ORIP_XXI Computer Programs for Isotope Transmutation Simulations

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ORIP_XXI software suite is developed for study of radioactive and stable isotope transmutation chains, i.e. networks with feedbacks. Using the programs from this suite it is possible to estimate various quantitative characteristics of a transmutation chain both for nuclide irradiations in neutron fluxes and in case of pure radioactive decays. The main parts of *ORIP_XXI* are *NKE*, the electronic nuclide chart, *ChainFinder*, the program for finding transmutation chains, and *ChainSolver*, the program for simulating transmutation. Only the open-source subprograms and licensed software products were used in the coding. *NKE*, *ChainFinder*, and *ChainSolver* source codes are accessible via NEA OECD Computer Program Service.

All programs use a common data file. The data file contains nuclear constants and decay data for more than 2800 nuclides with atomic weights from 1 up to 293 (nuclear charge from 1 up to 118) and characteristics of chemical elements. The file includes data on fission product yields for thermal and fast neutron induced fission of 22 heavy isotopes. Users may edit data as necessary for carrying out transmutation calculations. The transmutation calculation code *ChainSolver* allows users to take into account neutron flux depression and self-shielding factors, the latter using additional data from the resolved resonance parameters file. All data are taken from freely available public nuclear data libraries.

NKE program

NKE program (http://www.nea.fr/abs/html/iaea1384.html) is the latest version of *NuclideExplorer* program described in detail in [1]. The user interface (Fig. 1) has not been significantly changed. The data on radioactive decays, neutron reaction cross-sections and fission product yields has remained the same (the data sources are specified in publication [1] and in the program help file). The most important change is that the data are now stored in a freely available format, whereas in *NuclideExplorer* they were stored in Microsoft Access database format, legal use of which requires users to have Microsoft Jet database engine license. In addition to resolving the license issues the change of data format has allowed to significantly decrease data loading times and to noticeably reduce the data file size.

The program to search for transmutation chains *ChainFinder*

The main function of *ChainFinder* program (http://www.nea.fr/abs/html/iaea1405.html) is searching for nuclide chains which may be realized in nuclear reactors. Though the primary production chains are well known, sometimes it may be necessary to obtain new nuclides with unknown production chains. This program also allows the user to find out the reason for appearance of unexpected isotopes in irradiated material. *ChainFinder* automatically builds possible transmutation chains, given the start and finish states (Fig. 2).

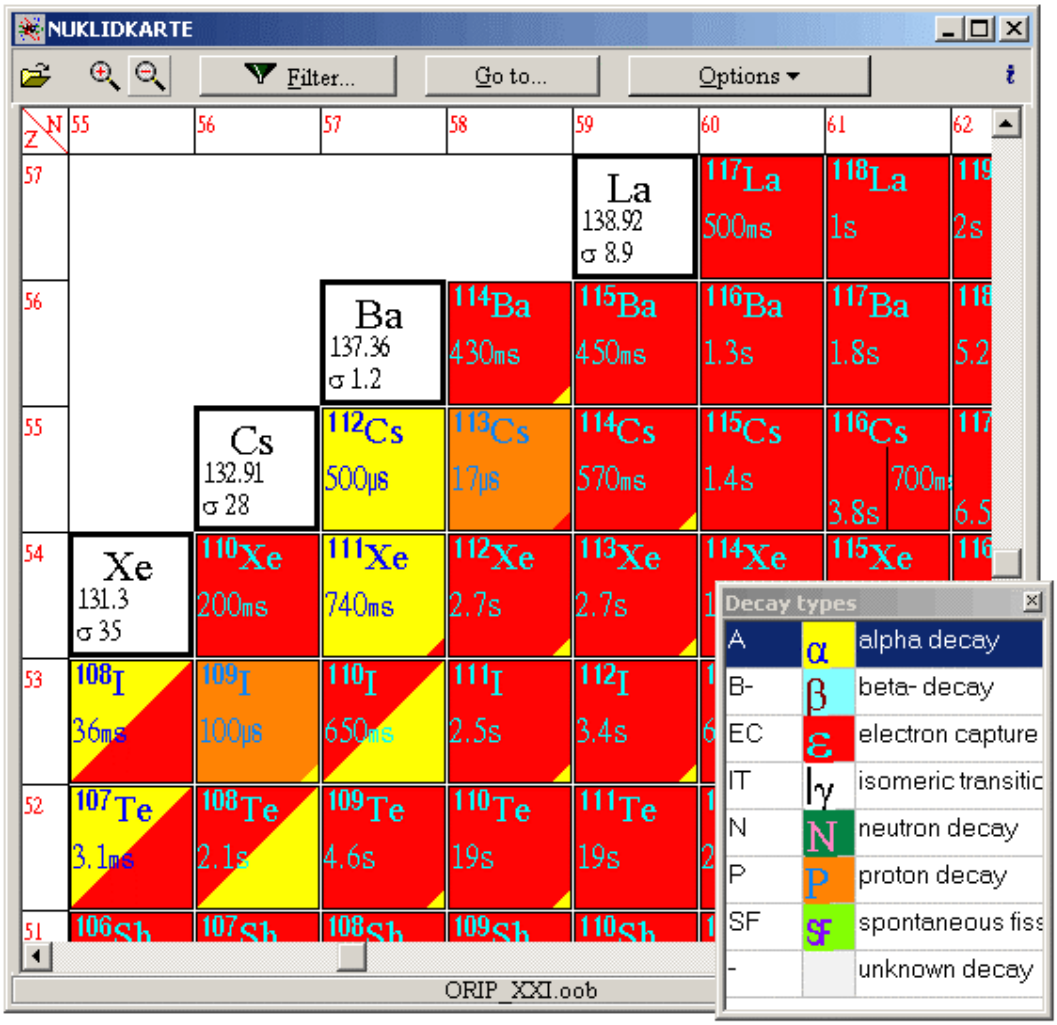

Figure 1. *NKE* program main window (with the legend)

The chain search process takes into account data on decay "subbranchings" available in the data file. For example, β-decay of ^{95}Zr nuclide produces the descendant ^{95}Nb isotope in both ground and metastable states. *ChainFinder* allows the user either to take into account or not, as desired, decay reactions, thermal neutron captures, neutron induced fission, and fast neutrons threshold reactions. This capability is useful, e.g., when trying to find out what transmutations are possible during storage and transportation of non-fissionable nuclides, when only decay reactions can happen. In cases where fissionable isotopes are absent, excluding fission reactions from search significantly reduces chain search time. Similarly, if fast neutrons reactions are negligible (for example, in a thermal reactor), excluding threshold reactions simplifies the analysis.

The user can copy the found state list into Windows clipboard or save the chain in a file to load it later into *ChainSolver* program for carrying out transmutation calculations. *ChainSolver* code can construct a transmutation network on the basis of a given nuclide list.

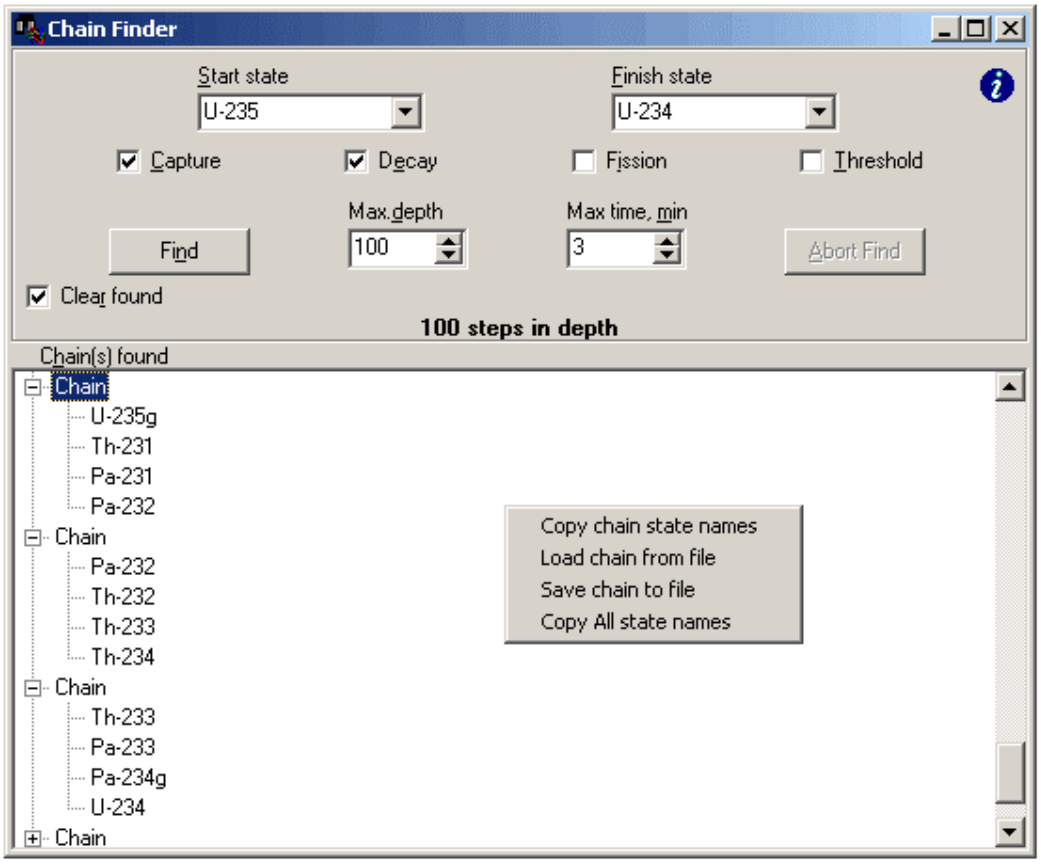

Figure 2. *ChainFinder* program window

ChainSolver transmutation simulation program

ChainSolver program (http://www.nea.fr/abs/html/iaea1404.html) is developed in order to automate the calculations at the final stage before the irradiation or before the isotope shipping. The neutron capture resonance self-shielding, thermal neutron flux depression and the schedule of the irradiation (the reactor schedule and rearrangement of the irradiated target in various positions in one or different reactors) can be taken into account.

These calculations are extremely tedious since at each irradiation time step the specific neutron fluxes, reaction cross-sections, and the initial isotopic composition all have to taken into consideration. The calculations allow to choose the irradiation mode more precisely and to predict the outputs of both products and inevitable impurities. The main approximation used for transmutation simulations is the assumption that only the change characteristics of a reactor as a neutron source due to the composition of the irradiated material is negligible, that is, the specified neutron spectra don't change.

The 'Chain' tab of *ChainSolver* program window (Fig. 3) allows the user to create a transmutation chain, to change its structure, and to edit the chain. Editing here means changing the characteristics of the chain states and/or the chain links (a link is a connection between two isotope states, possibly between two states of the same nuclide) and adding new states and links. The chain can be saved to or loaded from a file, including files created by *ChainFinder*.

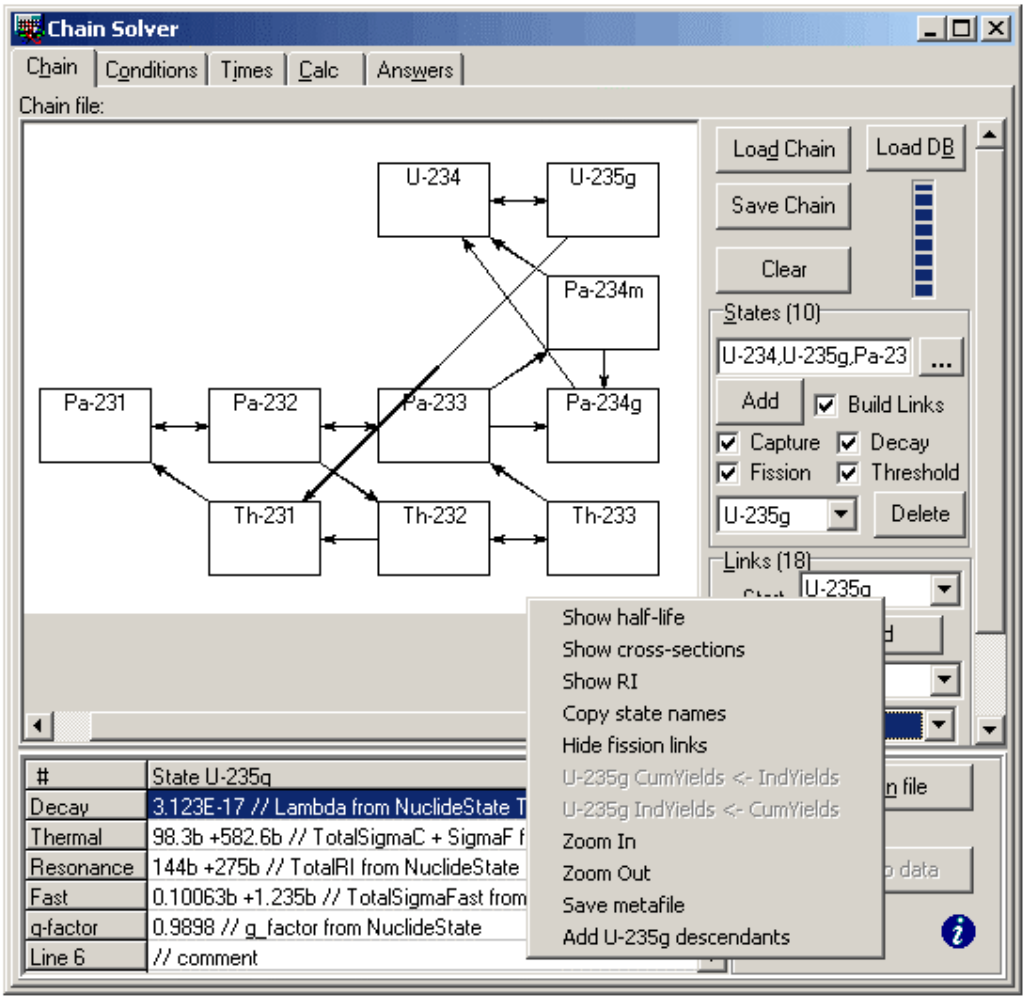

Figure 3. Page 'Chain' of *ChainSolver* programs

The bottom part of the 'Chain' tab shows the detailed information on the selected link or state and can be edited. For example, when nuclides ^{14}N and ^{14}C are added to the chain, the link corresponding to the fast neutron (n, p) transmutation between them is automatically created. However, the information on the same reaction induced by thermal neutrons is absent from the data file, so it is necessary to add it manually. For this purpose it is enough to add values of reaction cross-sections in thermal and resonance energies into the table. The latest program versions create this link automatically, as well as some other links for known (n, p) and (n, α) reactions.

'Conditions' tab is where the irradiation conditions are assigned: the initial material composition, required accuracy, and data to take thermal flux depression and resonance self-shielding into account. 'Times' page is for irradiation schedule parameters. 'Calc' page gives the interface to various solution methods for the system of ordinary differential equations (ODE) arising from the transmutation network. The ODE coefficients vary in time due to neutron flux changes and changes of nuclide concentrations, which alter depression and resonance self-shielding factors. It is well known that there is no single ODE system numerical solution method, which is "excellent" for any system of equations (see e.g. [2]). Users can apply four ODE solvers: VODE, LSODA, RADAU, and MEBDF [3-6]. VODE [3,4] uses variable-

coefficient Adams-Moulton and backward differentiation formulas (BDFs) methods in Nordsieck form. 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. LSODA (Livermore Solver for ODE Automatic, by Linda Petzold and Alan Hindmarsh) uses automatic method switching for stiff and non-stiff problems. It uses Adams methods in the non-stiff case, and BDF methods (the Gear methods) in the stiff case. The user does not have to determine whether the problem is stiff or not, and the solver will automatically choose the appropriate method. LSODA always starts with the non-stiff method. RADAU [5] uses implicit Runge-Kutta method of fifth order for problems of the form My'=f(x,y) with possibly singular matrix M; with dense output (collocation solution). MEBDF subroutine [6] uses modified extended BDFs of moderate to high order with better stability. Stability is not the only issue, however: the formulas also are computationally efficient. These subroutines were tested by means of a special utility program for linear transmutation chains having simple analytical solution [7]. Typical calculation time doesn't exceed one-two minutes. After calculations are finished, 'Answers' tab shows various characteristics obtained from calculated isotope densities: isotope masses, element masses, activities (α, β-, EC, IT, total), isotope specific activities per element gram, isotope parts, mass yields, depression coefficients, self-shielding factors, and fission energy deposition estimations for all time steps.

Since year 2000 *ORIP_XXI* freeware programs have been successfully used in Division of Radionuclide Sources and Preparations of State Scientific Centre of Russia - Research Institute of Atomic Reactors.

References

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