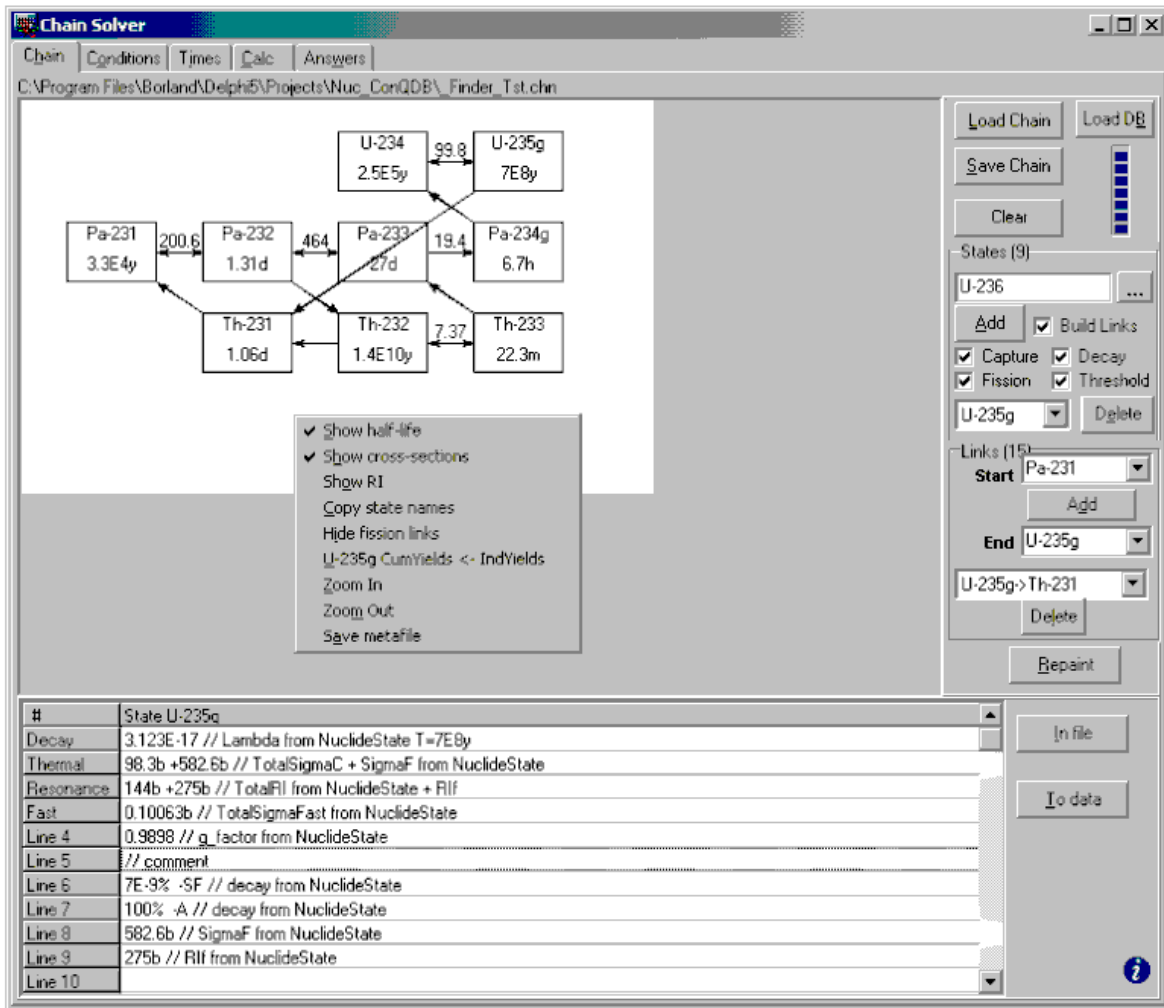
Fig.1. The 'Chain' page

There is the 'Links' panel on the page, which is intended for a work with the chain links (a link is a connection between two isotopes or two states due to nuclear transmutation reactions). By means of dropping out lists 'Start' and 'End' it is possible to choose initial (Start) and final (End) states for a new link in the chain. Then it is possible to add new link between the states by means of the panel button 'Add'. The dropping out list of links serves for the following purposes: having chosen some links (the link name is given in the format 'the start/parent state->the end/child/descendant state') it is possible to remove the link by button 'Delete' or to edit it (see below). The detailed data of the chosen link (on 'Links' panel) or the chosen state (on 'States' panel) is displayed in the bottom part of the

'Chain' page. The choice of a link or a state is made or by means of the appropriate drop-down lists, or simply with the mouse click inside the chain image (it is necessary to say that images of two different links may coincide, for example, for a neutron capture induced link and a (n, 2n) threshold reaction one).

The table in the bottom part of the 'State' page displays the detailed information on the link or the nuclide state and can be edited. A rare case of necessity for such editing is the following: when isotopes N-14 and C-14 both are added into a chain the link between the isotopes according to the known information about (n, p) fast neutrons reactions is automatically constructed. The information on the same reaction for thermal neutrons is absent in the software suite data file and it is necessary to edit the information manually. For this purpose, we should add the information on the reaction cross-sections for thermal and resonance neutrons (see Fig.2).

Fig.2.The table on page 'Chain' before and after editing

The double slash symbol '//' is a comments mark. The program warns the user in the case of unit absence in numerical expression for cross-sections or resonance integrals. 'To data' button is intended for modification in the given chains to be applied. For a changes cancel before their mapping into the given chains (pressing of 'To data' button) user can pass the focus to another link or nuclide state, having refused in appeared dialogue from preservation of changes. 'In file' button allows to see the information about the focused state or link available in the ORIP_XXI data file.

There exists a pop up menu for the chain image (on a mouse right button click), which gives access to the following operations: 'Show half-life' - to show/hide half-life values for states, 'Show cross-sections' - to show/hide cross-sections of thermal neutron capture reactions, 'Show RI' - to show/hide values of resonance integrals. The click on the menu item 'Copy state names' copies all nuclide state names of the chain to Windows clipboard, 'Hide fission links' - to hide/show the links caused by fission (its frequently encumber the chain image), 'Zoom In/Zoom Out' - to change the image scale. At nuclide state addition into a chain, all the state yields as a product of heavy atoms fissions are initiated by values of cumulative yields from the data file. Such initialization may not be appropriate for the chain. For example, the case takes place if in the chain alongside with the nuclide state there exists also the state which is the direct predecessor (parent) of the former by the way of nuclear transformations (by radioactive decays only). To avoid manual updating of fission yields in such cases; there is 'CumYields<-IndYields' item in the menu. The item automatically replaces cumulative yields on individual ones (for the given nuclide state as a fission product). Having chosen menu item 'Save metafile' it is possible to keep the chain image in metafile format file using EMF (Enhanced Metafile Format) or WMF (Windows Metafile Format).

'Conditions' page Fig.3 is intended for the input of initial conditions of the irradiation: initial nuclide masses, the account of thermal flux depression and resonance self-shielding.

In the table (the left part of the page) initial weight nuclide portioning of the chain is set, weights of elements are set in 'Masses, g' table. The lump of a sample is set in 'Total mass, g' edit control. This information is used for preparation of final results and is optional (if 'Total mass, g' field is not filled, then the initial weight is determined as the sum of the element weights). Parameters in 'atol' and 'rtol' columns define a maximum deviation for each variable for the system of the ordinary differential equations describing the nuclear transmutations in time. The local allowable error of integration for i-th variable y(i) on each time step is defined as rtol*abs(y(i))+atol(i). The time step

integration stops (it is considered to satisfy the accuracy requirements) if the difference of two consecutive approximations on absolute size does not above the local allowable error. Default values (about 1.0E-7) are used if 'atol' and 'rtol' fields are blank.

To take into account depression of thermal neutron flux it is necessary to check 'Depression' check-box and to input values of the irradiated sample volume and average chord.

Calculations taking into account resonance self-shielding are extremely tedious and demand a lot of additional parameters. Since resonance self-shielding factors calculations are rather long, there is an opportunity to save the factors table in a file in order to load and use it in the program later ('Save Table' and 'Load Table' buttons). 'Build Table' button is used for the table construction. The table is constructed on the basis of the approach described in work [2] in approximation of intermediate resonance with Doppler broadening. The user sets type of a resonance absorber block lattice ('No' - the single block in a external moderator, 'Sq' - rectangular (square) lattice, 'Hex' - a hexagonal prism lattice, 'Simple' - the single block in an infinite external moderator environment, this option is realized at the request of users of an old software suite with 'SELF' program for resonance self-shielding calculation, the algorithm was not tested in the frame of this work). For resonance self-shielding factors calculations some additional parameters are to be known: nuclear weight, neutron scattering cross section, and nuclear concentration for mixed moderators ('Mixed moderator', usually, is a material of a target matrix) and for an external moderator ('Outer moderator'), the external moderator volume.
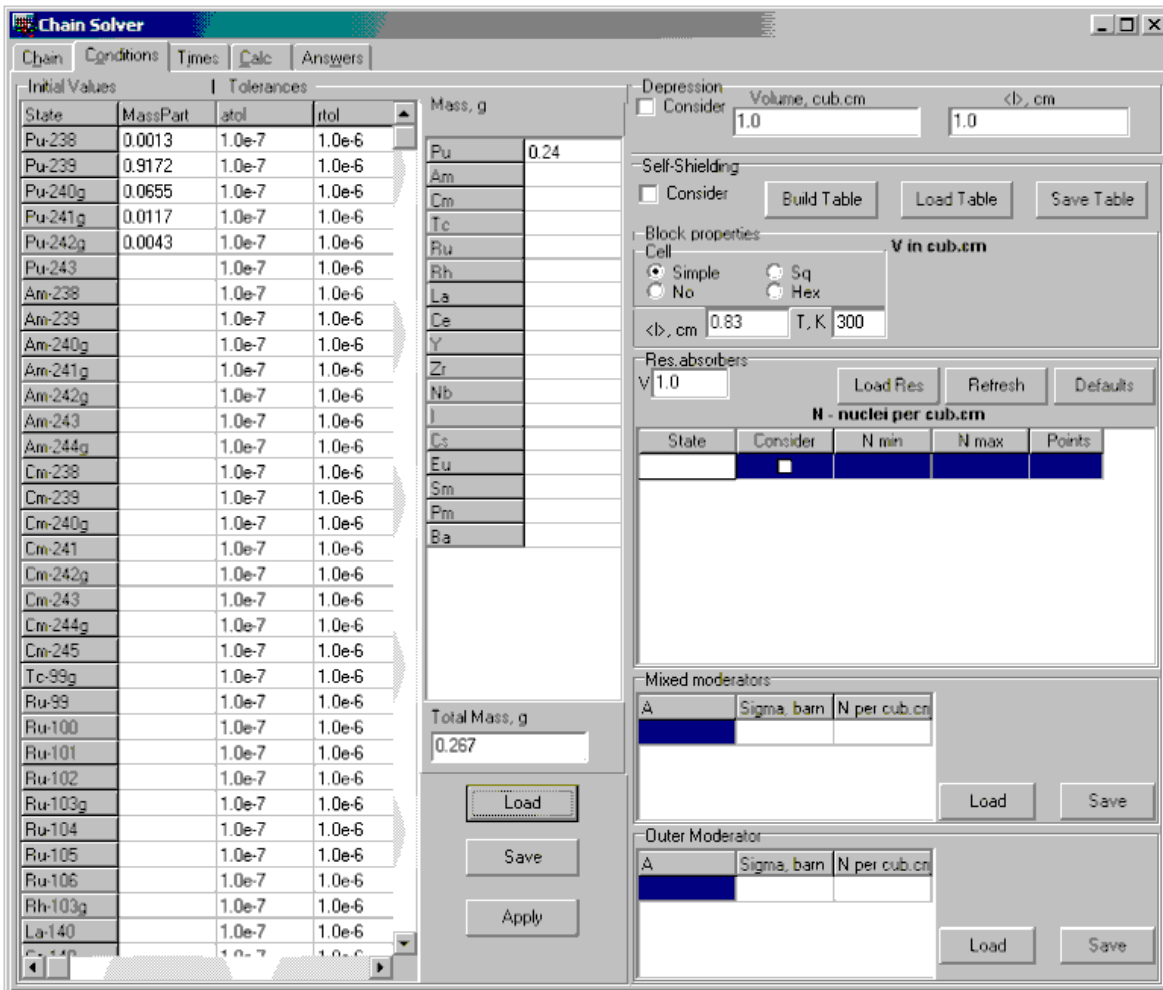
Fig.3 'Conditions' page

Resonance parameters for neutron cross-sections are loaded from an external file on pressing the 'Load Res' button, after pressing 'Refresh' button among loaded nuclides are searched the chain states and if are found, its will be output in the table of 'Res. absorbers' panel (in new versions these two buttons are combined). For construction of the resonance self-shielding factors table it is necessary to check a field in the left most column of the appropriate line of the table and to input values of the minimal and maximal nuclear concentration of a resonant absorber nuclide and number of intervals for the factor table (the table is constructed in logarithmic scale on nuclear concentration). The stand-alone service utility SelfShieldingCalculator and the program MCNP [3] (for calculations of neutron fluxes and speeds of neutron reactions) were used for calculation algorithms testing.

The detailed resonant absorber information available with a mouse double click on the corresponding line in 'Res. absorbers' panel table (Fig.4).

Res.type	E0, eV	A.avg.	2*I	2*J	Xs,b	I	Edown	Eup	GT	GN	GG	GF	GFB
MLBWR	426	236.17	0	1	11	0	1.05	412.5	0.09298	0.04768	0.034	0.0113	
MLBWR	496	236.17	0	1	11	0	1.05	412.5	0.050154	0.0093540	0.034	0.0068	
MLBWR	473	236.17	0	1	11	0	1.05	412.5	0.05935	0.02305	0.034	0.0023	
MLBWR	465	236.17	0	1	11	0	1.05	412.5	0.12631	0.08561	0.034	0.0067	
MLBWR	461	236.17	0	1	11	0	1.05	412.5	0.0903	0.0496	0.034	0.0067	
MLBWR	419	236.17	0	1	11	0	1.05	412.5	0.11622	0.05322	0.034	0.029	
MLBWR	59.8	236.17	0	1	11	0	1.05	412.5	0.035985	0.001315	0.034	0.00067	
MLBWR	151.1	236.17	0	1	11	0	1.05	412.5	0.07258	0.02938	0.034	0.0092	
MLBWR	139.7	236.17	0	1	11	0	1.05	412.5	0.043137	0.002837	0.034	0.0063	
MLBWR	132.4	236.17	0	1	11	0	1.05	412.5	0.040152	0.000851	0.034	0.0053	

Fig.4. The detailed resonant absorber information

'Times' page (Fig.5) is intended for input of parameters and the schedule of an irradiation.

In the multi line editor paired values should be entered: a time interval (days) and the corresponding power (a.u., see below). The blank line is the terminator of the time intervals list. In the one-line editors the following values are: 'Tn.g' - neutron gas temperature in Kelvin degree (for the account of neutron reactions cross-section dependence from thermal neutrons spectrum characteristics, also it is necessary to check the check-box near to the edit window). 'Th', 'Res', 'Fast ' - thermal, resonant and fast neutrons flux accordingly for the reactor nominal power. 'Nominal ' - value of the nominal power. During the subsequent calculations the neutron flux is defined as a product of flux value for nominal power on the ratio of the actual (entered for the time interval) power to the nominal. Calculation of neutron fluxes are usually carried out by means of high precision codes, for example, MCNP [3]. To say formally, any reaction velocity is the product of the state/link characteristic value by the corresponding flux.
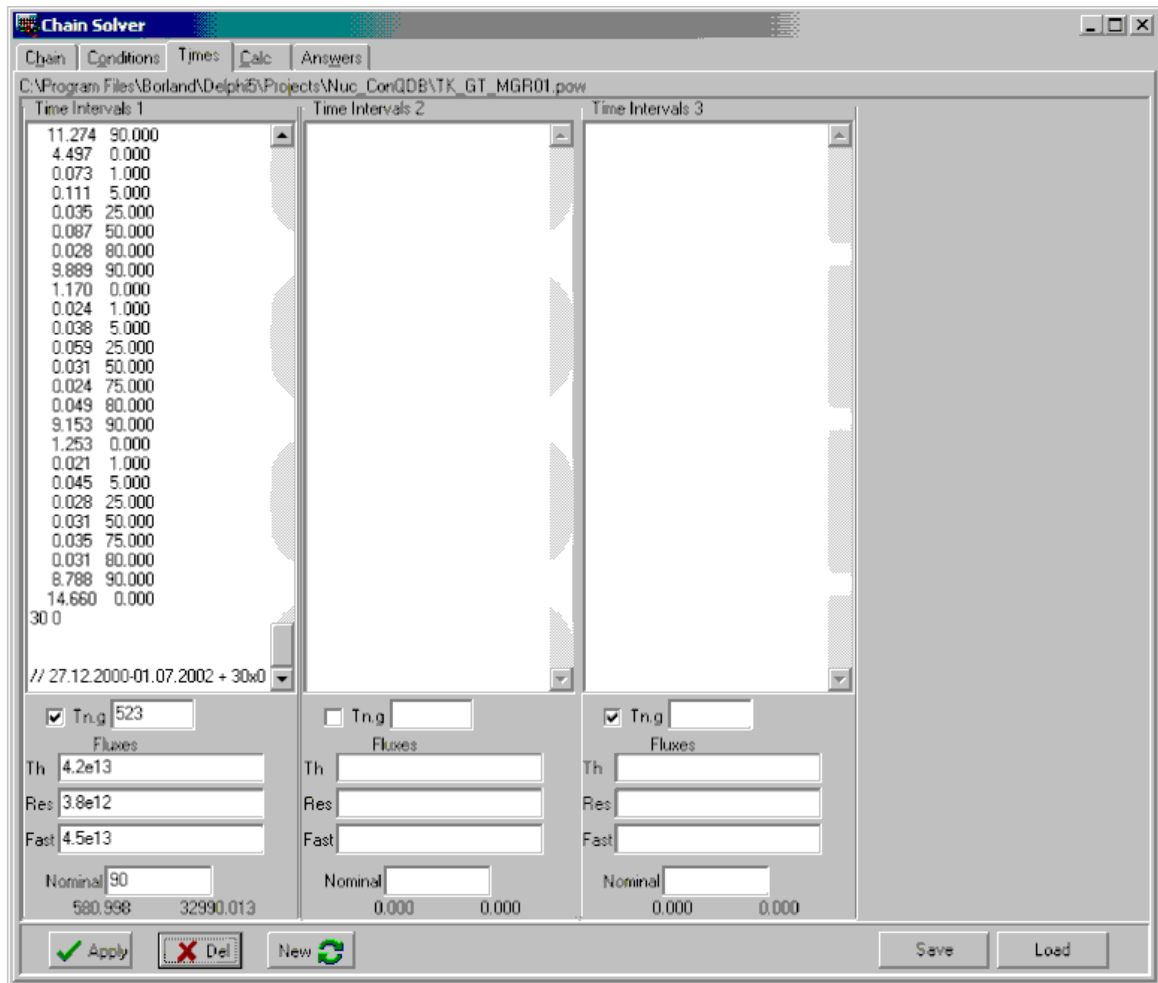
Fig.5 'Times' page

The program allows describing of multi step processes of an irradiation in a reactor; when the irradiated material at different stages is placed in various irradiation positions of the reactor (probably even in various reactors and/or endurance pool). Such situation is characteristic, for example, for production of transplutonium elements. It is impossible to place the starting material immediately in irradiation position with extremely high neutrons flux, which necessary for transmutations, because of impossibility to provide sufficient target cooling that is required for the elimination of heat caused by neutron fission.

For the task of bng time material storage it is enough to specify the endurance duration and zero reactor power for this time interval.

In order to set a multi stage irradiation, there is two buttons: 'Add' - to add an irradiation stage and 'Del' - to remove the last one. At a new irradiation stage addition a panel with the same set of input fields for the added stage is created, at removal - the last panel from available leaves. 'Save' and 'Load' buttons are intended to save in a file and to load from an earlier kept file the schedule of the irradiation, generally, multi step one.

'Calc' page Fig.6 gives the interface for various methods to solve the ordinary differential equations (ODE) system that describes nuclide transmutation in the chain. The ODE coefficients generally depend on time, both because of dependence of neutron flux on the irradiation schedule and dynamics of nuclear concentrations, resulting in changes of thermal flux depression and resonance self-shielding factors.

Fig.6. 'Calc' page

The user may take advantage of various subroutines for the ODE integration: VODE, LSODA, RADAU, and MEBDF solvers. Presence of several subroutines is based on the fact that there exists no

subprogram to be the best suitable for all ODE systems (see, for example [4]). Any solver from ChainSolver program may be called from dynamically loaded libraries (DLLs). Subroutines LSODA and VODE may be called from the main program without DLL use also (the check box 'DLL' is not checked). The subroutines use different methods of Jacobian calculations for the systems of ODEs. If the check box 'JAC' is checked, Jacobian is calculated in the main program. If the check box leaves unchecked, then Jacobian is internally generated in a solver by means of difference relation calculation (additional function calls for calculations of the ODEs right hand side are required).

Pressing 'Calc' button launches the calculation process. It is possible to see the calculation advance on the operation performance progress-bar. Full filling of the progress-bar corresponds to the calculation completion for the last time step. There is a memo for diagnostic messages (if the solver subroutine outputs them) in the right hand part of the program page.

The calculated weights of chain isotopes for each time step are shown in the table. For the user convenience the first two left most columns of the table have the following meanings: the interval initial time and the corresponding thermal neutrons flux.

LSODE - the base program of family of codes for the ODE solving: ODEPACK [5]. LSODE solves the initial value problem for stiff or non-stiff systems of first order ODEs ($Dt/Dt=f(y, t)$, y is a vector). The solver can use both banded and dense (few zero elements) Jacobian matrix. LSODA [4], in comparison with LSODE, has new feature: it is automatically switched with "backward differentiation formulas" (BDF) method (stiff equations) to Adams method (non stiff systems) with Petzold's algorithm [6]. The basic purpose of automatic switching is to release the user from decision about the system stiffness that may occur enough frequently. In general the ODE stiffness depends on time length of the interval for integration. So, for example, LSODA uses non-stiff algorithm for transitive time areas when there are fast changes of the irradiation conditions.

VODE [7] is the subroutine of stiff and non-stiff ODEs systems solving for problems with known initial values conditions, VODE uses variable-coefficient Adams-Moulton method and BDF methods in Nordsieck form as taken from the older solvers EPISODE and EPISODEB, treating the Jacobian as full or banded. Unlike the older codes, VODE has a highly flexible user interface. VODE authors have made several algorithmic improvements. First, a change in step size and/or order that is decided upon at the end of one successful step is not implemented until the start of the next step, so that interpolations performed between steps use the more correct data. Secondly, a new algorithm for setting the initial step size has been included, which iterates briefly to estimate the required second derivative vector. Efficiency is often greatly enhanced by an added algorithm for saving and reusing the Jacobian matrix J, as it occurs in the Newton matrix, under certain conditions. Finally, the modified Newton iteration is relaxed by a scalar factor in the stiff case, as a partial correction for the fact that the scalar coefficient in the Newton matrix may be out of date.

RADAU [8] applies implicit Runge-Kutta method of order 5 with use of linear algebra package LAPACK.

MEBDF [9] - the stiff ODE systems solving program uses modified extended BDF. Because the stability of these formulas deteriorates rapidly as the order increases within the family, a great deal of the MEBDF authors effort has been devoted to finding formulas of moderate to high order with better stability. Stability is not the only issue, however: the formulas also are computationally efficient.

Each the subroutine for ODEs systems solving has passed sets of tests, both common for initial values problems [10] and specific ones for transmutation problems. The service utility BatemanLSODA was written for the solver of systems describing transmutations tests. The utility allows comparing results of calculation to the simple analytical results for a so-called Bateman ODEs system having the simple analytical solutions.

On 'Answers' page (fig.7) the various measures derived from calculation results are shown.
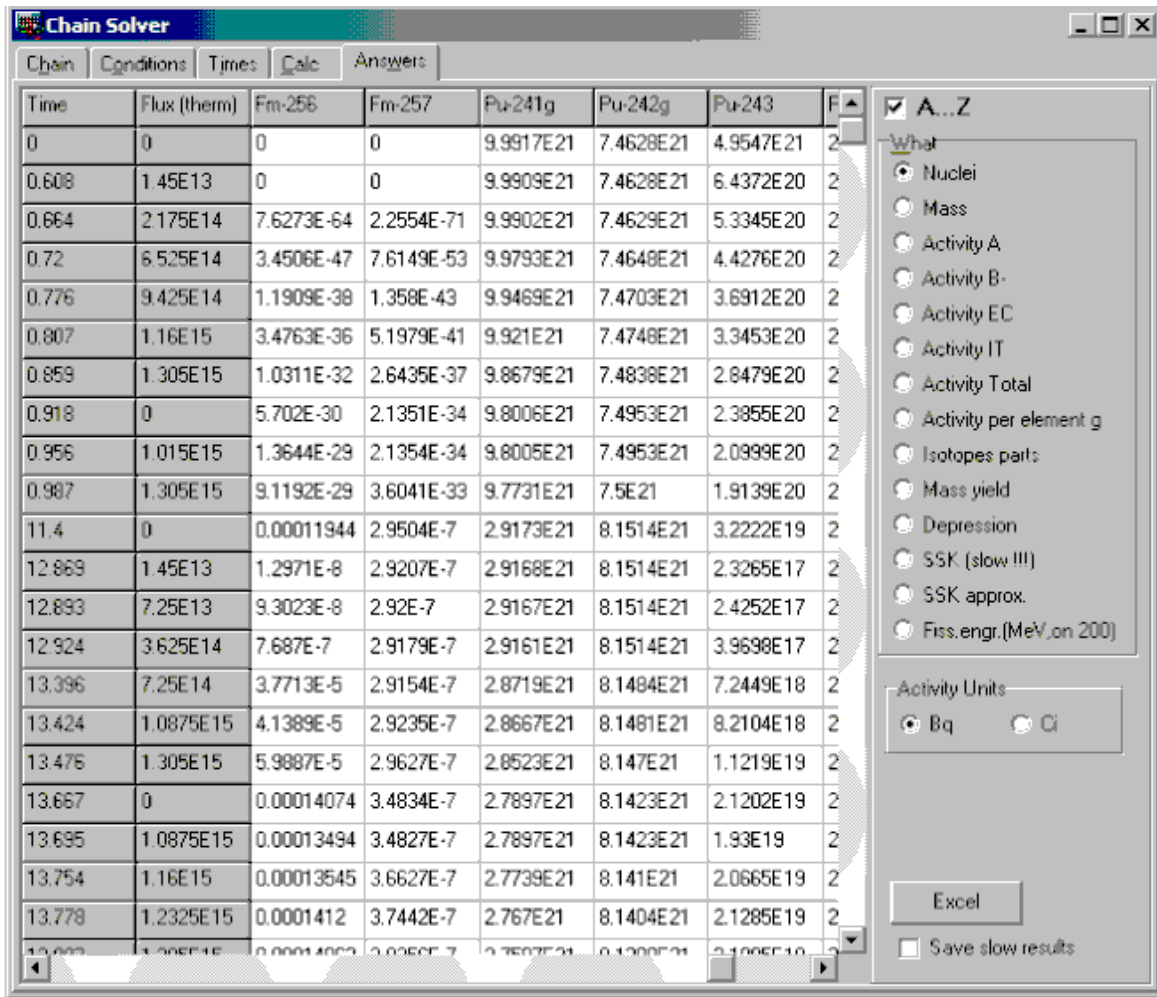
Fig.7. 'Answers' page

The check box 'A_Z' allows alphabetical ranking of the chain nuclide state names for the first table row (at the unchecked check-box 'A_Z' the rank goes in that order in what states appeared at ODEs calculation). The choice of activity units is made on the 'Activity Units' panel: Ci - activity in curie, Bq - in besquerel. What measure will be shown in the table is determined by a choice from the radio group 'What ':

'Nuclei' - number of the chain state nuclei for each time point,

'Mass' – weights (in gram),

' Activity A ' - alpha activities,

' Activity B-' - beta- activities,

' Activity EC ' - activities on disintegration by electronic capture (or beta+),

' Activity IT ' - activities on disintegration through isomeric transition,

' Activity Total ' - full activities,

' Activity per element g ' - full specific activities per 1 gram element mass,

' Isotopes parts' - isotope portions (it is considered that all isotopes of the element are submitted in the calculated chain),

' Mass yield ' - yield per gram mass of starting materials,

'Depression' - factor of depression (the only value for each time interval),

'SSK (slow!!!)' - resonance self-shielding factors (exact values of factors, the program gives out a warning to prevent probable duration of the calculation procedure),

'SSK approx.' - resonance self-shielding factors (approximated values of factors, which have been used actually for the calculations).

'Fiss.engr. (MeV, on 200)' - energy deposition value (MeV). At energy deposition calculations it is assumed that the significant contribution in thermal deposition brings only neutron-induced fission, on 200 MeV per fission. The energy deposition value is important for the reason that the irradiation of weight quantities of actinides and trans-uranium elements lead to significant difficulties because of significant thermal deposition owing to fissions of starting or intermediate isotopes. In some cases the basic thermal deposition occurs due to division intermediate, instead of a starting isotope. So, for example, at an irradiation Am-241, the maximum of energy deposition is achieved at accumulation of the Am-242 maximum. Frequently, the thermal deposition reserve factor should be equaled 10 [1], what is usually rather difficultly Therefore at energy deposition calculation it is considered that at division of any neutron fissionable element by neutrons of any energy it is determined to be equal to 200 MeV.

All results can be saved in a file of MS Excel spreadsheet on pressing the 'Excel' button. The check box 'Save slow result' is designed for above procedure. When checked, results with the word 'slow' in their names are saved automatically, otherwise omitted.

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