nucleonica

www.nucleonica.com

web driven nuclear science

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What is Nucleonica?

As a result of recent developments on issues such as energy security and sustainability, nuclear safety, security, and non-proliferation, and protection of the environment, we are witnessing a resurgence of interest in nuclear power and the nuclear sciences in general. The next generation of reactor energy systems aimed at addressing many of these issues – the so-called *Generation IV* systems – are expected to become available for commercial introduction in the period between 2015 and 2030 or beyond. There is also large range of "non-power" applications of radioisotopes and radiation in a variety of diverse fields such as medicine (e.g. cancer therapy), agriculture (e.g. pest population control), food irradiation (e.g. to increase shelf-life) and in industry (e.g. tracers, radiography, gauging, radiation processing, etc.), where such nuclear skills are also required. In order to support this renewed interest in the nuclear sciences, we will need a nuclear skills renaissance and it is within this context that the Nucleonica nuclear science web portal (www.nucleonica.com) has been developed. With its roots in the traditional paper-based Karlsruhe Nuclide Chart, Nucleonica has grown to become the leading online resource in the nuclear sciences. Nucleonica is particularly suitable for education and training of young scientists, engineers and technicians in the nuclear domain. A variety of our applications enable researchers and specialists to make complex and precise calculations in state-of-the-art fashion.

The Portal is already being used by thousands of scientists and students worldwide in over 92 countries. Due to its advanced IT features, user friendly and intuitive environment, the platform has recently been endorsed by the Sustainable Nuclear Energy Technology Platform (www.snetp.eu):

> "Nucleonica plays … an important role in making nuclear education more attractive and in building nuclear knowledge for a new generation of engineers and scientists"

The Nucleonica Nuclear Science Portal is an innovative professional and technical resource for knowledge creation and competence building in nuclear science for the worldwide nuclear community. Nucleonica provides a customisable, integrated environment and collaboration platform, using the latest internet "Web 2.0" dynamic technology. A unique feature of Nucleonica is its "electronic knowledge objects", which cover web-based scientific applications, an online wiki and blog as well as forums that enable collaborative research and scientific projects in a worldwide accessible online laboratory.

Who is Nucleonica aimed at?

Nucleonica is aimed at scientists, engineers and technical personnel working in the fields of nuclear power, health physics, radiation protection, nuclear and radiochemistry, decommissioning, nuclear medicine, etc. Nucleonica is particularly suitable for education and training of young scientists, engineers and technicians in the nuclear domain. It can also be used by professionals for everyday calculations, obtaining quick results in various fields of applications and testing, validating and verifying complex computer models.

Nucleonica also provides a range of consultancy services and industry co-operations. Examples of some recent studies include an analysis of the handling problems arising in the dismantling of radioactive sources, a decommissioning study of neutron sources, shielding analysis for a minor actinide laboratory, and a comparison of the radiotoxicities of wastes from fission, fusion, and coal fired power stations. Our clients include the Bundesamt für Strahlenschutz (BfS), Fichtner Engineering and Consulting, and Europol.

How can Nucleonica help you?

Nucleonica provides you with user friendly access to the latest reference data from internationally evaluated nuclear data. A unique feature is the wide range of web-based nuclear science applications for decay calculations, dosimetry & shielding, etc. A variety of social networking tools are provided for scientific collaboration.

In addition Nucleonica offers a range of introductory and advanced training courses in various areas of nuclear science. One of the main aims of these courses is to contribute to establishing a safety culture among the scientists and especially the younger scientists. This safety culture is a necessary prerequisite for a general acceptance of nuclear energy worldwide. Recent courses include: Illicit Trafficking and Radiological Consequences (ITRAC) with special focus on nuclear security; Nucleonica Training on Nuclear Science (NuTRONS) with special focus on environmental radioactivity; etc. Shorter courses on gamma spectrometry, nuclide charts, Karlsruhe Nuclide Chart, introduction to Nucleonica are also offered.

For more information on training courses see the Nucleonica wiki at http://www.nucleonica.com/wiki/

Nuclide Explorer
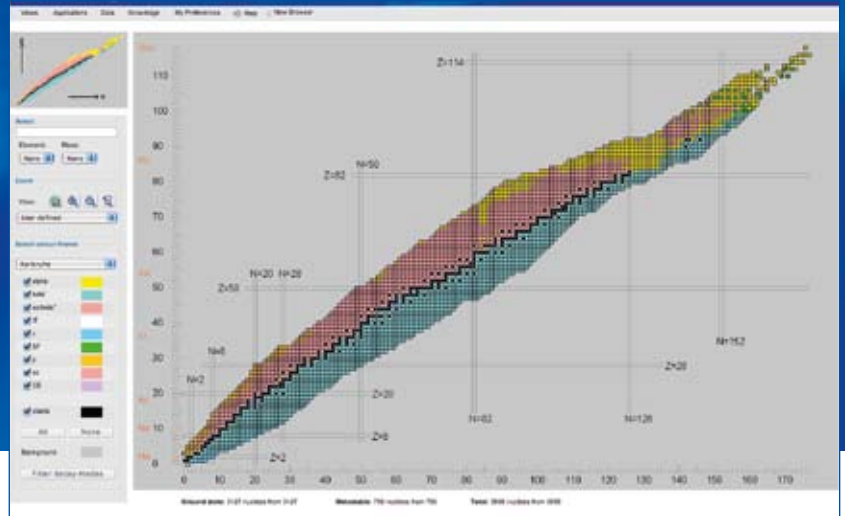
Nuclide Charts

Nuclide charts contain information on the basic nuclear properties of known atomic nuclei or nuclides – both stable and unstable. In these charts, the vertical and horizontal axes represent the number of protons and neutrons respectively in the nucleus. Stable isotopes (represented by the black boxes in the figure) lie within a relatively and almost diagonal narrow range. Radioactive nuclei (coloured boxes) mostly lie outside this range. At low atomic numbers, the neutron to proton ratio is unity. At higher atomic numbers, this value increases indicating a higher ratio of neutrons to protons in heavy atoms. The extremities of the coloured regions above and below the region of stability are known as the proton and neutron "driplines" beyond which nuclei are extremely unstable. As nucleons are successively added to a nucleus on the stability line, the binding energy of the last nucleon decreases steadily until it is no longer bound and the nucleus decays at the proton and neutron driplines.
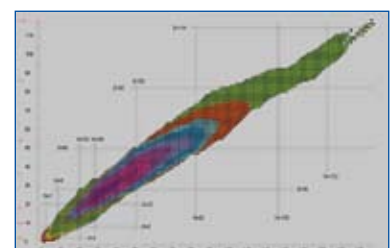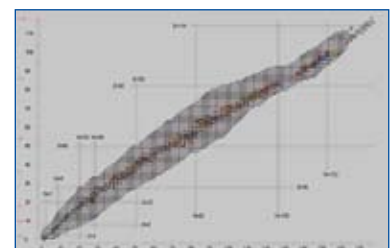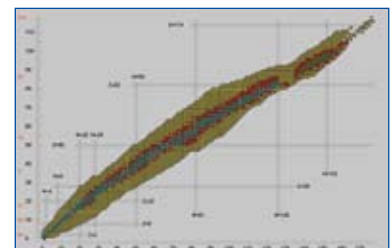
Nuclide Explorer

Nucleonica's Nuclide Explorer is a powerful online nuclide chart which allows the user to display internationally evaluated data based on decay modes, half-lives, binding energies, spin & parity etc. Navigational tools allow zooming to a region or nuclide of interest, highlighting of daughters, decay chain, etc. The chart can be used to search for rare decay modes (e.g. cluster emission, beta delayed particle emission, etc.). The Nuclide Explorer is of great didactic value in education and training. It is used in many training courses and in school and university courses.

Which data is used in the Nuclide Explorer?

The data used by the Nuclide Explorer is from the internationallly evaluated Joint Evaluated Fission and Fusion (JEFF3.1) radioactive decay datafile. Supplementary information has been taken from the NUBASE 2003 and for A≥266 from M. Gupta et al., (see also the Karlsruhe Nuclide Chart, 7th Edition). For a more detailed discussion see the Nucleonica Database wiki page. On right-clicking on a nuclide a context menu appears which offers direct access to nuclide specific information, such as the reference data, and applications.
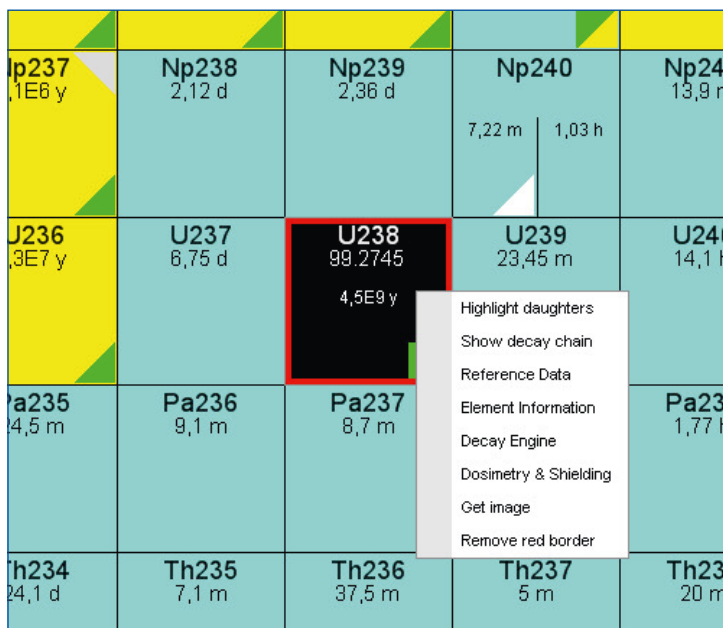
Decay Mode Filter

The nuclides shown in the chart have a single colour referring to the main decay mode. Nuclides – both ground states and metastable states – can have subsidiary decay modes in addition to a main mode. These subsidiary modes can be accessed through the *Filter decay mode* button. To see all nuclides which have a particular decay mode – either as main mode or as subsidiary mode – the user should use the frame *Filter decay mode*, select the mode or modes of interest and press the *Update* button. The results are shown in the nuclide chart.

Build your own nuclide chart

With the *Build your own nuclide chart* in the Nuclide Explorer, the user can create his/her own nuclide chart. By clicking on the coloured boxes adjacent to the modes of decay or the half-life range (see the left hand panel in the main interface overleaf), the user can introduce a new colour scheme based on the mode of decay, the half-life, binding energy, spin, parity, etc.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki

DataSheets

Nuclide DataSheets

The basic nuclear data in Nucleonica is contained within the DataSheets shown above. The active tab shows the Reference Data for the nuclide Co-60. Additional tabs provide access to *Description*, *Derived Data*, *Cross Sections*, *Radiations*, and *Prompt Gamma* radiation data. The *Reference Data* includes density, mass excess, atomic mass, half-life, spin, parity, abundance, binding energy, effective dose coefficients for inhalation and ingestion e(50), mean decay energies for alpha, electron and photon, types of decay, branching ratios, decay energy and daughter nuclides. The *Description* tab gives literature references for the basic data. This data originates from the JEFF3.1 nuclear datafile with some corrections.

Derived Data

Derived Data are obtained from the basic data and include the specific activity; the isotopic powers for α, $\alpha+\beta$, and $\alpha+\beta+\gamma$ (heat generation); specific gamma dose rate in air at 1m and gamma dose rate constant (gamma emission); spontaneous fission and neutron emission rates (neutron emission); annual limits of ingestion and inhalation (radiotoxicities) and derived air and water concentrations; the A1 and A2 activity and activity exemption limits for packaging and transportation.

Radiations

In the radioactive decay process, a variety of particles and/or photons can be emitted including alpha particles, electrons, gamma and X-ray photons. In the Radiations tab, a list of the energies and emission probabilities of the emitted particles/photons is given in both tabular and graphical forms. The underlying data is from the JEFF3.1 datafile or the 8th Table of Isotopes. In the *Prompt Gamma* tab, prompt gamma activation data for thermal neutron activation analysis is listed. Additional data include photon mass attenuation and mass energy absorption coefficients, and build-up factors to model the scattering effects in the shield material.

Cross Sections

Averaged thermal cross section data is based on JEF Report 14, *Table of Simple Integral Neutron Cross Section Data from JEF-2-2, ENDF/B-VI, JENDL-3.2, BROND-2, and CENDL-2*. The data include the averaged cross sections (2200 m/s, Maxwell average, resonance integral, 14 MeV, and fission spectrum average) for a range of important nuclear reactions including (n,gamma; n,fission; n,2n; n,3n; elastic; inelastic and total) and from a variety of databases. Point-wise, average (multi-group), and (x,xn) cross sections as a function of energy are shown in graphical form (where available).
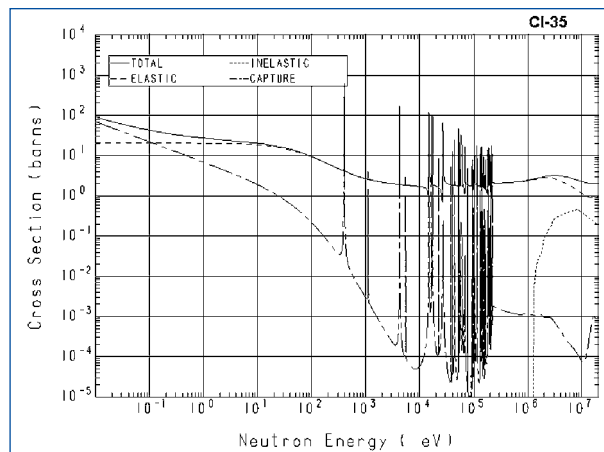
Physical Constants

The physical constants page contains basic physical constants such as masses of neutrons, protons, electrons, etc. The values of the constants provided are recommended for international use by CODATA and are the latest available and are generally recognized worldwide for use in all fields of science and technology.

Conversion Factors

Conversion Factors are given for mass, energy, energy dose, ion dose, time and activity. There is an additional tab for prefixes and the Greek alphabet.

Radiological Limits

Radiological Limits give radiation limits for workers, apprentices and students, and members of the public. The values given are recommended by international organisations such as Euratom, ICRP, and IAEA and the national German authorities. Dose limits given are for whole and partial body (eyes, hands, skin, etc.) exposure. For apprentices and students, data is given for ages less than 16 years, 16-18 years and over 18 years old.

More information can be found on www.nucleonica.com/wiki

Nuclear Data Retrieval

Nuclear Data Retrieval

Nuclear Data Retrieval

The Nuclear Data Retrieval pages in Nucleonica allow access to international evaluated nuclear data through searchable databases. The user interface is shown above. The various databases that can be searched are shown in the top set of tabs. These include the Nucleonica (JEFF3.1) database, EGAF prompt gamma database, ICRP database of effective dose coefficients, and the 8th Table of Isotopes database. Within each of these database categories, a number of further searches can be made covering nuclide search, radiation search and an advanced search.

Nuclide Search

In the example shown, the Nucleonica database is searched for nuclides of Co which have a half-life in the range 2 weeks – 100 years. In the results (see figure), four Co nuclides are listed that satisfy the criteria. In the Table Print Options, check box selection determines which additional information is shown in the results table.

Nuclides	Half-life
55 Cs 134	2.0651 (± 6) y
55 Cs 134	2.0651 (± 6) y
55 Cs 137	30.04 (± 3) y
55 Cs 137	30.04 (± 3) y

Dose Coefficients from the ICRP database

In another example (results shown), the ICRP Dose Coefficients database is searched for the effective dose coefficients of plutonium isotopes. The results are shown for both the inhalation and ingestion dose coefficients e(50) with units of Sv/Bq from both the ICRP (International Commission for Radiological Protection) databases, ICRP 68 and the more recent ICRP 72. The Evaluated Gamma-ray Activation File (EGAF), is a database containing prompt and delayed neutron capture γ-ray cross sections. EGAF contains thermal cross sections for approximately 35,000 prompt and delayed γ-rays from 262 isotopes. The 8th edition of the Table of Isotopes contains nuclear data for over 3,100 nuclide ground states and isomers. This data is mostly based on the ENSDF datafile.

Radiation Search

In the figure the results of a radiation search are shown. The search was performed for three gamma lines at 81, 303, and 356 keV with an uncertainty of 1 keV. The search returned two nuclides, Pa228 and Ba133. Since the emission probabilities of the protactinium nuclides are very small, the nuclide searched for is almost certainly Ba133 an isotope used in the nuclear medicine.

Fission Yields

Nuclear Fission

The discovery of fission by neutrons is credited to Hahn and Strassmann (1938), and to Meitner and Frisch (1939) for their explanation of the phenomena and introduction of the term nuclear fission. Spontaneous fission was discovered in 1940 by Petrzak and Flerov. Neutron induced fission follows the same process as the above described spontaneous fission. A neutron is absorbed by a heavy nucleus forming a compound nucleus which deforms and splits into two fast moving lighter nuclides, called fission products, and free neutrons. Fission is basically a binary process. Much less frequently (about once every few hundred events), fission can lead to the formation of a third light particle (ternary fission). Fission reactions differ according to the mass and nuclear charge of the fissioning system and, typically, more than 900 fission products are produced as a result of the fission process. The amount of a specific nuclide produced is generally expressed as fission yield.

Fission Fragments and Fission Products

The daughter nuclei showing up right at scission of a fissioning mother nucleus are called primary fission "fragments". In the large majority of the cases, the fragments will be sufficiently excited to evaporate neutrons in times less than 10^{-15} s. This means that the nuclei detected in experiments are not the primary fragments, but instead secondary fragments having lost a varying number of neutrons. The secondary fragments are called the fission products (i.e. fission fragments after prompt neutron evaporation).

Independent Fission Yield

The independent fission yield is the number of atoms of a specific nuclide produced directly (after emission of prompt neutrons but excluding radioactive decay) per 100 fission reactions.

Cumulative Fission Yield

The cumulative fission yield is the number of atoms of a specific nuclide produced directly and via decay of precursors per 100 fission reactions. If the nuclide is stable, the cumulative yield is the total number of atoms of that nuclide remaining per fission after the decay of all precursors (ignoring the effects of other nuclear reactions e.g. nuclear capture). Similarly, for a nuclide with a much longer half-life than any of its precursors, the cumulative yield is very nearly equal to the amount produced at a time short compared to its half-life but long compared to the half-life of its precursors. However, for a radioactive nuclide for which this is not the case, some atoms will have decayed before all have been produced. In such a case, the reported cumulative yield of atoms per fission will never actually be reached.

Chain Yield

The chain yield is the number of isobars of a specific mass, produced in 100 fission reactions. In other terms, the chain yield is equal to the sum of all stable or long-lived cumulative yields for a given mass chain. The cumulative yield of the last (stable or long-lived) chain member is generally identical to the chain yield. These chain yields apply to fission products after emission of prompt neutrons that takes place in a time of 10^{-14} s after scission.

Element: Mass:
U — 235

Select | Fission Yields

Library: JEFF-3.1
Type of Fission: Thermal fission
Total number of fission products: 24

	Nuclide	Half life	Independent Yield	Error	Cumulative Yield
Compare	55 Cs 138	33.41 (± 18) m	1.30E-03	4.72E-04	6.69E-02
Compare	55 Cs 135	2.3 (± 3) My	3.06E-06	1.06E-06	6.62E-02
Compare	55 Cs 133	Stable	1.67E-09	6.00E-10	6.60E-02
Compare	55 Cs 139	9.27 (± 5) m	1.19E-02	3.66E-03	6.31E-02
Compare	55 Cs 137	30.04 (± 3) y	7.22E-04	2.56E-04	6.22E-02
Compare	55 Cs 140	1.062 (± 5) m	2.11E-02	4.99E-03	5.02E-02
Compare	55 Cs 141	24.94 (± 6) s	3.27E-02	4.98E-03	4.84E-02
Compare	55 Cs 142	1.70 (± 2) s	2.40E-02	4.89E-03	2.92E-02
Compare	55 Cs 143	1.791 (± 7) s	1.57E-02	4.25E-03	1.65E-02
Compare	55 Cs 144	994 (± 4) ms	2.06E-03	7.35E-04	3.17E-03
Compare	55 Cs 144m	1.0 (± 0) s	2.06E-03	7.35E-04	2.06E-03
Compare	55 Cs 138m	2.91 (± 8) m	1.95E-03	6.70E-04	1.95E-03
Compare	55 Cs 145	594 (± 13) ms	8.98E-04	3.17E-04	9.02E-04
Compare	55 Cs 146	323 (± 6) ms	8.96E-05	3.12E-05	8.96E-05
Compare	55 Cs 136	13.03 (± 7) d	4.52E-05	1.57E-05	5.84E-05
Compare	55 Cs 136m	19 (± 2) s	2.65E-05	9.20E-06	2.65E-05
Compare	55 Cs 147	225 (± 5) ms	5.96E-06	2.12E-06	5.96E-06
Compare	55 Cs 135m	53 (± 2) m	1.87E-06	6.65E-07	1.87E-06
Compare	55 Cs 148	146 (± 6) ms	1.58E-07	5.94E-08	1.58E-07

Comparison of fissioning system | Libraries

Libraries

Cs-135 for U-235 Thermal fission

	JEFF-3.1	ENDF-BVI	JENDL-3.2
Independent Yield	5.29E-06	1.03E-06	7.61E-06
Error (I)	1.93E-06	6.59E-07	0.00E+00
Cumulative Yield	6.33E-02	6.60E-02	6.57E-02
Error (C)	1.84E-03	4.22E-02	0.00E+00
Y(A)	6.34E-02	6.63E-02	6.59E-02
Error (A)	1.20E-02	1.16E-02	0.00E+00

Download | ⦿ Excel ○ CSV Separator: Semicolon (";") ☑ Use field qualifier (")

Universal Nuclide Chart

Universal Nuclide Chart

Universal Nuclide Chart is a Java applet which simulates radioactive decay and reaction paths in nuclear reactors for over 3000 nuclides. The term "Universal" refers to the multi-purpose nature of the chart. There are two basic settings which can be made under the Options button on the taskbar (see above) – setting the language for the element name and the colour scheme (described below). The element names shown in the taskbar can be set to English, German, French, and Spanish. From the *File* button on the taskbar, six nuclides listed – Uub283, Fm251, Re185, Sn118, Mn55, and N15. Selection of one of these nuclides will allow fast navigation to the region of interest in the chart. In addition, the last six nuclides used are listed below the separator. This is useful for returning quickly to a nuclide previously selected. Five different **colour schemes** are available from the *Options* corresponding to the paper-based nuclide charts in use in various parts of the world (the default colour scheme is Karlsruhe):

- Karlsruhe: colours depend on the main mode of decay (alpha, β–, β+, IT, n, SF, p, ec, stable).
- Strasbourg: in which different colours are used for the decay processes.
- General Electric: colours depend on the half-lives of the nuclides (<1 day, 1 – 10 days, 10 – 100 days, etc.)
- JAERI: colours depend on half-lives under 10 min., 10 min. to 30 days, 30 days to 5×10^8 years and stable.
- ITU: Colours shows the main mode of decay similar to the Karlsruhe Colour Scheme.

A variety of **chart sizes** can be selected ranging from a 5 × 5 grid (showing maximum 25 nuclides) to a 15 × 15 grid (where up to 225 nuclides can be shown. The possibility of changing the **background colour** has been implemented. This is useful, for example, if the user needs to make a screenshot of the application with a specific background colour.

Nuclide Chart Viewer

It can be seen (see above) that the selected nuclide is highlighted with a red border. The basic decay and cross section data is also shown to the left of the nuclide chart. To view the basic data for other nuclides one need only place the mouse cursor over the nuclide of interest (without pressing the mouse button). The following data is given as far as available: half-life, decay modes, daughter products, branching ratios, abundances, two most important gamma lines and emission probabilities, thermal neutron cross sections, burnout-time. An explanation of the "burnout time" is given in the Nucleonica glossary (see www.nucleonica.com/wiki). For likely fission products, the chain yields of the isobar is given for the thermal fission of U233, U235 and Pu239.

Decay Chain Simulator

Two applications can be reached from the main chart window (shown overleaf): the Decay Chain Simulator (button Decay Chain) and the Neutron Reaction Path Simulator (button Reaction Path). The radioactive decay chain simulator window simulates radioactive decay chains for over 3000 nuclides in two different arrangements (normal and compact plots) and with five different standard colour schemes. The *Selected Nuclide* – in this case U238 – is shown in the box in the top left hand side of the window. The decay chain for this nuclide is shown in the main frame of the window. The decay process is simulated on a Z vs. N nuclide chart, labeled Normal Plot in the taskbar, with the Z and N

axes shown. Alternatively, a more compact description of the decay process based on a plot of A – 2Z vs. Z, can be selected through Compact Plot. Nuclides with high gamma activity are indicated in the Decay Chain Simulator through "blinking". The field E(MeV) shows the threshold gamma energy per disintegration in MeV to initiate "blinking". This can be changed also while the simulation is running. As decimal separator, a point (.) must be used. The default value is 0.5 MeV.

Neutron Reaction Path Simulator

This application indicates the main neutron reactions likely to occur with the selected nuclide in a nuclear reactor with a thermal neutron spectrum, i.e. in most light water reactors (LWRs). The neutron reactions occurring are based on the cross sections, the burnout time and the half-life of the selected nuclide. The *Selected Nuclide*, in this case Th232 selected from the Nuclide Chart Viewer, is shown in the box in the top left hand side of the window. The neutron reaction path for this nuclide is shown in the main frame of the window. The neutron flux can be set in the taskbar. The default value of the neutron flux is 3×10^{14} neutrons cm^{-2} s^{-1} typical of light water reactors. Here the

user can "see" the activation or transmutation process in "slow motion" by changing the time interval in which the products are painted onto the screen. The value is given in milliseconds with a default value of 500 ms. By increasing the time interval to 1500, for example, the transmutation will be painted at one third of the default speed onto the screen.

Example

Depending on the neutron flux, there can be a competition between decay and burnout processes. Consider the case of Th232 in a thermal neutron flux. With a half-life of 1.4×10^{10} y and a burnout time of 9.9 y, the nuclide will transmute to Th233. This nuclide has a half-life (22 m) shorter than the burnout time (18 d) and will decay to Pa233. This protactinium isotope has a half-life of 27 d and a burnout time of 1.8 y. It will therefore decay preferentially to the fissile isotope U233. This uranium isotope is highly desirable in a thermal reactor since it fissions to produce energy. If however the flux in the reactor increases, the burnout time decreases. This implies that more Pa234 (which decays to U234) is produced at the expense of U233. This can be demonstrated by setting the flux to a very high value of 5×10^{15} neutrons cm^{-2} s^{-1}. More quantitative evaluations of the decay and activation processes in nuclear reactors can be obtained with the webKORIGEN module in Nucleonica.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki

Karlsruhe
Nuclide Chart

Karlsruhe Nuclide Chart

For almost 50 years, the Karlsruhe Nuclide Chart has provided scientists and students with structured, accurate information on the half-lives and decay modes of radionuclides, as well as the energies of emitted radiation. Beyond the more traditional physical sciences such as health physics and radiation protection, reactor physics, nuclear and radiochemistry, and astrophysics, the Chart is now in wide and common usage in the life and earth sciences (biology, medicine, agriculture, geology, etc.). An important characteristic of the Chart is its great didactic value for education and training in the nuclear sciences. It has been used in training programmes worldwide and is a valuable and welcome addition to many books on nuclear science including school physics textbooks. The paper-based Karlsruhe Nuclide Chart, with its fold-out and wall chart versions, remains an aesthetically appealing record of human achievement in nuclear science. It provides a unique overview of current knowledge and is for many the preferred medium for ease of use, convenience and practicality.

The 7th edition (2006) of the "Karlsruher Nuklidkarte" contains new and updated radioactive decay data on 612 nuclides not found in the previous (1998) edition. In total, nuclear data on more than 2950 experimentally observed nuclides and 690 isomers is presented. Most recent values of the atomic weights, isotopic abundances and cross sections are included together with the thermal fission yields for both ^{235}U and ^{239}Pu. The accompanying booklet has been considerably revised to include a history and overview of nuclear science. The multi-lingual "Explanation of the Chart of the Nuclides" has been extended from the original four languages (English, German, French, Spanish) and now includes Chinese and Russian.

The Karlsruhe Chart of the Nuclides is available as both a 44 page brochure with 20 page fold-out nuclide chart and as a wall-chart (1.00 x 1.40 m). More information can be found on the Nucleonica wiki at www.KarlsruheNuclideChart.net

Karlsruhe Nuclide "Carpet" for International Year of Astronomy

The Karlsruhe Nuclide "Carpet" (approximate dimensions 1.3 x 8 m) was displayed at the International Year of Astronomy 2009 exhibition in Paris. The chart (shown), was presented to the public in an exhibition dedicated to astrophysics and nucleo-synthesis in the stars – 2009 being the International Year of Astronomy. It was exactly 400 hundred years ago in 1609 that Galileo first pointed his telescope to the skies. 2009 was also the anniversary of the publication of Kepler's "Astronomia Nova" in which he corrected Copernicus's description of the solar system and the motion of the planets. In contrast to previous versions, this new chart is in the form of a "carpet". This "floor chart" was designed to be especially durable to resist wear and tear due to exhibition crowds walking over it. The dimensions of the floor chart are such that the nuclide information can be read easily.

50th Anniversary of the "Karlsruher Nuklidkarte"

This commemorative publication, to mark the 50th Anniversary of the "Karlsruher Nuklidkarte", provides a broad, state of the art overview of scientific research in the nuclear sciences. In total there are 30 scientific articles written by experts in their various fields together with the historical Nobel lectures by Becquerel and Soddy.

New Editions of the Karlsruhe Nuclide Chart

The 8th edition of the Karlsruhe Nuclide Chart, together with a new online version, is currently under development. The online version will contain many additional features such as web-based energy level diagrams and nuclide references.

More information can be found on the Nucleonica wiki at
www.nucleonica.com/wiki
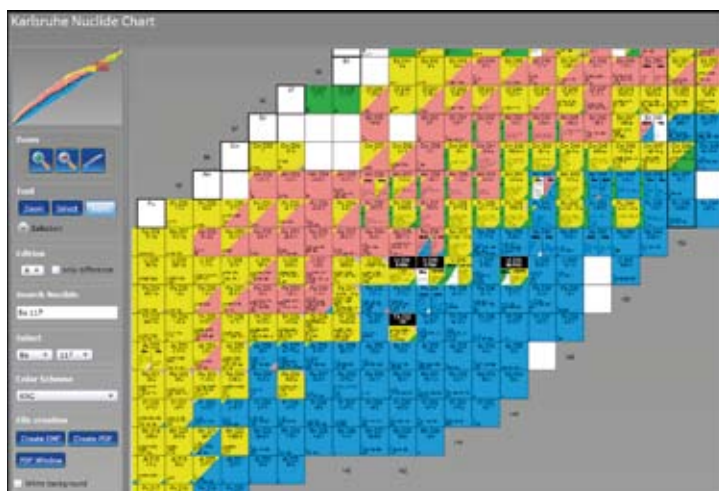
Mass Activity Calculator
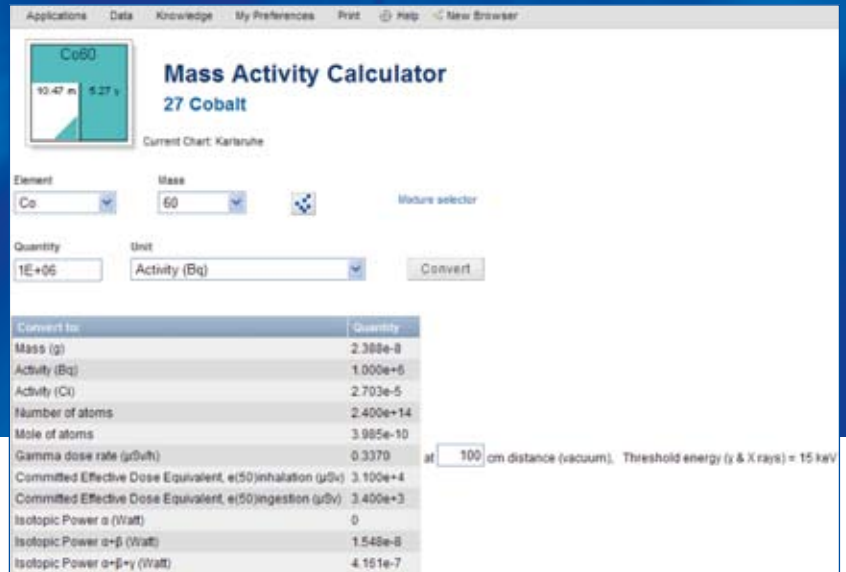
Nucleonica's Mass Activity Calculator

The mass activity calculator is a popular tool for conversion between different physical quantities (e.g. mass, activity, number of atoms, etc.). A particularly useful feature is that in addition to single nuclide, the mass activity calculator can also be applied to nuclide mixtures. These nuclide mixtures can be created with the Nuclide Mixtures module. The *Convert to* box shows the full list of quantities. In addition to the standard list (mass, activities, etc.), conversions can also be made using:

- external and internal dosimetry quantities such as the gamma dose rate (where the distance is required)
- the committed effective doses for inhalation and ingestion.
- the amount of heat generated – isotopic power – through radioactive decay for α, $\alpha+\beta$, and $\alpha+\beta+\gamma$.

In the above example, the nuclide Co-60 is selected. A different nuclide can be selected from the element and mass drop-down menus. The default source strength is 1 MBq. In the *unit* drop-down menu, the source strength is shown in becquerel (Bq), curie (Ci), number of atoms, etc. The user can also select a previously defined nuclide mixture (by clicking on the *Mixture selector*). Further information is given in the Nucleonica wiki.

Nuclide Mixtures

The mass activity calculator can also be used for nuclide mixtures. In the top diagram, the nuclide mixture "natural uranium" has been selected. This mixture has been previously created in the Nuclide Mixtures module for 1 mole (of atoms) of natural uranium containing 0.9927 mole U238, 7.114×10^{-3} mole U235 and 5.310×10^{-5} mole U234.

As can be seen, even 1 mole of atoms of natural uranium, with a mass of 238 gram and activity of almost 6 MBq (without daughters), has a negligible gamma dose rate and heat emission rate (isotopic power).

In the bottom diagram, a nuclide mixture containing 1 g (4.172×10^{-3} mole) of actinides in spent fuel has been selected. Again this mixture was previously created in the Nuclide Mixtures module. Here it can be seen that 1 g of the transuranics, has a substantial activity (11 Ci or 4.25×10^{11} Bq) gamma dose rate (21 μSv/h at 1 m).

Mass Activity Calculator
Natural Uranium

Mixture
| Natural Uranium | Nuclide selector |

Quantity | Unit
| 1 | Mole of atoms | Convert |

Convert to:	Quantity
Mass (g)	238.0
Activity (Bq)	5.981e+6
Activity (Ci)	1.617e-4
Number of atoms	6.022e+23
Mole of atoms	1.000
Gamma dose rate (µSv/h)	2.922e-3
Committed Effective Dose Equivalent, e(50)inhalation (µSv)	5.199e+7
Committed Effective Dose Equivalent, e(50)ingestion (µSv)	2.811e+5
Isotopic Power α (Watt)	4.356e-6
Isotopic Power α+β (Watt)	4.368e-6
Isotopic Power α+β+γ (Watt)	4.373e-6

at [100] cm distance (vacuum). Threshold energy (γ & X rays) = 15 keV

Mass Activity Calculator
Transuranics in 1 ton Spent Fuel

Mixture
| Transuranics in 1 ton Spent Fuel | Nuclide selector |

Quantity | Unit
| 1 | Mass (g) | Convert |

Convert to:	Quantity
Mass (g)	1.000
Activity (Bq)	4.247e+11
Activity (Ci)	11.48
Number of atoms	2.513e+21
Mole of atoms	4.172e-3
Gamma dose rate (µSv/h)	21.12
Committed Effective Dose Equivalent, e(50)inhalation (µSv)	4.285e+12
Committed Effective Dose Equivalent, e(50)ingestion (µSv)	8.960e+9
Isotopic Power α (Watt)	0.03413
Isotopic Power α+β (Watt)	0.03454
Isotopic Power α+β+γ (Watt)	0.03457

at [100] cm distance (vacuum). Threshold energy (γ & X rays) = 15 keV

Decay Engine
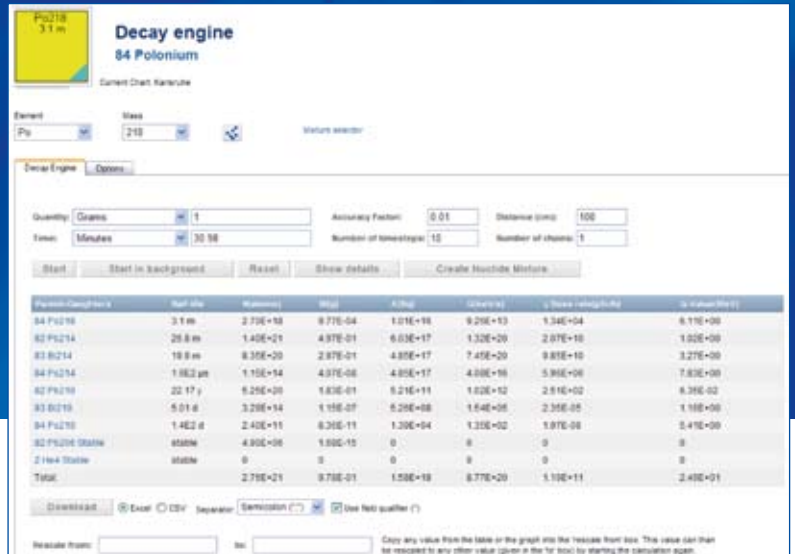
Simple Radioactive Decay

Radioactive decay is a random process where it is not possible to predict when a particular nucleus in a sample will decay. The basic relation governing radioactive decay, first identified by Rutherford, is given in the margin, where the left hand side gives the rate of decay of the atoms in terms of the number of atoms N(t) and a decay "constant" k which is the probability per unit time that a nucleus will decay. The minus sign indicates that N is decreasing with time. One can, however, evaluate the probability that a nucleus will decay in a time interval. The basic relation can be easily integrated to give the number atoms at time t. From this, various useful quantities such as half-life, mean-life, activity, etc. or can be derived.

$$\frac{dN(t)}{dt} = -kN(t)$$

Radioactive Decay Chains

It is very often the case that the daughter product of a nuclear decay is also radioactive. In such cases one speaks of radioactive decay "chains". As an example, consider the decay chain $N_1 \rightarrow N_2 \rightarrow N_3 \rightarrow \ldots$ in which the starting or "parent" nuclide N_1 decays to the "daughter" N_2. This daughter in turn is radioactive and decays to N_3. More generally each nuclide in the decay chain can "branch" to more than one daughter. This general process of radioactive decay was first investigated systematically by Bateman in 1910.
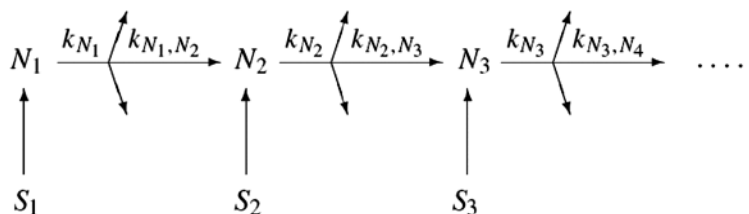
Nucleonica's Decay Engine

Nucleonica's Decay Engine is a very powerful tool for investigating the radioactive decay of nuclides and nuclide mixtures. It based on the exact mathematical solution to the Bateman equations. The user interface is shown overleaf. The first step is to select a particular nuclide, its activity, mass etc.

Number of time-steps

This input box is used to set the number of intermediate times at which the decay is evaluated. The default number of time-steps is 10, such that a graph can be drawn. The maximum number of time-steps is 40.

Accuracy Factor

This input box is used to set the accuracy of the calculation. The Accuracy Factor sets the minimum product of branching ratios which are accounted for in the calculation. To evaluate all possible paths, the Accuracy Factor should be set to zero. The number of pathways or "Chains" accounted for in the calculation is given in the *Number of Chains* box. A good compromise between accuracy and speed of the calculation can be obtained with an accuracy factor of 10^{-2}. For calculations involving many "chains", the calculation may be run in the background (*Start in Background*). In this case the job will be placed in a queue. When the web-server is not so busy, the decay calculation will be run and the results posted to the user through an alert.
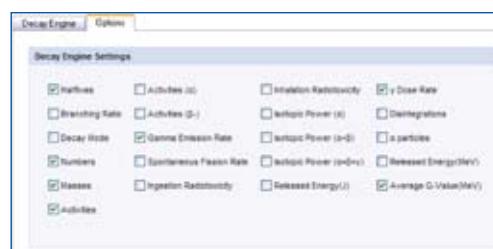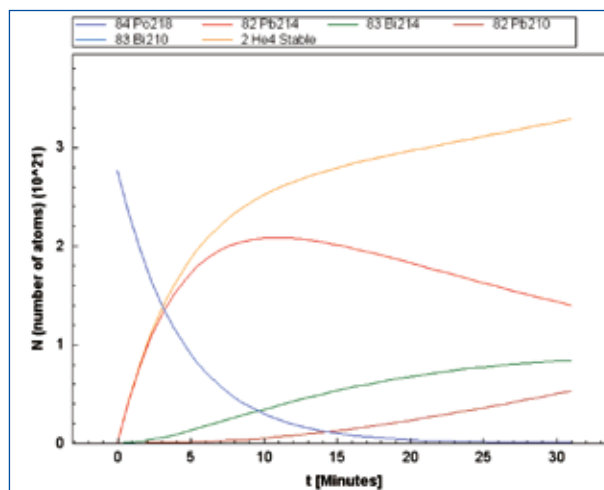
Results

On pressing the *Start* button the results are shown in both tabular and graphical form. In addition to calculating the amounts of parents and daughters, various additional quantities such as the number of disintegrations, the He production (from alpha particles), isotopic powers, radiotoxicities for ingestion and inhalation, gamma dose rate etc. are calculated. The choice of which properties to show can be set in the *Options* tab. The Reset button can be used to clear the input data used in the calculation.
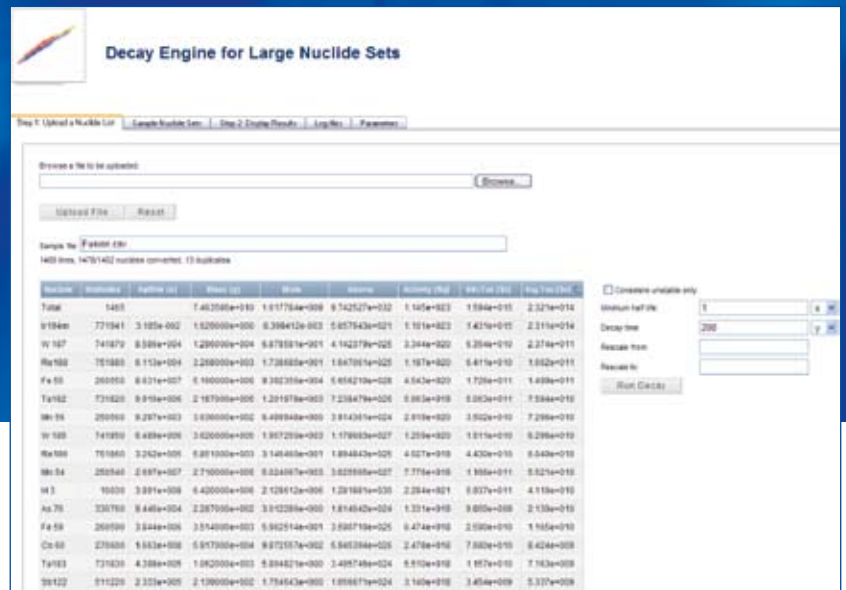
Rescaling

The rescaling feature allows the user to very simply rescale the input quantities to any other values.
Full details can be found in the Nucleonica wiki at http://www.nucleonica.com/wiki

Decay Engine for Large Nuclide Sets

Decay Engine
for Large
Nuclide Sets

Decay Engine for Large Nuclide Sets

There are a number of situations in which it is required to perform decay calculations for large numbers (typically many hundreds to thousands) of nuclides. In fission reactors, for example, more than one thousand nuclides can be present resulting from the irradiation process (a typical calculation using webKORIGEN produces more than 800 nuclides – although many of these are short lived). Similarly, fusion reactors can produce more than one thousand radio-nuclides due to neutron activation processes in the reactor walls. In the example shown (above) a fusion file containing 1478 nuclides has been uploaded into the application. The grid has been arranged such that nuclides with the highest ingestion radiotoxicity are at the top.

In principle such situations can be addressed by defining a nuclide mixture and decaying this mixture using the Decay Engine. However, there are problems associated with this approach. First of all, to create a nuclide mixture containing more than 50 nuclides is quite a tedious operation. Secondly, depending on the number of nuclides, the Decay Engine can take a considerable amount of time to obtain the solution. This latter problem can be partially resolved by running the decay calculation in the background (see Decay Engine). Nevertheless, this is not the optimum approach. Decay Engine calculations using nuclide mixtures should be restricted to nuclide mixtures with less 20 – 30 components.

In the case where the number of nuclides is significantly greater, an alternative approach is required which is fast (with running times of a few seconds) and accurate. The solution to such problems in Nucleonica is to use the Decay Engine for Large Nuclide Sets module. The underlying calculations engine used here is based on the decay routines in webKORIGEN which can be applied to many hundreds of nuclides and have running times are around a few seconds.

Example: Radiotoxicity Reduction in Different P&T Strategies

By removing the hazardous actinides from spent nuclear fuel (by partitioning), the radiotoxicity of the waste can be significantly reduced, especially in the long term. These effects can be studied by using the web-KORIGEN module in Nucleonica using different partitioning ratios. Following the reactor irradiation, cool-ing, reprocessing and decay, there are still many hundreds of nuclides present in the waste. These output nuclides are stored automatically as a sample nuclide mixture for the *Decay Engine for Large Nuclide Sets* module. The various mixtures can then be decayed over long time periods to investigate the effects of partitioning on the long-term radiotoxicity. A summary of the results is shown.

To investigate the effects of different P&T strategies on the radiotoxicity reduction, three cases have been considered in this study, as well as the open cycle. The resulting radiotoxicity curves (shown) have a crossover point indicating the time at which the radiotoxicity of the waste reaches the reference level. The following observations can be made:
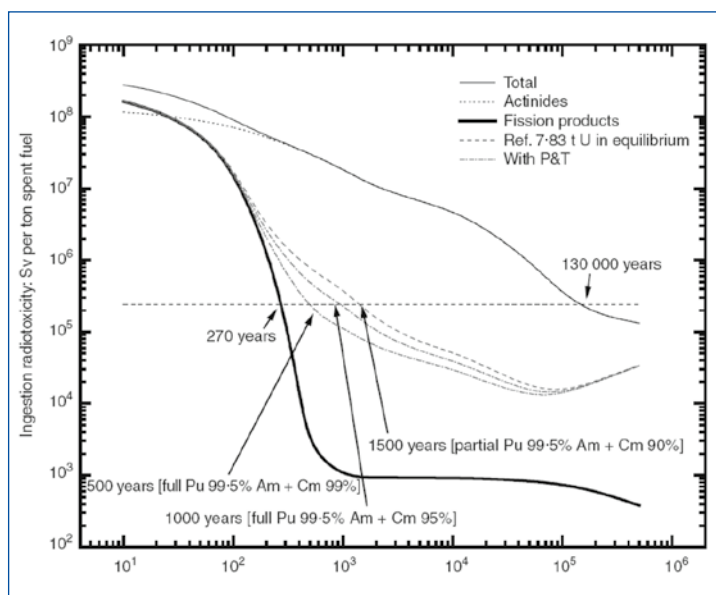
- The open cycle: the spent fuel is directly sent to long-term storage with no P&T. It takes 130000 years before the radiotoxicity reaches the reference level.

- The full multi-recycling of Pu as well as Am and Cm with high overall efficiency of P&T processes (99.5% for Pu and 99% for Am and Cm). The crossover point is 500 years. If the Cm is left in the waste, this time is extended to 1000 years.

- The full multi-recycling of Pu as well as Am and Cm with less overall efficiency of P&T processes (99.5% for Pu and 95% for Am and Cm). The crossover point is 1000 years.

- The partial multi-recycling: multi-recycling of the Pu (99.5% of P&T efficiency), and one single recycling of the Am and Cm. In this case the Am and Cm are transmuted in targets in a fast reactor, and then 90% of P&T overall efficiency is foreseen. Thus the crossover point is around 1500 years. In this strategy, we can also consider leaving the Cm in the waste, and then 3000 years are required.

Based on these results it can be concluded that partitioning of nuclear waste can help reduce the radiotoxicity of the spent fuel by more than two orders of magnitude after 500 to 1500 years. The fission products radiotoxicity curve gives the theoretical limit to the total radiotoxicity reduction in the case that all the actinides are partitioned and transmuted – that is, no losses. This time is about 270 years to reach the same order of magnitude in the radiotoxicity reduction.

More information can be obtained from the Nucleonica wiki at www.nucleonica.com/wiki

Gamma Dosimetry and Shielding
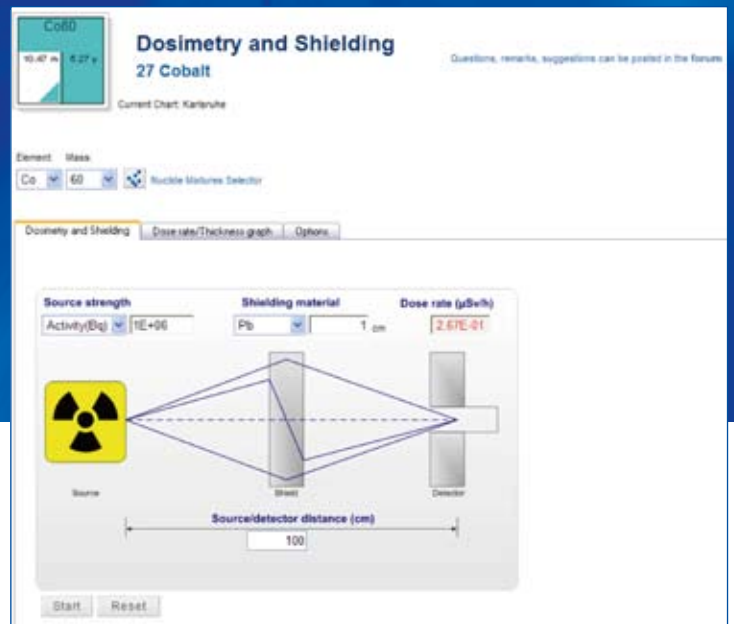
Nucleonica's Gamma Dosimetry & Shielding

One of the first modules developed within the Nucleonica portal was for dosimetry and shielding calculations for radioactive point sources and nuclide mixtures using the point source kernel method. The formalism is described in detail in the Nucleonica wiki. The module allows the user to calculate gamma dose rates from point sources of either single nuclides or composite mixtures. More than 1300 gamma and X-ray emitting nuclides with more than 53,000 gamma and X-rays are available in the Nucleonica database, together with a choice of ten different shield materials. The intuitive interface is ideal for quick and accurate dose calculations such as in health physics or to test more sophisticated Monte Carlo codes. It is ideal for workers in the lab to obtain a rough indication of the dose rate from the radioactive materials they are working with – only a web browser and internet connection required.

Modes of operation

There are three modes of operation:

1. Gamma dose rate for a given source and shield;
2. Shield thickness for a given dose rate;
3. Source strength for given shield and dose rate.

User Interface

The main interface, shown overleaf, allows the users to select the nuclide, the source strength, the source/detector distance, the shield material and shield material thickness. In the example shown, Co-60 ground state has been selected using the drop down menus. The source strength can be set in different units, namely Activity (Bq), Activity (Ci), Mass (g) or number of atoms. The default value shown is 1 MBq. In addition, the user has the choice of 10 shield materials. The calculation is initiated by clicking in the *Start* button. The detailed results are shown in tabular form and include the half value layer (HVL) and the tenth value layer (TVL) thicknesses required to reduce the gamma dose rate to 50% and 10% respectively of the initial value, and the specific gamma dose rate constant for the given nuclide. This information is followed by the number of gamma and X-ray energies together with the quantity $\Sigma_i E_i \cdot P_i$ which is the sum of the energies multiplied by their emission probabilities. In the table, the results include the contribution of each gamma-line or X-ray to the total dose rate, the mass absorption coefficients for tissue, the build-up factors, and the mass attenuation coefficients for the shield material. Clicking on the column header "Gamma Dose Rate (μSv/h)" re-arranges the table to show the main contributions to the gamma dose rate. In the case of Co-60 this is from the 1.33 and 1.17 MeV gamma lines.

Half-Value Shield Thickness(cm)	2.02E+00
Tenth-Value Shield Thickness(cm)	5.03E+00
Equivalent Dose Rate Constant Γ(mSv m²/GBq/h)	3.37E-01
Gamma Dose Rate (μSv/h)	**2.67E-01**
Effective Build-up factor	1.55E+00
Effective Number of Mean Free Paths (μ d)	6.70E-01

Number of lines (γ):	6	ΣE.P.(γ):	2.50E+06
Number of lines (X):	4	ΣE.P.(X):	8.35E-01
Number of lines (γ+X):	10	ΣE.P. (total):	2.50E+06

Nuclide	Gamma Energy (keV)	Emission Probability P (per disintegration)	Mass Attenuation Coefficient (shielding)(cm²/g)	Number of Mean Free Paths (μ·d)	Build-up Factor	Mass Absorption Coefficient (tissue)(cm²/g)	Gamma Dose Rate(μSv/h)
27 Co 60	1.33E+03	1.00E+00	5.64E-02	6.40E-01	1.53E+00	2.89E-02	1.43E-01
27 Co 60	1.17E+03	9.99E-01	6.20E-02	7.04E-01	1.57E+00	2.98E-02	1.25E-01
27 Co 60	8.26E+02	7.60E-05	8.50E-02	9.75E-01	1.60E+00	3.16E-02	5.83E-06
27 Co 60	3.47E+02	7.50E-05	3.05E-01	3.46E+00	1.80E+00	3.21E-02	2.18E-07
27 Co 60	7.48E+00	6.44E-05	2.71E+02	3.07E+03	1	1.22E+01	0
27 Co 60	7.46E+00	3.27E-05	2.72E+02	3.09E+03	1	1.23E+01	0
27 Co 60	8.26E+00	1.31E-05	2.11E+02	2.40E+03	1	9.01E+00	0
27 Co 60	2.16E+03	1.20E-05	4.54E-02	5.15E-01	1.49E+00	2.52E-02	2.86E-06
27 Co 60	8.50E-01	1.49E-06	7.16E+03	8.12E+04	1	5.38E+03	0
27 Co 60	2.51E+03	2.00E-06	4.39E-02	4.99E-01	1.48E+00	2.40E-02	4.97E-09

27 Co 60 spectrum: Gamma and X-rays
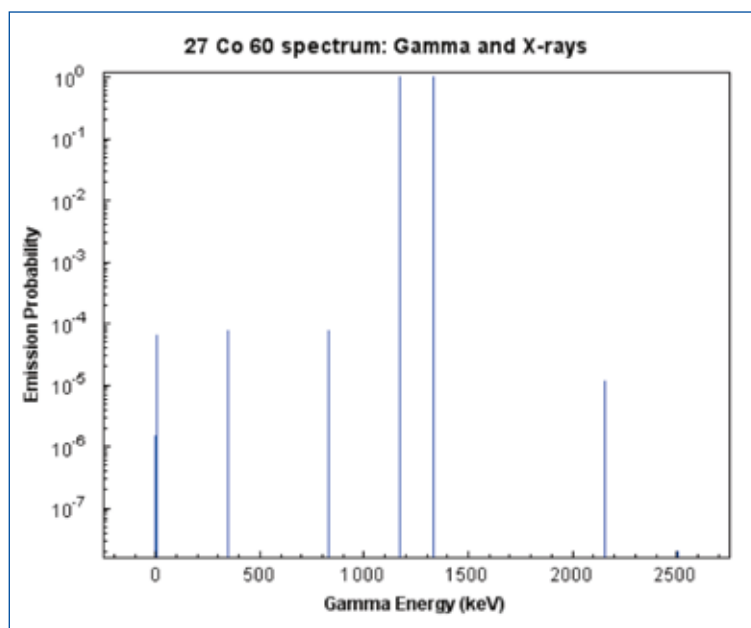
Range and Stopping Power
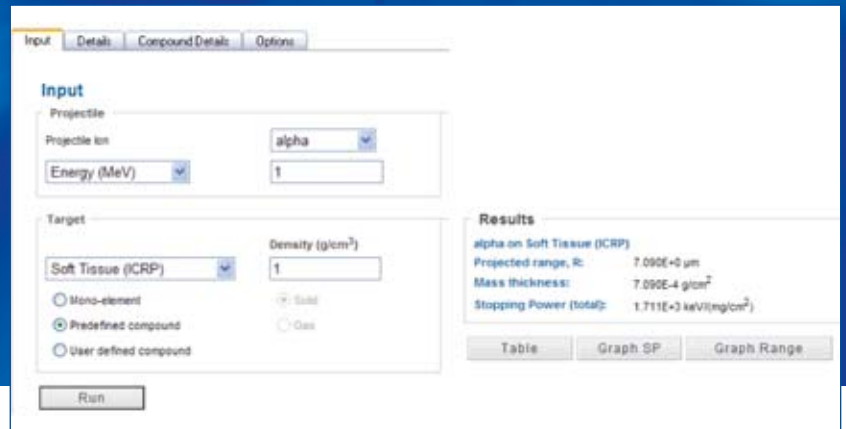
Stopping Power

In the interaction between charged particles and matter, the stopping power or the average energy loss per unit path length plays an important role in many fields such as impurity atom implantation in producing semiconductor devices, structure analysis of solid target by Rutherford backscattering spectroscopy (RBS), and plasma-first wall interactions in nuclear-fusion reactors. Stopping power can be considered in two parts: first is the interaction of incident particle with target electrons (called electronic stopping power), and second is the interaction with target nuclei (called nuclear stopping power).

Range

Another important quantity is the range of the charged particle in matter. The range is defined as the mean path length of particle in target matter before coming to rest. Generally, analytic transport theory and Monte Carlo calculations are used for the range calculations.

In Nucleonica, the Range & Stopping Power module provides a user-friendly interface for quick and accurate calculations on the range and stopping powers of charged particles – electrons, positrons, protons, alphas, muons and heavy ions – in matter. Target materials include the natural elements, pre-defined (e.g. tissue) and user-defined compounds. In addition, the user can also select the energy and stopping power units, etc. Range and stopping power results can be displayed in high quality graphs. The underlying calculation engine for stopping power and ranges on heavy ions is based on SRIM (Stopping and Range of Ions in Matter). For electrons, muons, and positrons, a new formulation, based on the work of *Gümüs et al.* for collisional stopping power, has been used. For radiative stopping power the standard ratio is used. Overall agreement is quite good especially for collisional stopping power and CSDA Range. On the other hand, for radiative stopping power agreement is better than 10%.

The user interface is shown overleaf. The first step is to select a **projectile** and specify the particle energy. In addition to protons, alpha particles and other heavy ions (Z=1 – 92), light ions (electrons, positrons, muons) can also be selected.

In a second step, the **target** needs to be defined. Here the user can select an element from Z=1 – 92, or a pre-defined compound. In addition the user can create own compounds.

In contrast to electromagnetic radiation (χ- and γ-rays), which exhibit an exponential decrease of intensity with penetration depth, heavy charged particles such as protons or heavy ions have a well defined range in matter (see diagram). The energy deposition of heavy ions is characterized by a low entrance dose and a pronounced sharp maximum near the end of range (Bragg peak). In nuclear medicine, for example, this characteristic allows treatment of the organs affected while sparing the healthy tissue.

The accuracy of the results is better than 5% for protons alphas, and heavy ions, 10% for electrons and positrons, and less than 7% for muons for the total stopping powers and the CSDA Ranges.

Full details are given in the Range and Stopping Power wiki page in Nucleonica at http://www.nucleonica.com/wiki/

Stopping Power for C-12 s on Soft Tissue (ICRP)

Bragg diagram for C-12 on Soft Tissue (ICRP) (2000 MeV)
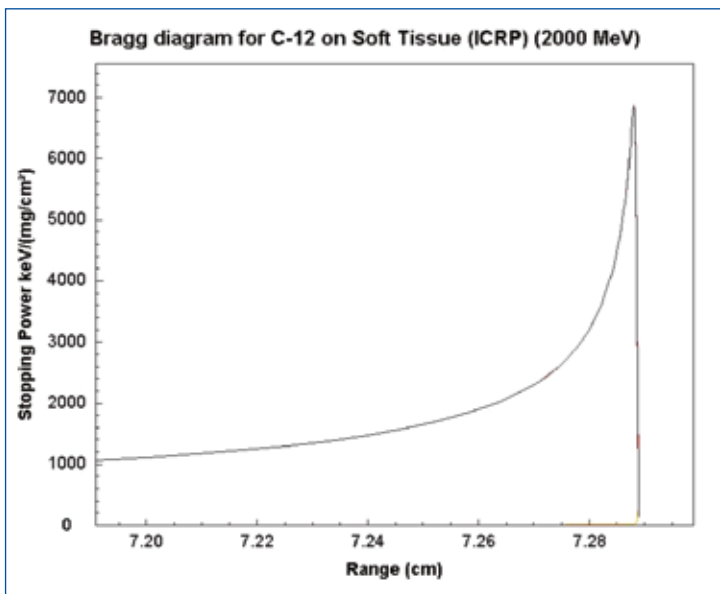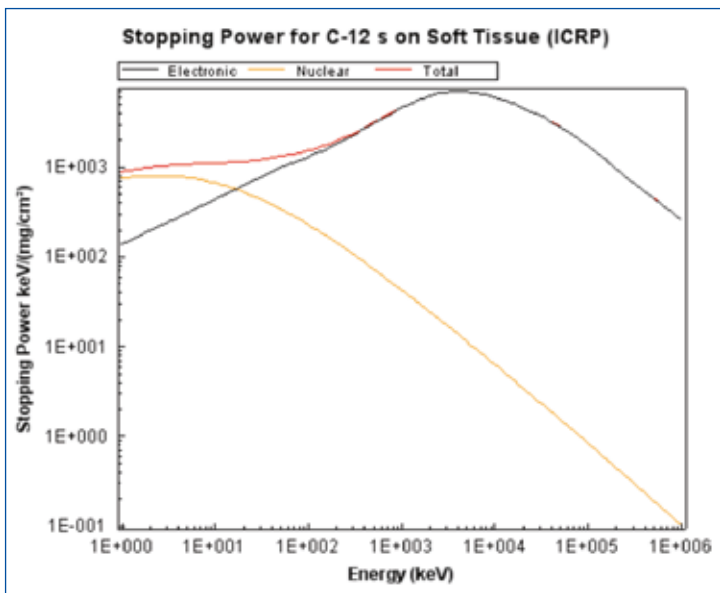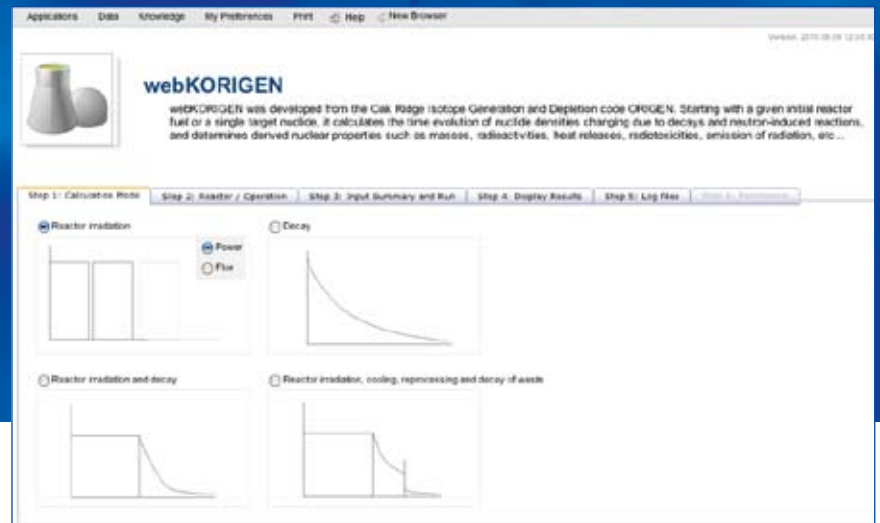
KORIGEN

KORIGEN originates from the ORNL computer code ORIGEN, and is used to determine characteristics of spent nuclear fuel, such as nuclide masses, radioactivities, decay heat, radiotoxicities, radiation sources etc. Optionally, it calculates fission products from spontaneous fission and the emission of neutrons from vitrified waste, taking account of (α,n)-reactions of light nuclides in glass constituents.

Nucleonica's webKORIGEN

Nucleonica's webKORIGEN is a very user-friendly and intuitive web-based version of KORIGEN which has been trimmed to three major classes of nuclear plants: Pressurized Water Reactors (PWR), Boiling Water Reactors (BWR), and the European Fast Reactor (EFR). Sub-critical systems can be analysed in the neutron activation mode.

Modes of Operation

There are basically four modes of operation (see figure):

- **1a:** **Reactor Irradiation** (constant power) of fresh nuclear fuel
- **1b:** **Reactor Irradiation** (constant flux) allows **Neutron Activation** of targets in PWR, BWR, Fast Reactor and Thermal Neutron spectra.
- **2:** **Decay** of single nuclides
- **3:** **Reactor Irradiation** (Mode 1) with subsequent period of decay storage
- **4:** **Reactor Irradiation** and Cooling with subsequent **reprocessing** and waste storage

Types of Fuel/Targets

Current fuel options are centered on UOX (uranium oxide) and MOX (mixed oxide fuels containing UO_2 and PuO_2). For UOX fuel the initial enrichment is specified, whereas for MOX the plutonium composition and the weight fraction of [241]Am/Pu is required together with the fissile plutonium in the initial heavy metal. Target **irradiations** are restricted to small samples of a single-nuclide material in the irradiation facility. In this way the neutron spectrum in the target is dominated by the reactor facility spectrum.

Results

A typical set of results is shown in the grids (see inset). Irradiation of UO_2 fuel (4% enriched) in a PWR for 4.8 years results in a total 833 nuclides from 64 elements (third panel). Graphical output can be obtained by clicking the appropriate buttons at the bottom of the window (Plot k_∞, Nuclides, Elements, Totals, Elemental Distribution). The items which have a tick in the check boxes are those which will be plotted in the graphs.

Filter

The output filter is a powerful tool for selecting which quantities are to be plotted. By the appropriate selection, entire groups or single nuclides can be selected. There are two modes of operation. First the chemical element, e.g. Pu, or the nuclide name La139 can be typed into the filter box. On clicking the Filter button, the results for this chemical element, i.e. the individual nuclides, are shown. The second mode of filtering is to make use of the check boxes shown. This is explained in the following example.

Example

Following irradiation of uranium fuel in a PWR and 30 years cooling (Mode 3), one is interested in the amounts of C137 and Sr90 produced. Since both these quantities are fission products, the fission products box is checked in the third panel in the output grid. Thereafter, the user clicks on the Filter button. In the central gird panel, the chemical elements of all fission products are listed. Since the fission products of the elements Cs and Sr are of interest, these boxes should now be checked and then clicking on the Filter button to activate the filter process. It can now be seen that the first grid panel contains all isotopes of Cs and Sr. It is now straightforward to check both Cs137 and Sr90 and then press the Plot Nuclides button. The activities of both Cs137 and Sr90 0ver the 30 year cooling period is shown in the inset.
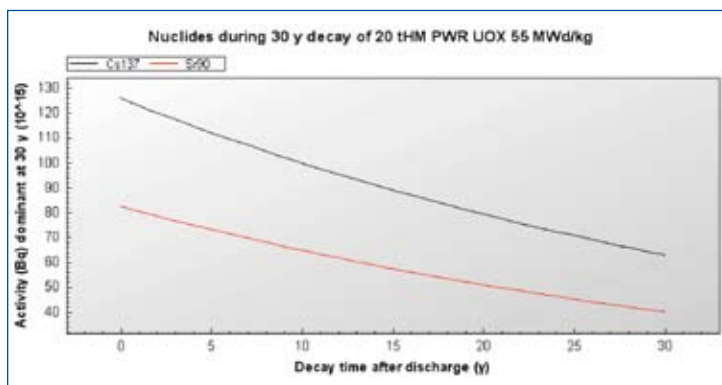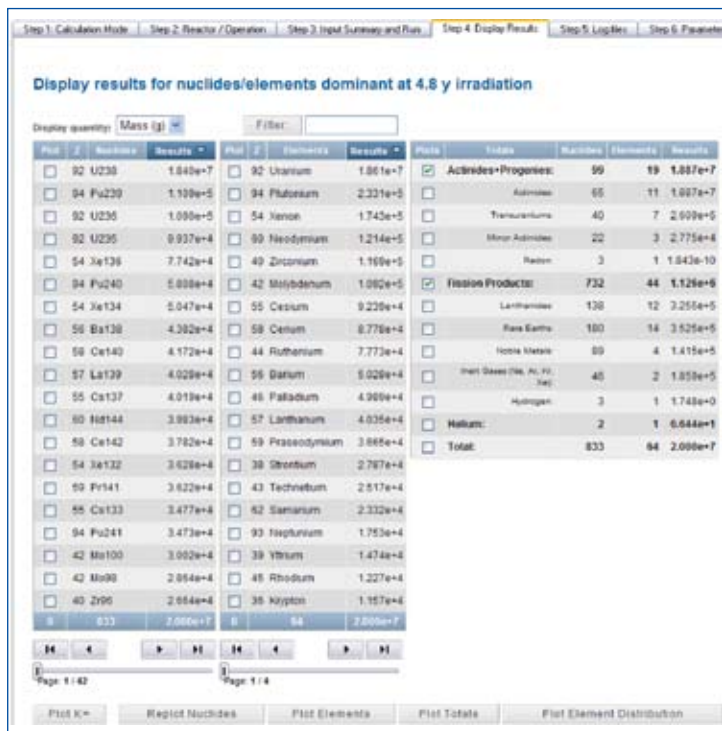
More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki

Neutron Activation with webKORIGEN
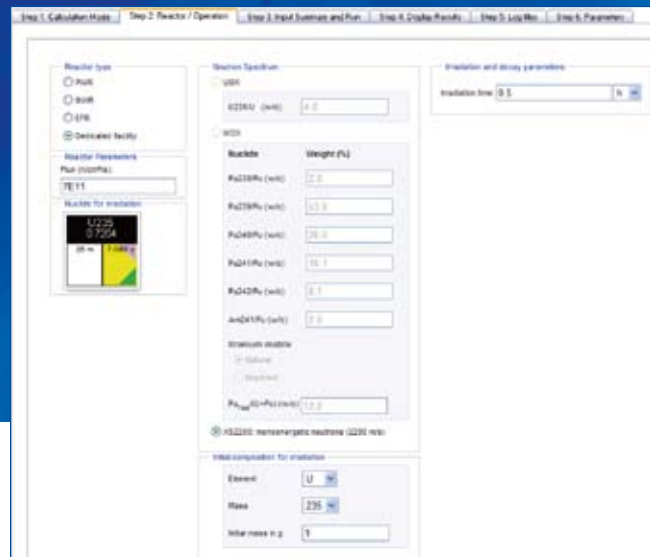
Neutron Activation with webKORIGEN

In addition to reactor irradiation simulations (for PWR, BWR, and fast reactors) with decay storage and reprocessing, webKORIGEN can also be used for neutron activation studies and sub-critical system analyses. Neutron activation can be investigated by choosing mode 1 (reactor irradiation) and selecting the constant flux mode. This mode of operation allows for target irradiations in the neutron spectra corresponding to PWR, BWR and Fast Reactors or a dedicated facility with thermal neutrons. Target irradiations are restricted to small samples of a single-nuclide material in the irradiation facility. In this way the neutron spectrum in the target is dominated by the reactor facility spectrum.

Example: Determination of the Fission Yield of Ba139

It is of interest to calculate the fission yield of Ba139 from the irradiation of 1 mg U235 (from enriched uranium) in a thermal neutron spectrum. The thermal neutron flux is 7×10^{11} cm^{-2}s^{-1}. In Step 1, Mode 1 (reactor irradiation) with constant flux is chosen. In Step 2 (see diagram above), the reactor type and neutron flux are set – Dedicated facility and 7×10^{11} cm^{-2}s^{-1} respectively. In the central panel, the nuclide and its mass are set – U235 and 1 g respectively. In the

third panel, the irradiation time is set to 0.5 h. In Step 3, the full input is summarised and the calculation can be started. In step 4, from the central panel in the output grid (shown), the element Ba is checked. On using the Filter button, the barium isotopes and their masses are shown in the first panel. By selecting Ba1239, a plot of the amount of Ba139 with time can be seen (shown).

Sub-Critical System Analysis with webKORIGEN

The neutron activation mode can also be used to investigate various aspects of sub-critical systems. In contrast to critical reactors, sub-critical systems need an extra source of neutrons in order to sustain a chain reaction. A reactor containing thorium (Th232) cannot sustain a chain reaction. A certain amount of fissile plutonium, for example, is required to make the system critical. An alternative approach is to irradiate the thorium in a thermal reactor. In this case the fissile U233 is produced (through neutron capture of Th232 to produce Th233 and then radioactive decay to U233). If enough U233 is produced, the system can become critical. This process can be simulated with webKORIGEN.

Example: Irradiation of Thorium in a Thermal Neutron Reactor

In Step 1, Mode 1 (reactor irradiation) with constant flux is chosen. In Step 2 (see diagram above), the reactor type and neutron flux are set – PWR and 3×10^{14} cm^{-2}s^{-1} respectively. In the central panel, the nuclide and its mass are set – Th232 and 1 kg respectively. In the third panel, the irradiation time is set to 2 y. In Step 3, the full input is summarised and the calculation can be started. In step 4, from the central panel in the output grid (shown), the element U is checked. On using the Filter button, the uranium isotopes and their masses are shown in the first panel. By selecting U233, a plot of the amount of how the U233 increases with time can be obtained. It is also of interest to plot the k_∞ value which shows the ratio of total neutron production to absorption rates. Low values of k_∞ indicated that neutrons are mainly absorbed by the system. At k_∞ close to unity, the neutron production and absorption are almost equal – this is a system near to criticality. In the example above, it takes more than 2 years irradiation of Th232 in a thermal reactor to produce enough fissile U233 to sustain a chain reaction.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki
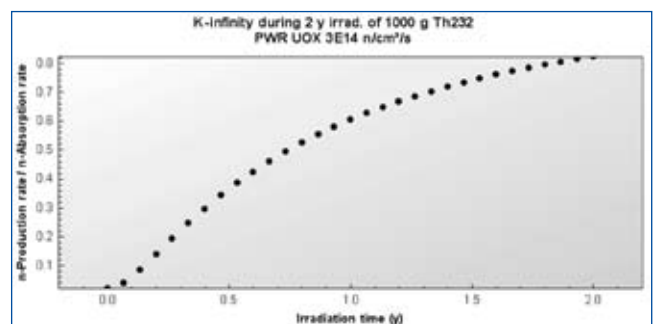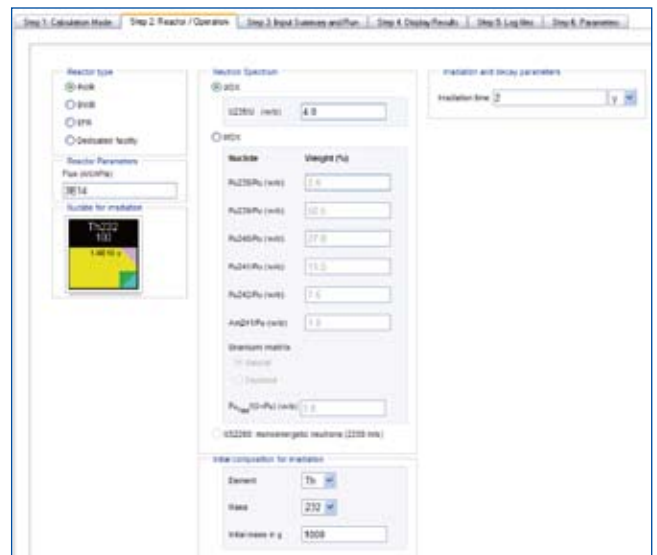
Transport & Packaging
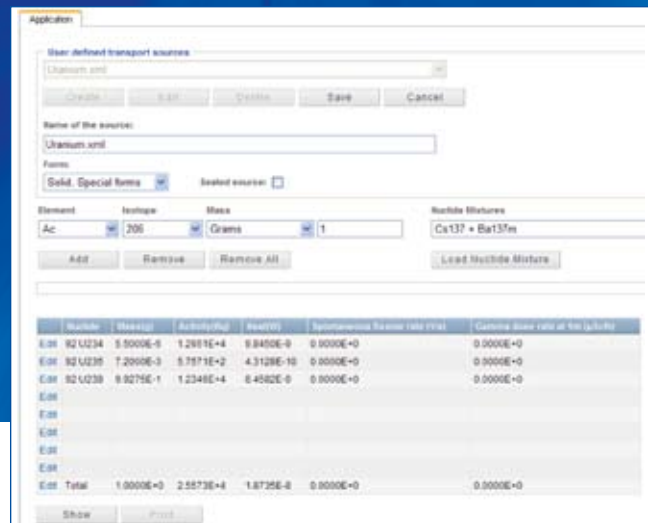
Background

Each year more than 10 million packages of radioactive materials are transported worldwide. Radionuclides are used for a variety of purposes e.g. in nuclear medicine, materials testing, oil exploration etc. For these purposes radioactive materials must be packaged and transported to the location of interest. Before these materials can be shipped, care must be taken that the shipping regulations have been strictly followed. The purpose of these regulations, of course, is to ensure safety by containing the radioactivity to make sure that there is no negative effect on the environment, to control the radiation emitted from the package, make sure that nuclear fission criticality conditions cannot be met, and to dissipate any heat generated within the package. The choice of packaging depends on the radionuclides involved, the amounts of radioactivity to be shipped and the form of the radionuclides. Restrictions on the amounts of material are determined by the so-called "A1" and "A2" values.

A1 and A2 Values

"A1" is the maximum amount of activity for a special form radionuclide that is allowed in Type A packaging, whereas "A2" refers to the maximum amount of activity in a Type A package for normal form materials. Usually the A1 or A2 values can not exceed 37 TBq (37×10^{12} Bq) or 1000 curies (Ci). For some materials, however, the limits have been set to 40 TBq or more (e.g. in the case of U-238). The A2 values refer to normal form radioactive materials and to both external and internal exposure. In contrast to the A1 value, the A2 value assumes that dispersal and contamination of the package content is probable. On this basis, the A2 values are always lower than the A1 values. The values of the quantity A1 arise through worst-case assumptions with regard to external gamma radiation from a known source at a certain distance. More exactly, the A1 value for a particular radionuclide is that quantity of radionuclide which will give rise to a dose rate of 0.1 Sv/h at a distance of 1m from the package. Since only external radiation is considered, it is assumed that the radioactive material inside the package will not be dispersed if the package is damaged. The A2 value also relates to the worst-case assumptions, but five different exposure pathways are considered rather than just the single pathway associated with the A1 value. The five pathways are: external gamma radiation, external beta radiation to the skin, inhalation, ingestion, external gamma radiation from immersion in a gaseous cloud of radioactive material released from a damaged package.

Packaging

Type A packaging is required for shipping radioactive materials when the radioactivity inside the package does not exceed the A1 or A2 values. If the radioactivity is higher, type A packaging, which is foreseen for normal transportation conditions and minor accidents only, cannot be used. The basic purpose of type A packaging is to prevent loss or dispersal of the package contents while maintaining proper radiation shielding under normal transportation conditions. Type A packaging must withstand water spray, drop, puncture and crash tests. When the level of radioactivity exceeds the A1 and A2 values, type B or type C packaging is required. Type B and C packaging must meet all the conditions of type A packaging and in addition have the ability to withstand serious accidents. Examples of type B packaging are spent nuclear fuel casks.

Example

Consider the radionuclides Cs137 and Co60. The A1 and A2 values are shown in the table below. It can be seen that the values for Cs137 are quite different and for Co60 are the same.

Maximum activities for special (A1) and normal form (A2) materials

Nuclide	A1 (special form)	A2 (normal form)
Cs137	2 TBq	0.6 TBq
Co60	0.4 TBq	0.4 TBq
U238	No limit	No limit

In the case of Co60, this means that even if five different exposure pathways are considered, there is no greater risk than if only the external gamma radiation pathway is considered. This is not the case with Cs137, for example, which does indeed depend on the exposure pathway. The special form referred to above refers to the fact that if the material were released from the package, the only hazard would be from external gamma radiation. An example of such a special form is that of a sealed (encapsulated) source of radiation. Here the durable metal capsule with high physical integrity ensures that the radioactivity will not disperse. In addition, only solid materials are classified as "special form". Special form encapsulation is designed such that the capsule cannot be opened unless it is destroyed. In contrast to special form materials, normal form materials may be solid, liquid, or gaseous. Examples here are waste materials in a plastic bag, a liquid-containing bottle housed with a metal contained, powder in a glass or plastic bottle, contaminated soil in a drum, or gas in a cylinder.

Nuclear Material Transport Report

The transport & packaging application (interface shown overleaf) is used to create nuclear transport reports. Before a nuclear transport report can be created at least one nuclear source has to be defined. A nuclear source consists of a list of nuclides, a name and a form. The desired form can be selected from the *Form* combo-box and the name can be entered in the *Name of the source* input field. *Sealed source* has to be checked for sealed sources. A new nuclide is added to the nuclide list by selecting the desired nuclide in the *Element* and *Isotope* combo-boxes and clicking the *Add* button. A nuclide can be removed from the nuclide list by selecting the nuclide in the nuclide list and clicking the *Remove* button on top of the nuclide list. The nuclide list is cleared by clicking the *Remove All* button. After entering the data of the nuclear source a new nuclear source is created by clicking the *Save* button. Previously defined nuclear sources can be selected from the "User defined transport sources". Following selection of a particular source, the component data is shown. Clicking the *Show* button will show the nuclear transport report which can then be printed. An example of a transport report for uranium metal is shown.

Nuclear material transport report

Transport report generated for source: Uranium metal on 8/9/2010

Source : Uranium metal   Irradiated fissile material: ☑
Form: Solid, Special forms

Nuclide	Mass(g)	Activity(Bq)	Heat(W)	Gamma dose rate at 1m (µSv/h)
92 U238	9.9275E-1	1.2346E+4	8.4582E-9	0.0000E+0
92 U235	7.2000E-3	5.7571E+2	4.3128E-10	0.0000E+0
92 U234	5.5000E-5	1.2651E+4	9.8450E-9	0.0000E+0
Total	1.0000E+0	2.5573E+4	1.8735E-8	0.0000E+0

Fissile Uranium Mass Content: $\dfrac{^{233}U + ^{235}U}{U_{total}} = 0.72\ \%$

Fissile Plutonium Mass Content: $\dfrac{^{239}Pu + ^{241}Pu}{Pu_{total}} = 0.00\ \%$

Total fissile material
U233 (g): 0.0000E+0
U235 (g): 7.2000E-3
Pu239(g): 0.0000E+0
Pu241(g): 0.0000E+0
Total fissile material (g): 7.2000E-3

Total heavy metal
Th(g): 0.0000E+0
U (g): 1.0000E+0
Pu(g): 0.0000E+0
Total heavy metal (g): 1.0000E+0

Container Type: $\sum_i \dfrac{A_i}{A_{l_i}} = 3.1628E\text{-}10$ Type A

Due to fission product activity, irradiated fissile material has to be transported in Type B container.

Gamma Spectrum Generator

Gamma-spectroscopy

Gamma-spectroscopy is an important nuclear and radio-analytical method. Most radioactive sources produce γ-rays of various energies and intensities. When these emissions are collected and analyzed with a γ-spectroscopy system, a gamma energy spectrum can be produced. A detailed analysis of this spectrum is typically used to determine the identity and quantity of γ-emitters present in the source. Today, γ-spectrometry is one of the most usable methods in different basic and applied fields of nuclear science & technology. A variety of instruments and measurement techniques, involving γ-spectrometry measurements, are employed routinely by nuclear and radio-chemists, health physicists, nuclear facility operators, radiation protection staff, safeguards inspectors, border police, customs and law-enforcement officers. Needs for *Education & Training* in these areas are high and, obviously, they will be increasing in the future as new challenges arise, such as strengthening international nuclear safeguards and security, nuclear terrorism prevention and implementation of new standards in radiation safety and protection.
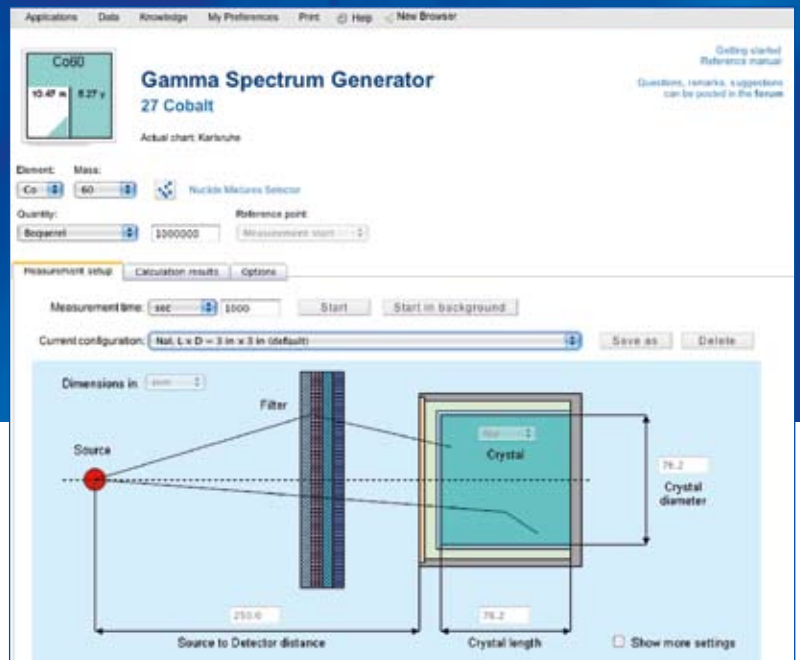
Nucleonica's Gamma Spectrum Generator

To address these growing demands in Education & Training, an interactive web-accessible simulation tool has been developed. The simulator presents an efficient visual teaching aid that is especially useful in training facilities, which have restrictions on the use of radioactive substances, or when sources of special interest (e.g. spent fuel, enriched U, weapon grade Pu or other highly radiotoxic materials) are not readily available. The module is setup (see overleaf) such that the user can run the program immediately through a simple "one-click" calculation with default parameters. This "one-click" calculation simulates the spectrum for a 10 MBq Co60 γ-source located at 25 cm distance from unshielded 3" x 3" NaI detector. A typical result of the calculation is shown.

Adapt the GSG to your specific problem

Choose an appropriate HPGe or NaI detector setup from a set of predefined measurement configurations or define your own setup using the interactive tools provided. Define the input window, crystal packaging and inactive crystal layers of the detector setup. Add up to 6 additional absorbing filters between source and detector. Specify energy resolution properties and ADC settings of the virtual γ-spectrometer. Save the configuration in your personal Nucleonica account for the future use and reference. Select from around 1300 γ-emitting nuclides available in Nucleonica, or choose a predefined or user-defined mixture of nuclides as a γ-source. Specify the source cooling and measurement time intervals and enable decay calculations to allow radionuclide decay and build-up during the source cooling and measurement.

Validation

The Gamma Spectrum Generator has been extensively validated by experiments and Monte Carlo calculations. Details can be found in the following publications/reports:

A. Berlizov, et al., A Collection of Reference HPGe Gamma-Spectra for Shielded / Unshielded Radionuclide Sources and Special Nuclear Materials, Technical Note JRC-ITU-TN-2009/25, 2009. See also: Fast and Accurate Approach to γ-Spectrum Modelling: A Validation Study with a Shielded / Unshielded Voluminous Uranium Sample, Applied Radiation and Isotopes 68 (2010) 1822–1831.

V. Kleinrath, a Study of Gamma Interference Scenarios for Nuclear Security Purposes, Measurements and Modelling using the Nucleonica Tools, JRC-ITU-TN-2010/21.

Cambio File Converter
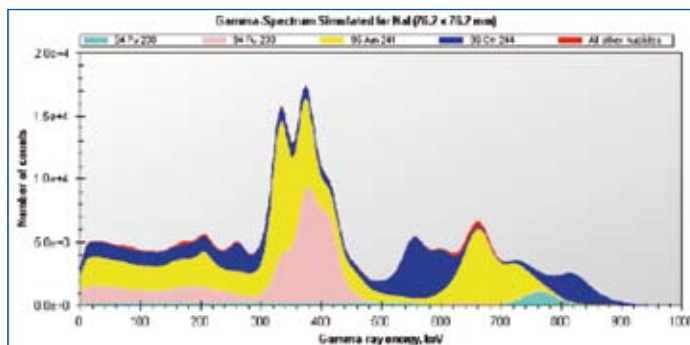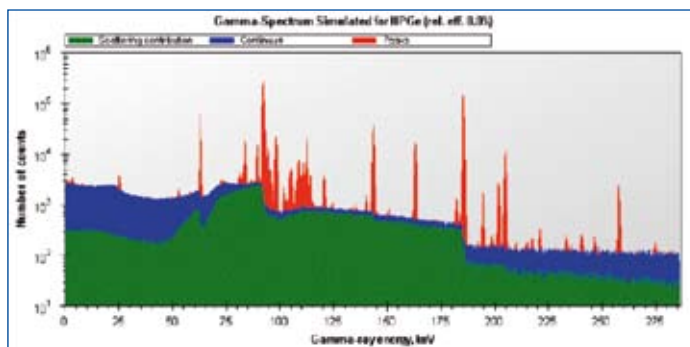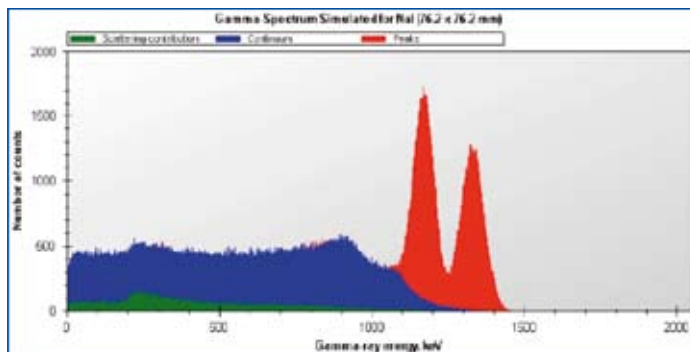
Cambio File Converter

Cambio File Converter

Cambio was developed in response to a need of nuclear emergency response analysts everywhere to be able to quickly read the data from any of a widely growing number of formats used by both commercial and government detector systems worldwide. As the number of manufacturers of nuclear detection instrumentation grows, so does the number of data formats that must be able to be read by emergency analysts. Manufacturers of instrumentation often need to create new and more complex versions of their own formats as technology advances and as new user requirements lead to new, more sophisticated instruments.

File Conversion in 4 steps

The user interface is shown. The file conversion is completed as follows:

1. Select a file to be uploaded for conversion (e.g. Eu152_HPGe.txt shown above). The full filename of the file to be uploaded is shown. After selection of the appropriate input file, this can then be converted to one of the eight general file formats.
2. Select one of eight target file formats from the drop-down menu. The eight conversion formats are: IaeaSpe, N42Xml, OrtecChn, DetectiveSpc, IdentiiFinderSpc, Gr130Dat, Gr135Dat, and GadrasPcf.
3. Start the conversion; If the input file is converted to the IaeaSpe or N42Xml formats, then a graph of the data can be viewed in the *Spectrum* tab.
4. Download the converted file.

Further information on the Cambio file conversion process is given in the *Diagnostic* tab where the input and output data are given.

Sample Spectra

As an alternative to uploading a spectrum, or if a spectrum is not readily available, a number of sample spectra are provided in the *Sample Spectra* tab. These spectra have been created using the Gamma Spectrum Generator and converting the output .txt files to IaeaSpe or N42.Xml files. Using this approach, the user can create any desired spectrum either from single nuclides or nuclide mixtures.

Spectral data at cursor position			Gamma Lines near cursor (from standard lib, 580 lines)				
Energy, keV	Channel	Counts/keV	Nuclide	Decay	Halflife	Energy, keV	Emission Probability (%)
345.021	1149	1.59726e+5	Eu152	EC	13.33 y	344.28	2.659E+01
344.421	344	3.23782e+4	Bi210	α	3.00My	344.95	7.629E-01
			Pu239	α	24.11ky	345.01	5.560E-04

Example

The file conversion process is illustrated by a simple example. In a first step the Gamma Spectrum Generator is used to create a gamma spectrum e.g for the nuclide Eu152. This spectrum is then downloaded and saved as a .txt file – Eu152_GSG.txt – on the user's desktop. This file is then uploaded to the Cambio File Converter application. Thereafter, the desired conversion format is selected (in this case IaeaSpe, see figure). The uploaded file is then converted. Finally, the converted file can now be downloaded. If the spectrum conversion is to IaeaSpe or N42Xml, the spectrum graph can be viewed in the *Spectrum* tab together with title and date.
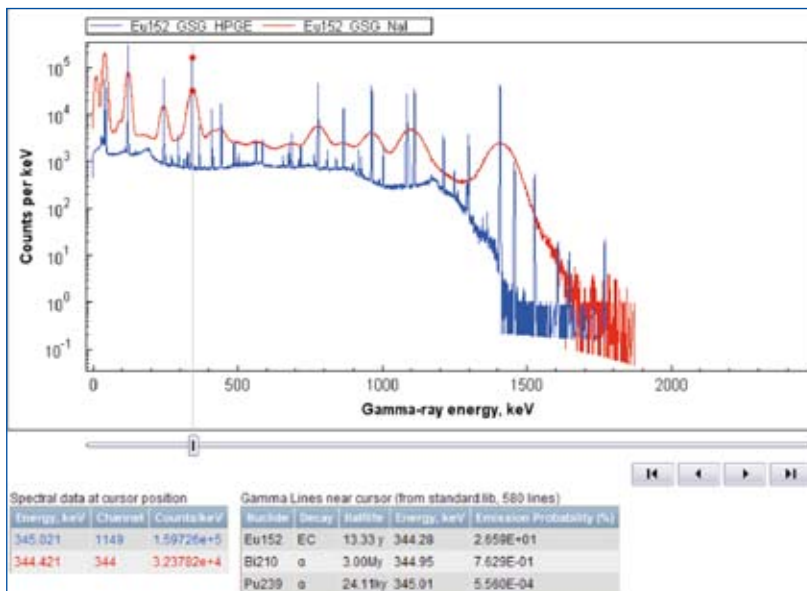
Spectrum analysis

In the *Sample Spectra* tab, previously created spectra can be compared with each other (i.e. a simplified spectrum analysis). In the example shown, two Eu-152 spectra – one taken with a NaI detector (in red) and one with a HPGe detector (in blue) – can be seen. By using the slider control, trackball, and crosshair, the individual peaks can be analysed to see which nuclides have gamma lines in this region of interest. More sophisticated analyses can be made with Nucleonica's WESPA (WEb Spectrum Analyser) module.

Testimonial from a Nucleonica user

"The Cambio file converter is a very nice new feature. One of our customers uses Ortec instruments and we use Canberra instruments. Now we can exchange our measurement data. This is very interesting, since with most software it is difficult to obtain a print-out with all details we need. We are performing purity measurements for radiopharmaceutical products, and, need to prove the absence of certain peaks."

For more information, see www.nucleonica.com/wiki

WESPA –
Web Spectrum Analyser
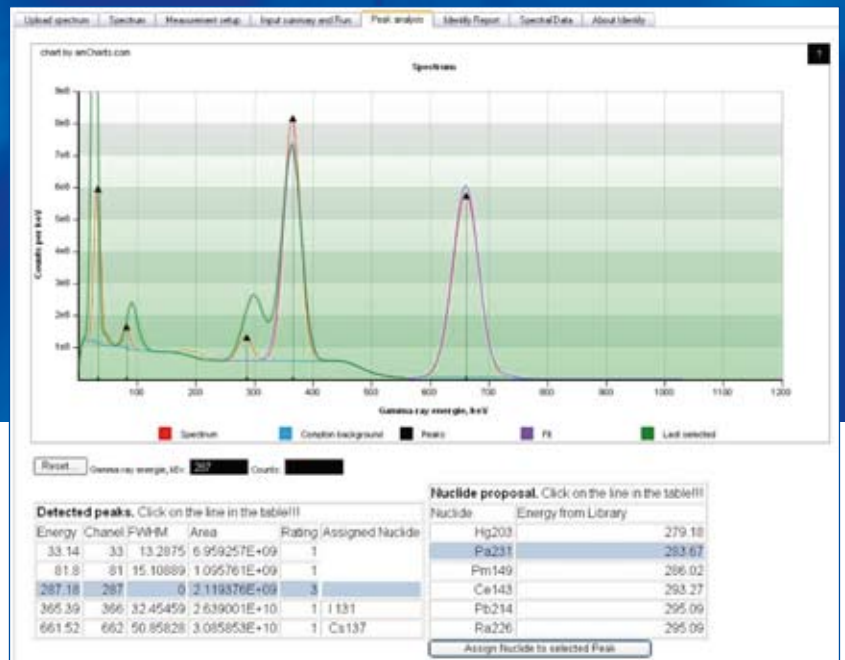
WESPA

WESPA (**We**b-based **Sp**ectrum **A**nalyser) is an interactive peak-search based gamma spectrum analysis tool. Through an intuitive interface, it allows the user to assist in the identification process. One of the basic principles is the use of dedicated gamma libraries for nuclides to be expected in the sample. This simplifies the analysis process and allows for fast identification of the nuclides concerned. The specific nuclide libraries can be created with Nucleonica's library creation tool. In addition, a general library can be used where there is no information on the sample content available. WESPA can process spectral files with the IAEA *.spe format directly. Other formats need to be first converted using the Cambio file converter application in Nucleonica. The program includes peak search, energy, efficiency, and FWHM calibration. Energy dependent efficiencies are calculated from the detector supplier data and information about source matrix and absorbers.

The WESPA web application provides a wide range of advantages for the user as well as the developers. The proven user-friendliness of the Nucleonica applications is a key feature – the user can concentrate on the science rather than on the computing. In addition, learning times are kept to a minimum making WESPA a standard for education and training.

The WESPA gamma spectrum analysis and nuclide identification module is aimed primarily at education and training within the field of nuclear security. For simplicity of use, a number of sample gamma spectra are available for test purposes. Inexperienced users can start by analysing these spectra and obtaining a first list of possible matching nuclides. Through this "learning by doing" process, students obtain direct, first-hand experience in the problem of gamma spectrum identification. Within this context, the Gamma Spectrum Generator (GSG) in Nucleonica is also of interest. With this tool, the user can generate gamma spectra for any mixture of radionuclides. With WESPA the aim is the opposite: starting with a gamma spectrum, the goal is to identify the nuclides. By combining the GSG and WESPA modules, students have a powerful combination of tools for spectrum creation and analysis. With these tools, many of the problems encountered in gamma spectrum analysis for nuclear security can be demonstrated. The WESPA gamma spectrum analysis module is under continuous development through a collaboration between the Nucleonica team and international experts in the field of radionuclide identification.

The **first step** in the identification process is to upload a spectrum. For testing purposes, the user can select a number of pre-defined or sample spectra.

In the **second step**, the user should select the type of detector used during the measurement of the spectrum and also should specify or create a nuclide library containing a list of gamma lines from the expected nuclides.

In the **third step**, the user should run WESPA to make a peak search and to prepare a nuclide proposal for each peak based on the selected library. Thereafter, through the user friendly interface, the user can check the proposal for each peak and how the proposed nuclide fits the peak. The user can accept or refuse the proposal.

WESPA profits from the latest internationally evaluated nuclear data available in Nucleonica. In addition, full standardised technical documentation is provided in the Nucleonica wiki. Users can post questions, comments, and suggestions in the Nucleonica forum and obtain answers from experts in the field.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki

Energy	Chanel	FWHM	Area	Rating	Assigned Nuclide
21.32	71	2.604911	2986.789	1	
25.45	85	2.288658	1483.72	1	
31.16	104	2.671621	96989.14	1	
35.29	118	2.365115	64820.25	1	Ba133
53.46	178	2.589359	32932.02	1	Ba133
71.42	238	2.898974	2921.501	1	
81.31	271	2.673545	769852.3	1	Ba133
160.91	536	3.145461	16105.94	1	Ba133
223.54	745	3.492194	9857.624	1	Ba133
276.69	922	3.64309	137005.9	1	Ba133
303.14	1010	3.749711	329040.6	1	Ba133

Nuclide	Energy from Library
Ba133	34.96
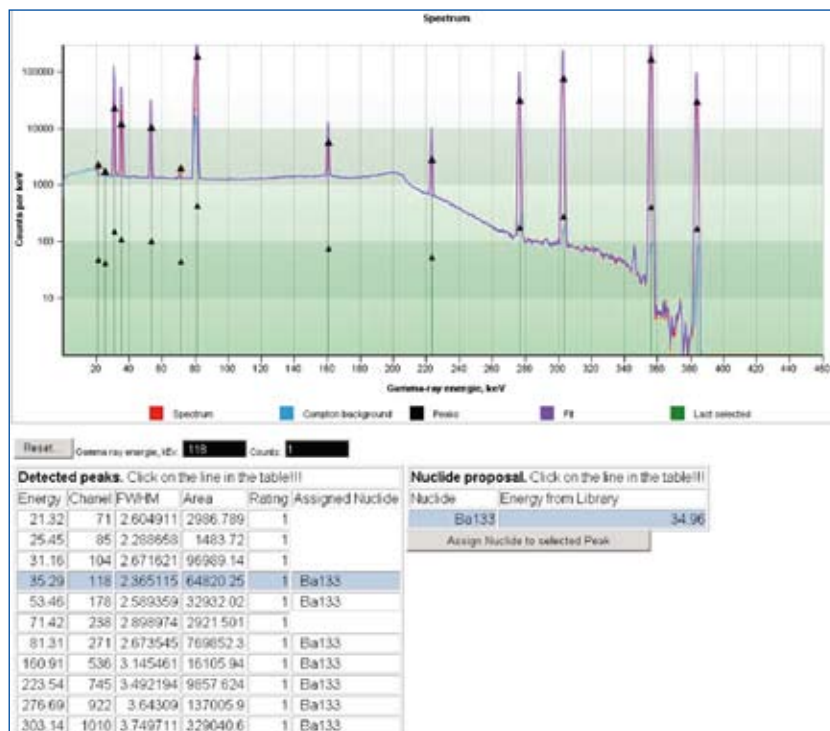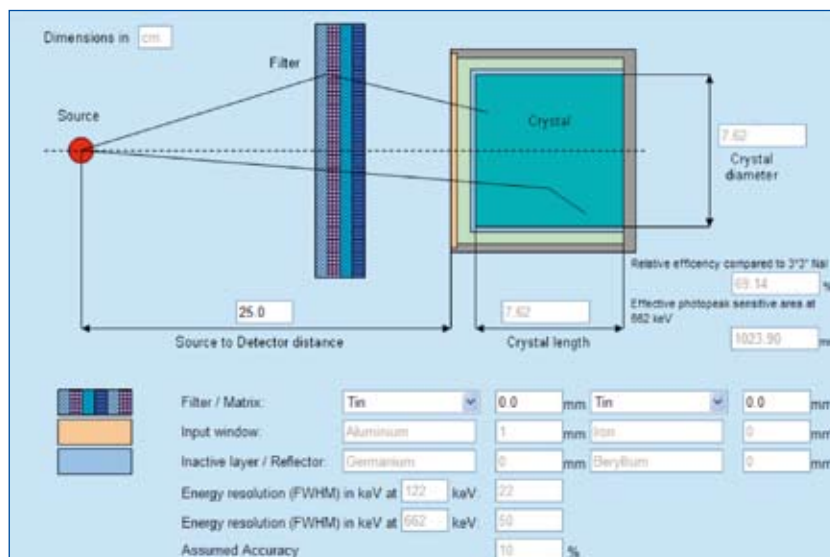
In Silico Dosimetry

What is Radiation Therapy?

Radiation therapy for cancer treatment has been in use for over 100 years. Radiation therapy, also known as radiotherapy or radiation oncology, refers to the medical use of ionising radiation for cancer therapy by controlling malignant cells. The therapy uses ionising radiation to damage DNA cells. The damage is caused directly by photons, neutrons or charged particles or indirectly through released free electrons. These free electrons can further damage DNA by breaking molecular bonds, causing ionisation or creating free radicals. The total dose is usually spread out over time. This procedure allows normal cells to recover between irradiation phases. Typical treatments involve irradiation levels of around 2 Gray per day, five days per week. There are three main divisions of radiation therapy: external beam therapy where the radiation source is outside the body; brachytherapy where a sealed source is used in the area under treatment; and unsealed source therapy given by infusion or oral ingestion. Particle therapy (also known as hadron therapy) is a special case of external beam radiotherapy where the particles are protons or heavy ions. Tumours can be located with 3D images from X-ray computer tomography (CT), magnetic resonance imaging (MRI) and positron emission tomography. The total treated volume as well is defined using the CT information on different tissues of the patient.

Radiation Therapy Studies

Through a collaboration with the Turin based company I-SEE, a web-based module is being developed to determine high energy particle dose rates in tissue. Through Nucleonica's web interface, users can specify the simulation parameters and send those for calculation. I-SEE is active in the field of particle therapy and specialises in services for the simulation of beam delivery lines for cancer treatment for

Courtesy Heidelberg Ion Beam Therapy Center at the University Hospital Heidelberg, Germany

both proton and carbon ion beams. The key innovation here is through the use of a distributed Monte Carlo computing environment (based on the delocalization of resources and adopting a parallelized architecture, to minimise calculation times) and the use of web browser interface for running, checking and displaying results. With I-SEE's expertise in radiation therapy, and Nucleonica expertise in web services, browser based applications and training, the collaborative partnership is in the position to provide a unique service to oncology centres for particle and radiation therapy and to companies operating in this area of healthcare.

Beam Simulations

are performed with a dosimetry module for calculating the energy loss in 3D for X-ray, proton and carbon ion beams. In contrast to electromagnetic radiation (X- and -rays), which exhibit an exponential decrease of intensity with penetration depth, heavy charged particles such as protons or heavy ions have a well defined range in matter (see diagram). The energy deposition of heavy ions is characterized by a low entrance dose and a pronounced sharp maximum near the end of range (Bragg peak). This allows treatment of the organs affected while sparing the healthy tissue. To deliver a radiation dose accurately requires high accuracy in the simulation and the treatment plan.

Heavy ion beams used in the field of hadron therapy provide additional advantages because of the radiobiological efficiency of heavy ions and especially carbon ions beams. The production of secondary particles, however, requires a very precise estimation of the fragments created and their distribution in the target volume.

Radiobiology Effect Estimates

When using heavy ion beams for radiation therapy, it is mandatory to estimate well the radiobiological effect in patients before treatment. Using the Monte Carlo algorithms, one can estimate the tissue responses to radiation and cell survival when irradiated with specific beams.

Dose distribution for X-ray and ion beams in biological tissues
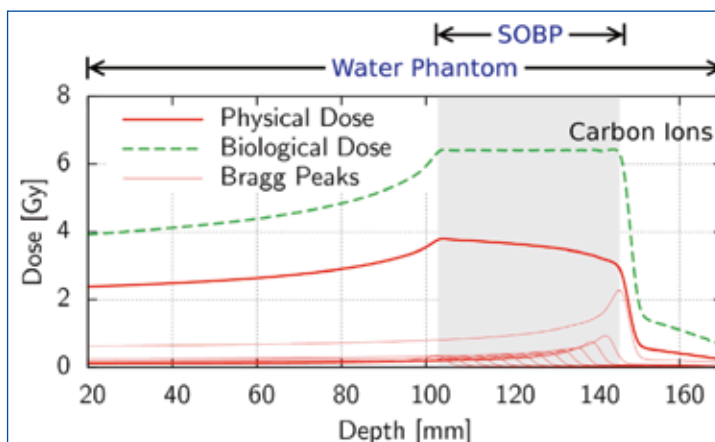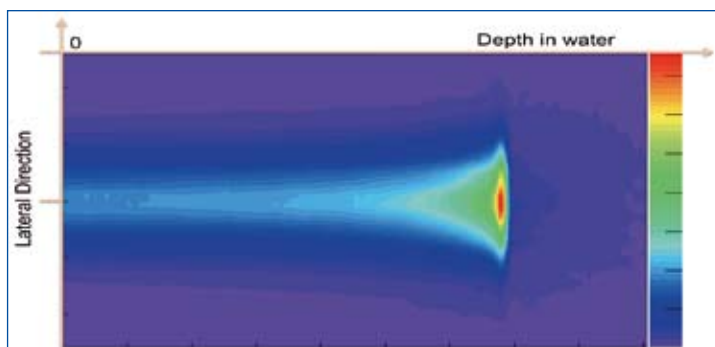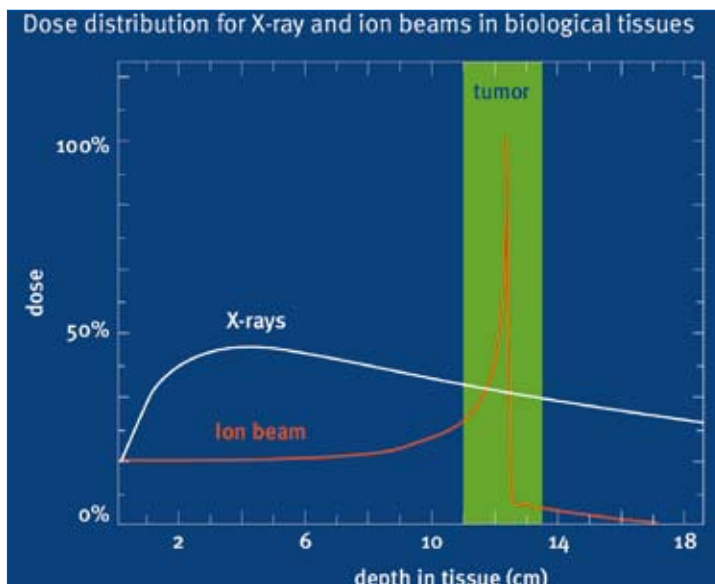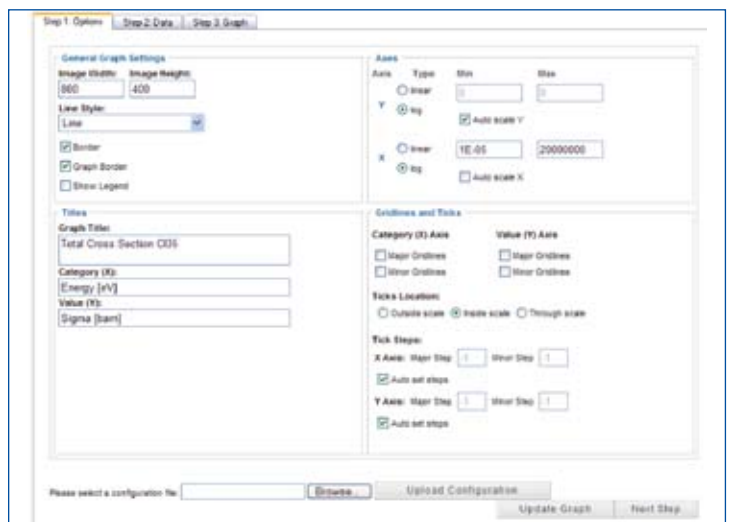
webGraph

Nucleonica webGraph

Nucleonica's webGraph is an easy to use web-based graphics module which allows the user to plot data and create publication quality scientific graphs. There is no software to install. The module can be accessed at any time from any location – only requirements are a web browser and an internet connection. In addition, webGraph provides graphical output for the many nuclear science applications available in Nucleonica (e.g. decay engine, dosimetry & shielding, etc.). Basic graphs can be produced simply by inserting data into the *Data* tab and viewed in the *Graph* tab using default values for the graph settings.

For a more "hands-on" approach, graphs can be created in three basic steps: In the **first step**, general graph settings are specified in the Options tab. These include the image width and height (in pixels), line style (column, line, line with symbols, symbols only), the use of borders and legend, graph title, and labeling for the x- and y-axes. In addition the types and ranges of axes can be specified (linear or log) together with gridlines and ticks. For more advanced users, an entire graph configuration containing both the data and graph settings, can be uploaded (*Upload Configuration*) as an xml file.

In a **second step**, the data to be plotted can be entered manually using the Data tab. A simple example is shown of the input data for two linear plots. In the first line, the data structure is defined e.g. x, y1, y2 (this is also used for the legend). In this case, both curves y1 and y2 have the same x values. Thereafter, the data is listed using commas to separate the x, y1, and y2 values. Using this approach, multiple curves can be displayed by using comma separators following each y value provided the x vales are the same. If the curves y1, y2, etc. have different x values, the data format is slightly different (see below). The resulting plot can be seen in the the the *Graph* tab (shown as an

inset here). Curve interpolation between the data points can either be linear or polynomial. As an alternative to entering the data manually, an Excel file can be uploaded (shown at the bottom of the *Data* tab) or by "cut and paste" directly from the spreadsheet). In this case the separators are blanks.

In the case where the various curves have different x values, a slightly different format should be used. The datasets (x1,y1), (x2,y2), (x3,y3), etc. should be separted by a comma. Hence the data is structured as: x1, y1,, x2, y2,, x3, y3,, etc. The Data tab for five sets of data (circle, x^2, x^3, $x^{1/2}$, $x^{1/3}$) is shown.

In a **third step**, the plot can be seen in the Graph tab. At this stage, the graph can be finalised by specifying the graph settings (titles for graph and axes, types and ranges of axes, gridlines and ticks, etc.). The graph can then be saved in a number of standard formats or the entire data and graph settings can be stored in an xml configuration file. These are described in more detail.
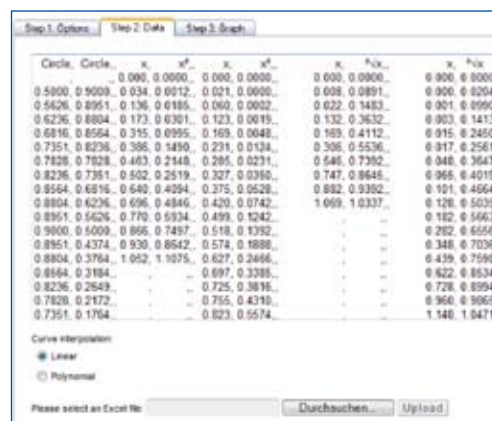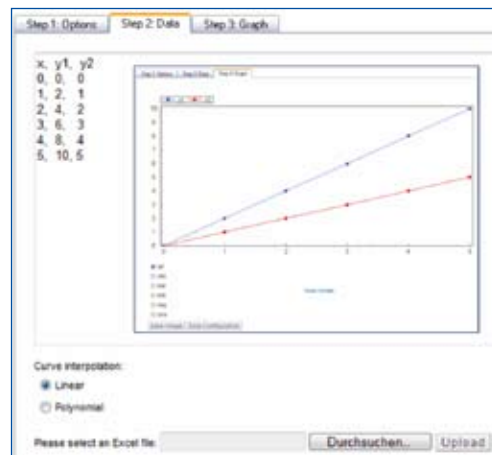
Graph Formats

The image can be saved in a number of graphical formats. GIF, JPG, PNG are best suited for web pages; EMF (Enhanced Metafile Format) for use in programs such as MS Word, Powerpoint; EPS (Encapsulated PostScript), for use in programs such as Adobe Illustrator, Quark Express; and SVG (Scalable Vector Graphics) which requires the Adobe SVG Viewer, and is best used for printing.

Configuration File

A graph is finalised when, in addition to the basic data, the general graph settings have been specified. This entire information can then be saved in a configuration file in xml format. This has the advantage that at a later time, this configuration file can again be uploaded into the graphics module, with not only the data but all the graph settings.

More information can be found on the Nucleonica wiki at
www.nucleonica.com/wiki
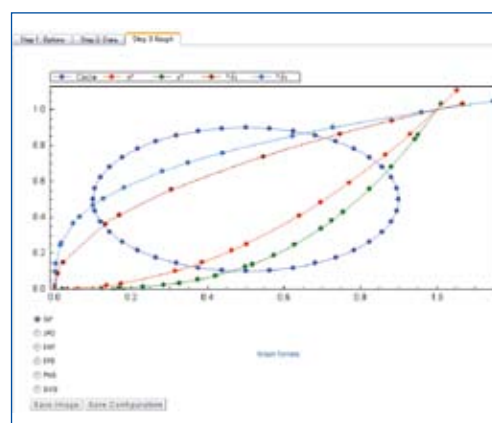
Scientific Calculator and Conference Calendar

Scientific Calculator

Nucleonica's scientific calculator is an easy to use web-based scientific calculator. The basic scientific functions (exp, 1/x, x^2, etc.) are shown above. By clicking on "Select and copy result", the results of a calculation - shown in the results window – can be selected and copied into another application. In addition, there are two other modes of operation of the calculator – for obtaining commonly used physical constants and performing routine conversions. These are briefly described.

Commonly used Physical Constants

The commonly used physical constants are reached by clicking on the *CONST* button. The following constants are available:

Speed of light in vacuum, $c(ms^{-1})$
Avogadro's number, N_A
Electrical charge, $e(C)$
Boltzmann constant, $k(J/K)$
Electron mass, $m_e(kg)$
Proton mass, $m_p(kg)$
Neutron mass, $m_n(kg)$
Atomic mass unit, $u(kg)$
Planck's constant, $h(Js)$

The user can return to the scientific calculation mode by clicking the *SCN* button (**SC**ie**N**tific Functions).
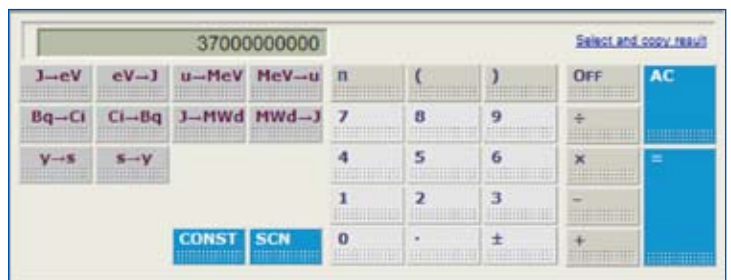
Unit Conversions

By clicking on the *CONV* button, the unit conversions are shown. These are:

J to eV; eV to J
U to MeV; MeV to u
Bq to Ci; Ci to Bq
J to MWd; MWd to J
y to s; s to y

To convert 1 curie to eV, enter 1 into the results window and click on the Ci → Bq button.

Conference Calendar

Nucleonica's conference calendar is both web-based and user generated (see figure). Clicking on an entry on a particular date will take the user to the conference / meeting website. The calendar can be scrolled on a month by month basis. Below the calendar, more details on individual events are given in chronological order. Again these details contain hyperlinks to the respective websites.

The calendar can be used for various events. The calendar has two tabs: 1 Conferences 2 MyConferences. If the user clicks on the MyConferences tab, he sees only his own meetings. If the user clicks on the Conferences tab, he sees all the conferences meetings his peer users have entered.

Entering a New Event in the Conference Calendar

To enter information on forthcoming events, meetings, conferences etc., the user must first click on the MyConferences tab. The date of the event is then selected in the calendar (in the example shown, the 8th November 2008 is selected). Thereafter information on the event is entered: Number of days (i.e. the duration of the event), Conference Name or title, a brief description of the event and a link to the Conference Web Site.

Finally, the user can decide if he wishes to share this information with other users. If he wishes to share the information, a tick should be entered in the checkbox "Share with other users". In this way a user-generated calendar of events is generated. If this box is not checked, the information will not be seen by the other users. In this case the Conference Calendar contains only personal event information.

More information can be found on the Nucleonica wiki www.nucleonica.net/wiki
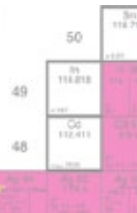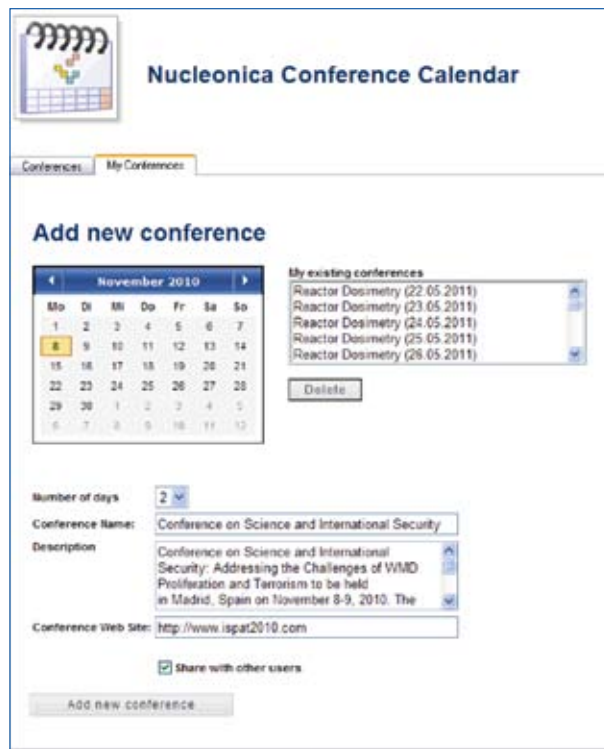
Nuclide Mixtures
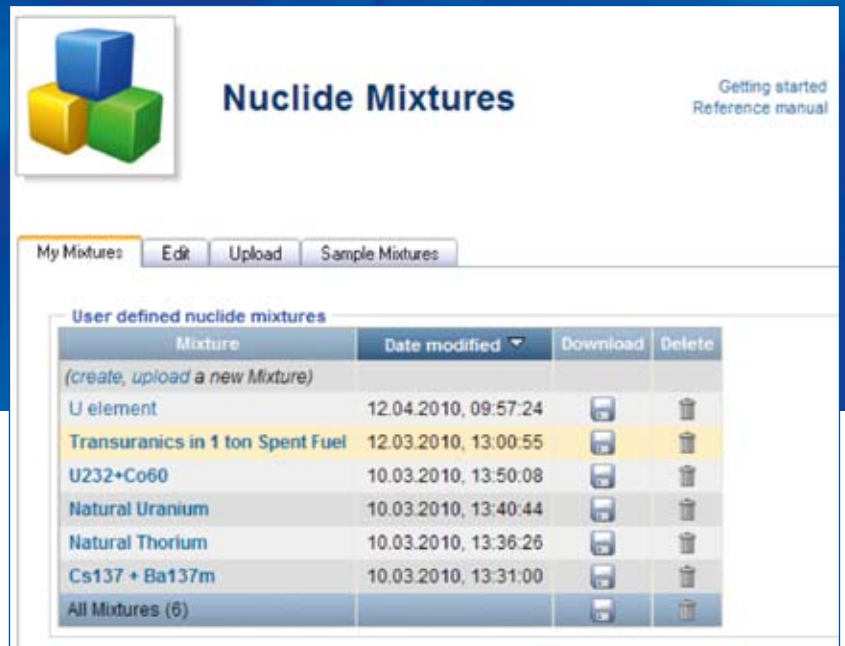
Nuclide Mixtures

The Nuclide Mixtures module is used to create and edit nuclide mixtures. Thereafter, these mixtures can be used in the Nucleonica applications (e.g. decay engine, dosimetry and shielding, gamma spectrum generator, etc.). The nuclide mixtures user interface is shown above. The My Mixtures tab contains a list of sample (default) mixtures together with user defined mixtures. The mixtures shown are sample mixtures as examples: *U element, Transuranics in 1 ton spent fuel, U232 + Co60, Natural Uranium, Natural Thorium, and Cs137+Ba137m*. The last nuclide created/edited – *U element* – is shown at the top of the list highlighted (arranged according to date modified). The last mixture viewed is shown highlighted. Just above this most recent mixture, there are two hyperlinks which allow the user to create or upload a new nuclide mixture. To the right of each nuclide mixture, the creation or last edit date is given. In addition, there are two icons with which the mixture can be downloaded (as an xml file) or deleted. At the bottom of the list, the total number of mixtures is given. The adjacent download icon allows the user to download ALL mixtures into a single xml file. This is useful for backup purposes for sending nuclide mixtures to other users. The second icon should be used with care since it allows the user to delete all mixtures in the list.

View/Edit mode

If a nuclide mixture is selected, the details (name, description, component nuclides, quantities, etc.) are shown in the Edit tab (see diagram). Input quantities can be in grams, number of atoms, activity (Bq or Ci) and moles or combinations of any of these units. Quantities entered in one unit (e.g. mass) are automatically converted into the other units (e.g. number of atoms, activity (Bq), moles) and shown in the grid. Additionally, the mass, mole and activity ratios are also listed. In the example shown, the nuclide mixture has the name "*Transuranics in 1 ton Spent Fuel*". These nuclides have been created mainly from the irradiation of U238 in a PWR reactor. There are 11 actinide nuclides of the elements Np, Pu, Am, and Cm with a total mass of 12.37 kg. The mixtures can be downloaded, either individually or all together as an xml file. This is useful for sending particular mixtures to a colleague, or for saving an entire mixture collection.

Creating a New Mixture

A new mixture can be created by clicking on the *create* link in the main interface (overleaf). Thereafter, the edit tab window will be shown with no content. The user should then specify the name of the mixture, provide a brief description, and then add the nuclide components. After each operation the mixture should be saved to avoid losing information. A new nuclide is added to the nuclide mixture by selecting the desired nuclide in the 'Element' and 'Mass' combo boxes, entering the desired quantity (mass, activity, number of atoms, or moles) and clicking the 'update' button. Similarly, the nuclide can be removed by clicking on the delete icon. All nuclides can be removed by clicking on the delete icon adjacent to the Total quantity in the nuclide column.

Rescaling

The rescaling feature allows the user to very simply rescale the input quantities to any other values. In the creation of a nuclide mixture for uranium, one could consider a total number of 100 atoms (see diagram). The numbers of U238, U235, and U234 atoms are then given by the isotopic abundances i.e. 99.2742, 0.7204, and 0.0054 respectively. If instead of 100 atoms (total), one would like to convert to say 25g uranium, this can be easily done by rescaling. By clicking on the "total", the user can then change the total mass, activity, number of atoms or moles directly.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki

Nuclide Mixtures

Getting started
Reference manual

My Mixtures | Edit | Upload | Sample Mixtures

Name
Transuranics in 1 ton Spent Fuel

Description:
Transuranics in 1 ton spent fuel. The fresh fuel has an initial enrichment of 4.2%. Values given are for a burnup of 50 GWd/t and following 6 years cooling. Total mass of transuranics is 12.37 kg per ton spent fuel.

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mass ratio	Mole ratio	Activity ratio	Delete
(add a new Nuclide)							
93 Np 237	1.937e+10	743	1.888e+24	0.06008	0.06074	3.689e-6	🗑
94 Pu 238	2.034e+14	321	8.121e+23	0.02596	0.02613	0.03872	🗑
94 Pu 239	1.354e+13	5900	1.486e+25	0.4771	0.4783	2.578e-3	🗑
94 Pu 240	2.242e+13	2670	6.698e+24	0.2159	0.2156	4.268e-3	🗑
94 Pu 241	4.786e+15	1250	3.123e+24	0.1011	0.1005	0.9113	🗑
94 Pu 242	1.138e+11	778	1.936e+24	0.06291	0.06229	2.167e-5	🗑
95 Am 241	5.946e+13	469	1.172e+24	0.03793	0.03771	0.01132	🗑
95 Am 243	1.293e+12	175	4.336e+23	0.01415	0.01395	2.462e-4	🗑
96 Cm 244	1.656e+14	55	1.357e+23	4.447e-3	4.367e-3	0.03153	🗑
96 Cm 245	1.587e+10	2.5	6.143e+21	2.022e-4	1.977e-4	3.022e-6	🗑
96 Cm 246	3.409e+10	3	7.342e+21	2.426e-4	2.363e-4	6.491e-6	🗑
Total: 11	5.252e+15	1.237e+4	3.107e+25	1	1.000	1	🗑

Element | Mass | Quantity | Unit
[ ] | [ ] | [1] | [Gram] | Update

My Mixtures | Edit | Upload | Sample Mixtures

Name
Uranium

Description:
100 atoms of uranium

Significant figures 6

Nuclide ▲	Activity(Bq)	Mass(g)	Number of Atoms	Mass ratio	Mole ratio	Activity ratio	Delete
(add a new nuclide)							
92 U 234	4.82737e-16	2.09862e-24	0.0054	8.29494e-26	8.53800e-26	1.49501e-21	🗑
92 U 235	1.42203e+4	0.177841	4.55654e+20	7.11404e-3	7.20439e-3	0.0440383	🗑
92 U 238	3.08579e+5	24.8200	9.27910e+22	0.992986	0.992796	0.955961	🗑
Total: 3	3.22909e+5	24.9987	9.32467e+22	1	1	1	🗑

Element | Mass | Quantity | Unit
[ ] | [ ] | [1] | [Gram] | Update

Save Mixture | Reset | Cancel

Gamma Library Creation
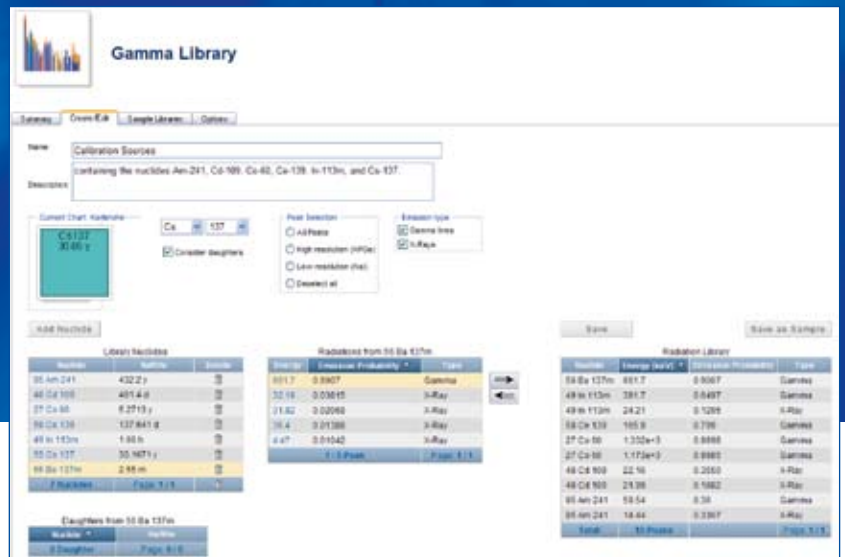
Gamma Library Creation

The library creation module can be used to create nuclide libraries using the latest internationally evaluated nuclear data. In addition to text formats, some proprietary formats (e.g. GammaVision) are also supported. Such libraries are required for example for radionuclide identification programs such as the WESPA (web spectrum analyser) module in Nucleonica. The libraries can be created using a range of commercial software, but usually the data (which includes nuclide, energies, emission probabilities, $T_{1/2}$, etc.) has to be entered by hand. Also the underlying databases may not be up to date with the most recent nuclear data. Using the Gamma Library Creation module in Nucleonica for this purpose makes life easier.

Create/Edit

The library creation interface is shown above. Before a new library can be created the nuclide list has to be filled with the desired nuclides. A new nuclide is added to the nuclide list by selecting the desired nuclide in the element and isotope combo boxes and clicking the *Add* button. A nuclide can be removed from the nuclide list by selecting the nuclide in the nuclide list and clicking the delete icon. The nuclide list is cleared by clicking the delete icon at the bottom of the list. In the example shown, a nuclide library for calibration sources is being created. The list of nuclides and the radiation library is shown. A new nuclide, Cs137 has just been added. If the *consider daughters* box is checked, it can be seen that Cs137 has the daughter Ba137m which is a strong gamma emitter with a main emission at 661.7 keV. Clicking on this daughter, the energies and emission probabilities of Ba137m will be transferred to the central grid. From this point, the main gamma lines can be selected and transferred to the *Radiation Library*.

The central grid lists all the gamma and X-ray energies and emission probabilities in the Nucleonica database. Depending on which radio button is checked in the *Peak Selection* box, either one or more emission lines are highlighted. The Peak Selection box allows the user to specify all peaks, or a subset of the peaks depending on which type of detector is being used. By clicking on the arrow icon, the highlighted radiations are transferred to the *Radiation Library*. At this point the library can be saved.

In the *Summary* tab (overleaf), the list of gamma libraries together with the creation dates can be seen. Since the Calibration Source library has just been created, this is shown highlighted in the grid. In the *Download* column, there are two icons. On selecting one of these icons – the tool-tip shows the text "GammaVision" Library – the library can be saved in GammaVision format. The other icon allows the user to save the library as a text file (for use in Nucleonica applications).

In the *Sample Libraries* tab, a list of pre-defined libraries is given. As an alternative to creating a library from "scratch", the user can then select and edit one of the existing libraries.

In the *Options* tab, the user can select the relational database from which the basic spectral data is to be taken: either Nucleonica, the 8th Table of Isotopes, or JEFF3.1. There is also the possibility to select the minimum branching ratio for daughter products. Clearly there is no sense in including small branching ratios since this will result in very small quantities of a particular daughter. The default value use is 0.01. This implies daughters with a branching ratio less than 1% will be omitted in the list of daughter products. Finally there are boxes for selection of gamma peaks for both high and low resolution detectors. In these boxes, the minimum and maximum energies can be specified together with the lower limits on the emission probabilities.

More information can be found on the Nucleonica wiki at www.nucleonica.com/wiki
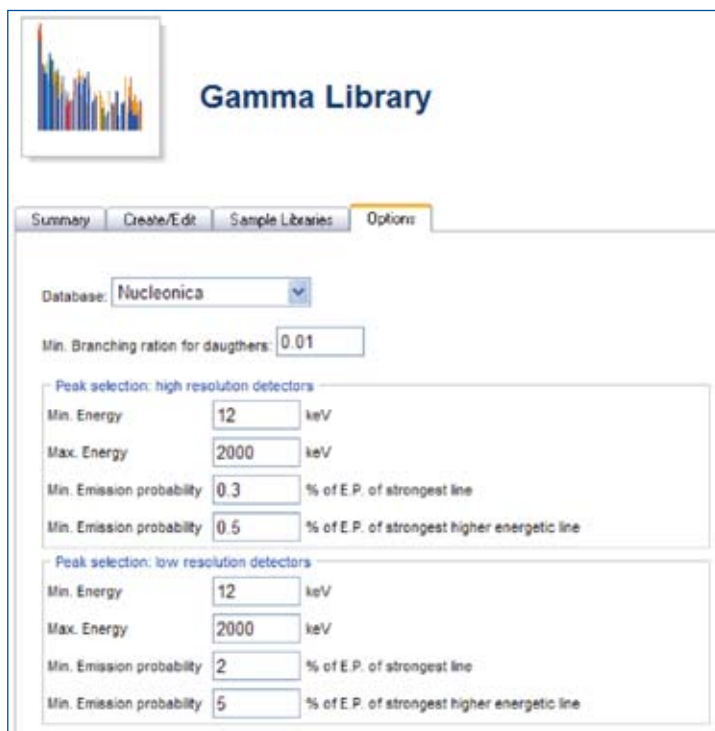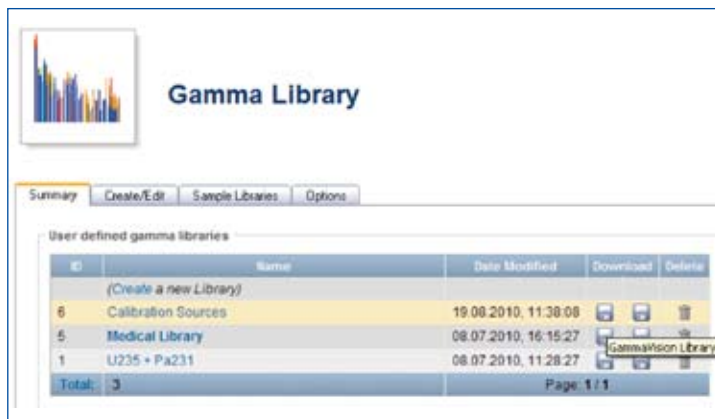
Nucleonica Scripting

The Nucleonica Scripting Language

The Nucleonica scripting is an object oriented language which is based on the physically intuitive classes, methods and properties. Through the script interface the user has access to the main Nucleonica applications and nuclear data. By combining results from multiple Nucleonica applications and nuclear data, users can go beyond the conventional single application approach for solving their specific experimental tasks and problems. Nucleonica applications are designed to be very user-friendly, intuitive, and require a minimum of learning time. For users, who prefer a more "hands on" approach, Nucleonica provides this with its scripting module. Scripting refers to a programming task, in which pre-existing components or applications are connected to accomplish a new task. In accordance with this definition, the Nucleonica scripting gives the user a powerful programming interface through which he/she can access basic nuclear data and run all the Nucleonica applications.

Class	Main methods	Related applications	Related classes
nuclide, vnuclide	Decay()	Decay Engine	decayResult
	Dosimetry()	Dosimetry and Shielding	doseResult
	DecayInfo()	Nucleonica database	decayInfo
	Radiations()	Nucleonica database	radiations
range	CalculateMono()	Range and Stopping Power	rangeResult
	CalculateCompound()	Range and Stopping Power	rangeResult
transport	Calculate()	Transport and Packaging	transportResult
korigen	callKorigen	webKORIGEN	korigenResult

The Nucleonica scripting is an easy-to-use physically intuitive object oriented programming language. The basics of the language, such as variable types (int, double, string or arrays), logical (&&, ll) and mathematical (+, -, *, /, %) operators, control structures (for and while loops, if statements) and built-in functions (sin, log, print, abs, exp, sqrt, pow etc.), are described in detail in the respective section of the Nucleonica wiki. This wiki also serves as an on-line reference on the features of the implemented classes, their properties and methods. With ready-to-use examples and pre-defined scripts, which are largely enriched with comments and explanations, users can easily learn the language and save the time when developing their own scripts. The basic components of the language (classes) are summarised (see table).

In the script, the classes are instantiated through the objects which provide access to specific properties (object.property) and methods (object.method(parameterlist)). The nuclide class is of the central importance in the Nucleonica scripting, as it gives access to all basic properties of nuclides and implements the most important Nucleonica applications, such as "Decay Engine" and "Dosimetry and Shielding".

Classes, Properties and Methods

One of the main classes is the nuclide class:
Properties: nuclide.Halflife as double 'half-life in second
nuclide.A as int 'integer mass
nuclide.Z as int 'integer charge
nuclide.Element as string 'element name (chemical symbol)
nuclide.Parity
nuclide.SpinFraction
etc …

Methods:
nuclide.Decay(quantity, unitQuantity, time, unitTime, steps, distance, accuracy, options)
nuclide.dosimetry(quantity, unitQuantity, energyRangeOption, shieldMaterial, distance, mode, thickness, threshold)
nuclide.transport()
etc …

A Simple Example

Ex: Specific functions has been defined such as the nuclide.Create(Z,A,Liso) method which loads into a nuclide object all the relevant properties (half-life, radiations, etc.) from the Nucleonica database. If one creates a nuclide object with the name Co_60,

```
nuclide Co_60;            // Declare the object Co_60, as an instance of the class nuclide
Co_60.Create(27, 60, 0);  // initialize the object Co_60 with data from the Nucleonica database
```

one can retrieve all its properties such as:
Co_60.A → 60 'mass number
Co_60.Z → 27 'charge number
Co_60.Element → "Co" 'element name (chemical symbol)

One can call the different methods in order to make a calculation or to retrieve further data based on this nuclide e.g.

```
decayResult Co_60_Decay;
Co_60_Decay = Co_60.Decay(1, "g", 5, "y", 20, 1, 0.01, "halflife, mass, activity, branching")
// launches the decay engine and
// gets results in Co_60_Decay object, an instance of class decayResult

radiations Co_60_gamma;
Co_60_gamma = Co_60.Radiations(0);     // retrieves radiations, where 0 is the code for gammas
```

Co_60_gamma.Count → 6 'number of gamma lines
Co_60_gamma.Energy(0) → 1332.5 'gamma-line n°1 in keV
Co_60_gamma.Probability(0) → 0.998 'emission probability of the gamma line n°1

Register as a Nucleonica User (free access)

Networking with Nucleonica

The networking features in Nucleonica provide tools to encourage the development of discussion communities around the applications and to enhance collaboration with a view to "capturing" the tacit knowledge (knowledge management) from the expert developers and passing this on to a wider community. The Networking Centre allows users to stay in contact with colleagues from workshops or conferences, meet scientists from similar areas of interest and build up an international contact list. The users can represent themselves (personal page) and their Institute/Organisation in the international science community. Nucleonica's Calendar can be used to enter information on forthcoming events, meetings, conferences etc. The user can decide if he/she wishes to share this information with other users. In this way a user-generated calendar of events is created. Alternatively, the user can decide to keep the information in his personal diary.

Registration

The entire registration process involves three steps: Registration, Change Login and Password, and Activate your Profile. To register with Nucleonica, go to the Nucleonica Homepage at www.nucleonica.com. In the left hand window panel, click on Free Access and Register as a Nucleonica User. Read the end user's license agreement. Tick the checkbox to agree to the terms of the license agreement. Fill out your details on the form and enter the automatically generated code. If you can't read the code please click on the image to generate a new access code. Submit the form by pressing the "Register" button. Access will be granted only to *bona fide* users. Shortly thereafter, you will receive an email with login and password. The login is just the email address you specified in the registration process. The password is an automatically generated combination of letters and numbers. Both of these can be changed after logging in to Nucleonica for the first time.

Change Login and Password

To login to Nucleonica, go again to www.nucleonica.com and enter your login and password in the top right of the page. This procedure will take you to the Nucleonica networking page. Following first login, it is recommended that you change both your login and password in My Settings – shown in the right panel of the main networking page. Both the login and the password can be changed.

Activate your Profile

To activate you profile, click on My Profile in the networking page (see the main screenshot overleaf) and then Edit. It is essential to check the tick boxes adjacent to the fields which you would like to share with other users. In the Profile tab, you can see the information which you have allowed other users to see. Adding a photo makes the community pages much more personal. Finally, remember to save this information by pressing the button *Save My Profile*. Additional information (for example publications, interests etc.) can be added in the *Additional Fields* at the bottom of the page.

Main Networking page

Following login, the user is directed to the main networking page (main graphic overleaf). This default setting can be changed in the My Settings such that following login, the user is directed to the Nuclear Science page. The networking page consists of three panels, from left to right: the navigation (with My Profile, My Community, etc.), Nucleonica Hot Topics and RSS feed from the Nucleonica Blog, and finally to the recent Nucleonica members and Forum. In addition to the left-most panel, further navigation buttons can be found at the top right of the page, above the blue banner. Here the user can directly access the pages: nuclear science, search, forum, calculator, etc. Also, in the taskbar, the user can directly access the Applications, Data, Knowledge, My Preferences, Print and Help. Access to the Nucleonica wiki is through this latter Help or by clicking on the [wiki] link in the left hand navigation panel.

My Community

The My Community page can be reached from the rightmost panel. Tabs provide access to community members, my contacts, and pending contacts. On the right hand side of each name, the user can send an email or add to contact list by clicking on one of the icons.

My Groups

A list of the Nucleonica groups can be seen in the All Groups tab in the My Groups page where the name of the group, the number of members, the group category and the group registration date are shown. A description of the group is given using the tooltip feature by placing the mouse cursor over the group name. Using the icons to the left of the group names, the group creator can edit or delete a particular group. In the tab My Groups, the user can see all the groups in which he/she is a member. In the tab Add/Edit Group, the user can create a new group of edit an existing group. There are open and restricted groups. All groups are defined as open by default. Group founders are able to change the group type in the Add/Edit Group tab. If the group is open, users can access as usual by clicking on the *Join* button. They will be accepted automatically. The group founder can reject a user. If the group is restricted, users can click on *Join* button. An email will be sent to the group founder in order to keep him posted about the join request. The mail is only sent to the group founder. The group founder can accept or reject the user's join request.

Wiki, Blog, Forum and Nuclear News
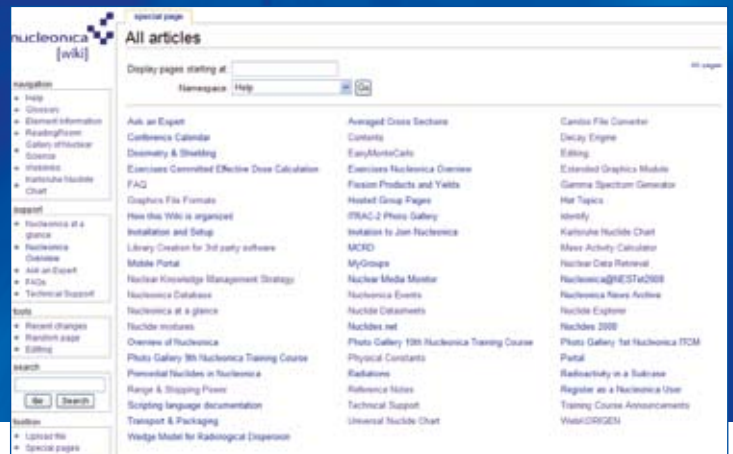
Nucleonica and Knowledge Management

Nucleonica is based on a number of "knowledge objects" ranging from the actual scientific applications to the wiki, blog and forum. In contrast to conventional paper-based documents, these are "electronic" knowledge objects. The aim here is to produce high quality information resources which are easily accessible to any user and can be maintained with the latest international nuclear data. In the context of Nonaka's knowledge spiral and the SECI model, these knowledge objects are aimed at supporting and enhancing the knowledge creation, transfer, and dissemination.

Nucleonica Wiki

The Nucleonica wiki is used to provide the technical documentation in support of the Nucleonica nuclear science portal. The basic characteristic of a wiki is that it allows the article author to directly edit and add content online (the word "wiki" means fast in Hawaiian) – there is no need for a web master or programmer to convert the text into html. In contrast to Wikipedia which can be edited by anyone, the Nucleonica wiki can only be edited by the Nucleonica experts and consultants. Most of the entries under "All Articles" or Help main wiki page are links to the technical documentation in support of the Nucleonica applications and nuclear data pages. Other main pages include: Glossary, Element information, ReadingRoom (articles, etc.), Gallery of Nuclear Science, Weblinks, Karlsruhe Nuclide Chart, Ask an Expert, FAQs, etc. Also shown is a search box for text searching in the entire wiki. A typical example of the documentation is shown for the "Decay Engine" application. Here the structure of this document is very similar to a chapter in a textbook. The advantage of using a wiki for such purposes is that the document can be kept up to date, and various versions of the document, and major and minor edits, can be followed (in the Recent Changes).

Nucleonica Blog

The Nucleonica Blog can be reached from the main Nucleonica web page or directly at www.nucleonica.com/blog. This page is used to provide latest information on Nucleonica nuclear science portal and related products such as the Karlsruhe Nuclide Chart. The blog provides an in-depth look at our activities in the field of nuclear knowledge management, and education and training in the nuclear sciences. It is also used as an archive for all such articles and has an own search box. The RSS blog feed is shown. There are two main categories in the Nucleonica blog: The Karlsruhe Nuclide Chart and Nucleonica.

Nucleonica Forum

The main goal of the Nucleonica forum is to capture the tacit knowledge of experts and peers alike within the specific context of the Nucleonica applications. Initially a user will have little knowledge of the application. However, after some experimentation, questions can be posted in the Nucleonica forum on a particular application. The approach is based on a question and answer interaction between the expert, who possesses tacit knowledge, and users. The knowledge or know-how flow is "externalized" by the fact that the question and answer dialogue is fully recorded in the forum database. The Nucleonica forum can be regarded as a "community of practice" to support this process. Scientists can assist each other on a reciprocal basis on research projects through this "social networking" and "crowdsourcing". The basic principle followed here is that knowledge can be created through dialogue and interaction between contributors and made explicit through mutual discussion in the online forum. The Nucleonica forum can be accessed directly from the main networking page. This forum can be read by anyone with an internet connection. To post a discussion topic (thread) or reply to an existing topic the user must register.

Nuclear News

The nuclear news aggregation service provides latest news and information on nuclear issues. This information is provided by our web crawler which scans thousands of newspapers worldwide for nuclear related news. The news is updated at least on an hourly basis. The user can select the number of displayed news articles, the language (English, French, German), and the news categories (Nuclear (General), Nuclear Decommissioning, Nuclear Medicine, Nuclear Reprocessing, Nuclear Safety).

How to Enter and Leave the Wiki

There are various ways to enter the wiki. From the main Nuclear Science or Networking pages, when the user clicks on the nucleonica [wiki] logo a new browser window opens with the main wiki page (All Articles) shown above. The user can then select an article from the main panel or a category from the navigation panel. The Decay Engine wiki page is shown. To leave the wiki, the browser window is closed. The wiki can also be reached through the Help link in the taskbar. This is of interest when using a specific Nucleonica application. When using the Decay Engine module, for example, clicking on the Help in the taskbar will open a new browser window with the technical documentation on the Decay Engine (shown). Finally the wiki can be reached from the Knowledge menu in the taskbar.

NUCLEAR NEWS

Defusing nuclear tension with Tehran | Johan Bergenäs

AUG 19 — Behind warlike rhetoric, the signs are that sanctions have been effective: the time is ripe for renewed diplomacy with Iran Ayatollah Ali Khamenei, Iran's supreme leader, said Wednesday that talks abo [...]

No major alarm once Bushehr NPP activated - Alon Ben-Meir

AUG 19 — John Robles : ";Voice of Russia"; world service. This is John Robles. I'm talking with Professor Alon Ben-Meir from the Center for Global Affairs at New York University. He is a Middle East expert. H [...]

Commander Extends Malrock Gold Zone With Initial Drill Results

AUG 19 — VANCOUVER, BRITISH COLUMBIA – (Marketwire) – 08/19/10 – Commander Resources Ltd. (TSX VENTURE: CMD) has expanded the size and potential of the Malrok Zone with results from the first nine holes rec [...]

Nuclear Science Training Courses

Background to the Courses:

Nucleonica training courses in nuclear science are aimed specifically at the areas of nuclear safety, nuclear security, and environmental radioactivity. The courses introduce the basic concepts of nuclear science and technology. Core topics range from the history of radioactivity, nuclide charts, radiation protection and health physics, gamma spectrometry, through to the storage and transportation of radioactive materials. Recent exciting developments in nuclear science are highlighted in a series of special topics covering nuclear forensic science / illicit trafficking, nuclear science with high intensity lasers, environmental radioactivity, radiation hormesis and the LNT hypothesis, etc. Lectures are followed by a series of "hands-on" case studies based on the use of the Nucleonica web-based applications to give the user direct experience in the above areas.

Who should attend

The courses are aimed at persons who provide technical support (measurements, interpreting results, drawing conclusions, making recommendations) for the actions in response to environmental radioactivity and nuclear security issues. The courses are suitable, for example, for physicists, radio-chemists, health physicists, technical experts etc. from the nuclear industry, nuclear research organizations, universities, regulatory authorities and nuclear medicine institutes. Completion of this course will enhance and support nuclear related decision-making as well as provide formal academic principles in nuclear science. Course requirements are a basic knowledge of nuclear science, physics and chemistry. The courses are held in English.

What makes the courses unique is the emphasis on interactive and hands-on learning through the use of Nucleonica – a suite of powerful and versatile web-based applications for calculations on radionuclides and their radiations. With examples, exercises and dedicated case studies, a whole variety of core and topical issues in nuclear science and technology will be presented by experts in their respective fields.

Key Advantages of Nucleonica

- Manage all your data in a single browser-based system: The web applications are browser and operating system independent and can be accessed with Internet Explorer, Mozilla-based browsers (Mozilla, Firefox, Netscape) and a variety of other browsers.

- Don't waste time writing and testing programs: Nucleonica provides you with user friendly, reliable, and fast modules (for decay, dosimetry & shielding, range and stopping power, transport and packaging, reactor irradiation calculations, gamma spectrometry, etc.)

- Improve the quality of your work: avoid the tedious task of searching for nuclear data. Nucleonica uses the most recently evaluated nuclear data from international datafiles (JEFF3.1, 8th Table of the Isotopes, ICRP72, etc.).

- Publication quality scientific graphs at any time from any location. Nucleonica webGraph is easy to use, and delivers publication quality graphs in a variety of formats (GIF, JPG, PNG, EPS, EMF, SVG).

- Keep informed on nuclear developments: NUCLEONICA web crawlers scan hundreds of websites every few minutes to bring you the latest nuclear news.

- Keep track of your recent activities: NUCLEONICA will "remember" your recent activities and store these in a Personalized Desktop with detailed user preferences.

Testimonials (from the ITRAC-2): 2nd Advanced Training Course on Illicit Trafficking and Radiological Consequences with Nucleonica, Karlsruhe, November 4 – 6th, 2009):
"… and I hope Nucleonica will be like a key word for nuclear chemists and nuclear physicists" (Zeynep Talip)
"First of all I would like to thank all of the people who put effort into this workshop and developing nucleonica. It was great to hear all those talks from specialists around the world. Sharing ideas and connecting with colleagues from other institutions was an excellent experience." (Tolga Inal)
"I found the course was very helpful to learn how the nucleonica works and what it is capable of doing. The various seminars were positive. They linked the theory with real life, so that it was possible to get a feeling for dangers involved and the security needed (handling radioactive materials)." (Marika Vespa)
"I deeply appreciated the wise combination of high quality lectures and exercises, as well as the efficient organization of the various activities." (Francesca Quinto)
"… Congratulations! Great and modern platform …" (Rolf Arlt)

Further information on the courses, together with full presentations are given on the Nucleonica wiki at www.nucleonica.com/wiki

Verification, Validation and Testing

For the physical scientist, it is primarily of importance to know if the calculated results are "correct" – i.e. to what extent the results agree with experiment and/or other computer programs. Validation assures that the results agree with experiments and/or other programs. Verification aims at checking that the product has been built according to the requirements and design specifications. Testing is the process by which bugs and error are eliminated. In this context the Nucleonica modules are undergoing continuous development based on user-feedback through questions, remarks, and suggestions, for example, in the Nucleonica Forum. In particular there are two main questions of interest:

How reliable is the nuclear data in Nucleonica?
How reliable are the results from the calculation modules?

Nuclear Data

A key advantage of Nucleonica is that the user has access to the most recently evaluated nuclear data from international datafiles. The user can thereby improve the quality of his work by using this nuclear data. The Nucleonica database is based on the Joint Evaluated Fission and Fusion (JEFF3.1) radioactive decay datafile [1] which contains decay data on 3852 nuclides in ground and isomeric states. The relational nature of the Nucleonica database allows for fast searching and data retrieval in comparison to the non-relational JEFF3.1 datafile. The Nucleonica database contains information on additional nuclides and their half-lives which are not listed in JEFF3.1 but are present in NUBASE ´03 [2], bringing the total number of nuclides (ground and isomeric states) in the Nucleonica database to 3896. In addition, NUBASE ´03 data on the atomic weights, binding energies, mass excesses, and abundances are included in the Nucleonica database. To support the nuclear science applications in Nucleonica, the database is further complemented by a variety of data from other sources, e.g. spectral data (energies, emission probabilities etc.) from the 8th table of isotopes [3] can be selected for comparison and for library creation for gamma spectroscopy. Further details are given in the Nucleonca wiki www.nucleonica.com/wiki
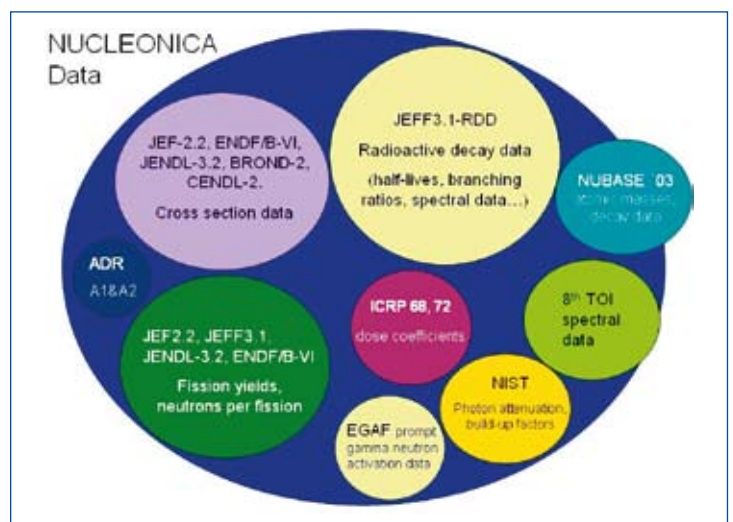
Nucleonica Calculation Modules

With regard to the reliability of the calculation modules, the following modules have been extensively tested: The **Mass Activity Calculator** relies essentially only on simple conversions from one set of units to another. The **Decay Engine** is based on an analytic solution to the Bateman equations and, as such, requires no experimental validation. Internal checks (such as conservation of total number of atoms and mass-energy) ensure no systematic errors. Calculation results can also be compared to those using webKORIGEN (in the decay mode).

Range and Stopping Power: The results have been compared with a number of programs such as Pstar, Astar and Estar for protons, alphas and electrons respectively. It has been shown that the accuracy of the results is is better than 5% for protons alphas, and heavy ions, 10% for electrons and positrons, and less than 7% for muons for the total stopping powers and the CSDA Ranges. Full details are given in the Range and Stopping Power wiki page.

webKORIGEN: Over the past three decades, a considerable effort was made to upgrade and extend the nuclear data and analysis capabilities of the KORIGEN code especially in the field of calculations for German power plants: PWRs and BWRs. During this period the code has been extensively validated wherever possible against experimental results. Recent developments enable the code to predict accurately the decay heat of advanced fuels. The KORIGEN results for transmutation (inert matrix) fuels irradiated in fast spectrum were validated in the framework of a benchmark for European First Industrial Transmuter (EFIT) [4]. WebKORIGEN has also been benchmarked in an international exercise on radiotoxicity evaluation of spent nuclear fuel [5].

Gamma Dosimetry & Shielding: There are a number of cases where the module have been directly tested against literature results (e.g. Co60, Na24, etc.). These are described in more detail in the Nucleonica wiki. More generally, the results have been tested directly against Monte Carlo codes (e.g. MCNP).

The Gamma Spectrum Generator: The measurements have been performed with Cs137, Co60 and Eu152 thin standard spectrometry γ-ray sources. The sources were located on the detector axis and measured twice, at 5 cm and 17 cm from the detector end cap. Results are shown: Top: comparison of the calculated (curve) and experimental (circles) detector responses for a HPGe detector and point Cs137 source located at 17 cm distance from the detector end cap; Bottom: comparison of the calculated (curve) and experimental (circles) detector responses for a HPGe detector and point Eu152 source located at 17 cm distance from the detector end cap. Further details can be found in the references [6,7].
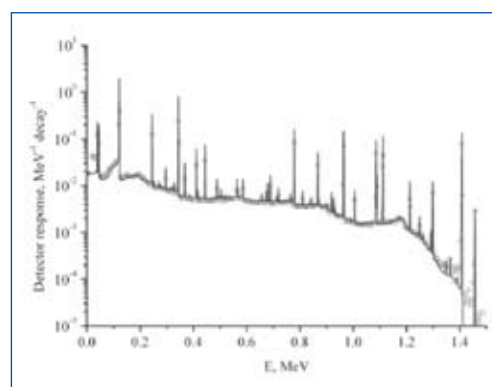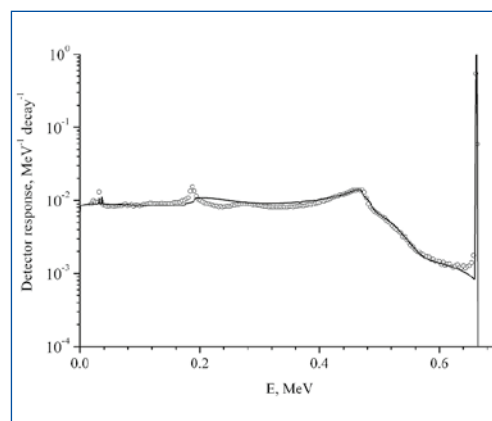
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[3] R.B. Firestone, "Table of Isotopes, 8th edition", John Wiley & Sons Inc., (New York, 1996). Updated in 1998.
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[6] A. Berlizov, et al., A Collection of Reference HPGe Gamma-Spectra for Shielded / Unshielded Radionuclide Sources and Special Nuclear Materials, Technical Note JRC-ITUTN-2009/25, 2009. See also: Fast and Accurate Approachto g-Spectrum Modelling: A Validation Study with a Shielded / Unshielded Voluminous Uranium Sample, Applied Radiation and Isotopes 68 (2010) 1822 – 1831.
[7] V. Kleinrath, A Study of Gamma Interference Scenarios for Nuclear Security Purposes, Measurements and Modelling using the Nucleonica Tools, JRC-ITU-TN-2010/21.

Nucleonica Knowledge Objects, Packages and List of Features

In the following table, "knowledge objects" refer to the individual programs listed in the table of contents (i.e. under the Nuclear Data, Applications, Tools, and Networking categories). These are listed in the first column. Columns 2 and 3 provide a list of features of each knowledge object for the Free and Platinum packages.

- The **Free package** provides user access to all the knowledge objects with restricted features. This gives users the opportunity to test the basic features and obtain a feeling for the portal.
- The **Premium package** provides user access to all the knowledge objects with full features. There is an annual user charge for the Premium package. Individual and institutional multi-user licenses are available.

Knowledge Objects	Free	✔	Premium	✔
Nuclide Explorer				
Types of charts	Decay mode	✔	Decay mode	✔
			Half-lives	✔
			spin, parity, spin and parity	✔
			Binding energy	✔
			Stable / unstable	✔
			create new charts / User defined	✔
Change background colour			yes	✔
Filter decay modes			All features	✔
Nuclide Datasheets				
Basic reference data	Half-lives, BRs, decay modes etc.	✔	half-lives, BRs, decay modes etc.	✔
			derived data (heat gammas neutrons, etc.)	✔
Cross sections			averaged	✔
			Point-wise (in graphical form)	✔
			Average (multi-group)	✔
			(n,xn)	✔
Radiation databases			JEF3.1, 8th Table of Isotopes	✔
			discrete energies, emission probs.	✔
Output			view data in graphical form	✔
			download tables in Excel, csv formats	✔

Knowledge Objects	Free	✔	Premium	✔
Fission Yields				
Nuclides	U-235, Pu-239	✔	U-235, Pu-239	✔
			All other fissionable nuclides	✔
Databases	JEF3.1	✔	JEF3.1	✔
			ENDF, JENDL	✔
Neutron spectrum	Thermal fission	✔	Thermal fission	✔
			Fast, 14 MeV, spontaneous fission	✔
Compare with other fission parents			yes	✔
Compare different libraries			JEF3.1, ENDF, JENDL3.2	✔
Output			download tables output in Excel, csv formats	
Nuclear Data Retrieval				
Databases	Nucleonica	✔	Nucleonica	✔
			8th TORI, ICRP 68 & 72, EGAF	✔
Nuclide search			yes	✔
Radiation search	yes	✔	yes	✔
Advanced search			yes	✔
Output			download table output in Excel, csv formats	✔
Mass Activity Calculator				
Sources	Single nuclides	✔	Single nuclides	✔
			nuclide mixtures	✔
Conversion to/from	mass/activity/atoms/moles	✔	mass/activity/atoms/moles	✔
			gamma dose rate	✔
			effective dose	✔
			isotopic powers	✔
Decay Engine				
Sources	single nuclides	✔	single nuclides	✔
			nuclide mixtures	✔
Calculated/output quantities	half-life, mass, activity, atoms	✔	half-life, mass, activity, atoms	✔
Options			branching ratios (BRs), decay mode	✔
			Isotopic powers (α, $\alpha+\beta$, $\alpha+\beta+\gamma$)	✔
			gamma dose rate, gamma emission rate	✔
			ingestion, inhalation radiotoxicities	✔
			Spontaneous fission rate	✔
			disintegrations	✔
			released energy, helium production	✔
Additional Features			create nuclide mixture from decay output	✔
			rescale output	✔
Output	as tables and graphs onscreen	✔	as tables and graphs onscreen	✔
			download tables in Excel, csv formats	✔
			download Graphs	✔

Knowledge Objects	Free	✔	Premium	✔
Dosimetry & Shielding				
Sources	single nuclides	✔	single nuclides	✔
			nuclide mixtures	✔
Modes of operation	gamma dose rate	✔	gamma dose rate for a given shield and source	✔
			shield thickness for given dose rate	✔
			source strength for given dose rate and shield	✔
Options			Set threshold energy, etc.	✔
			Dose Rate/Thickness Graph	✔
Output			download tables in Excel, csv formats	✔
			download Graphs	✔
Range & Stopping Power				
Projectiles	electrons, positrons, protons, alphas	✔	electrons, positrons, protons, alphas	✔
			positrons, muons, heavy ions	✔
Targets	elements	✔	elements	✔
			predefined compounds	✔
			user-defined compounds	✔
Options			alternative stopping power units	✔
Output			graphs of range & stopping power	✔
			Bragg curve	✔
			Output table	✔
webKORIGEN				
Number of nuclides	Top 20	✔	>800	✔
Modes of operations	reactor irradiation	✔	reactor irradiation	✔
			reactor irradiation and decay	✔
			decay	✔
			irradiation, decay, partitioning, cooling	✔
Neutron Activations			in thermal , PWR, BWR, FR neutron spectra	✔
Reactor type	PWR	✔	PWR	✔
			BWR	✔
			Fast reactor	✔
			Dedicated facility	✔
Types of fuel	UOX	✔	UOX	✔
			MOX	✔
Output	Actinides, FPs, and helium	✔	Actinides, FPs, and helium	✔
			additional chemical sub-categories	✔
			Plot k_∞, nuclides, elements, totals, etc.	✔
Universal Nuclide Chart				
	all features	✔	all features	✔

Knowledge Objects	Free	✔	Premium	✔
Nuclide Mixtures				
	Not available to "Free" users		Pre-defined mixtures	✔
			user-defined mixture	✔
			edit, save, delete mixtures	✔
			upload and download mixtures	✔
			rescale feature	✔
Nucleonica Scripting				
			all features	✔
Gamma Library Creation				
			all features	✔
Gamma Spectrum Generator				
Sources	Single nuclides	✔	Single nuclides	✔
			nuclide mixtures	✔
Detectors	NaI	✔	NaI, HPGe	✔
Configurations	two standard	✔	six standard	✔
			User defined detector configuration	✔
Options			Edit and save detector configuration	✔
			decay during cooling and counting	✔
			effects of backscatter radiation	✔
			display efficiency curves	✔
Cambio File Converter				
File input format	formats in general use	✔	formats in general use	✔
File output format	.spe (IAEA format)	✔	spe (IAEA format)	✔
			6 additional formats including n42	✔
Spectrum display			sample spectra provided	✔
			graphical display of converted files	✔
Spectrum analysis			slider control, cross-hair, trackball	✔
			analysis using standard libraries	✔
Output			Print graph	✔
			download graphs (multiple formats)	✔
webGraph				
	input data manually	✔	input data manually	✔
			input from Excel	✔
			Save configuration (graph + data) as xml	✔
			upload graph configuration (xml)	✔
			save graph as gif, jpg, emf, eps, png, svg	✔

Uuo 294
0.89 ms

118 Uuo

117 Uus Uus 293 14 ms Uus 294 78 ms

116 Uuh Uuh 290 15 ms Uuh 291 18 ms Uuh 292 18 ms Uuh 293 83 ms

176

Uup 287 32 ms Uup 288 87 ms Uup 289 0.22 s Uup 290 ~16 ms

114 Uuq Uuq 286 130 ms Uuq 287 0.48 s Uuq 288 800 ms Uuq 289 2.7 s

Uut 283 100 ms Uut 284 480 ms Uut 285 5.5 s Uut 286 ~20 s

174

Cn 282 Cn 283 Cn 284 Cn 285 29 s