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Activity Report of the ENEA Nuclear Data Project in 2008

Prepared by

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March 2009

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Activity Report of the ENEA Nuclear Data Project in 2008

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Abstract

Descriptions are given of the nuclear data activities undertaken during 2008 at the Bologna Research Centre of the Italian National Agency for New Technologies, Energy and the Environment (ENEA).

March 2009

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General Quantum Mechanics

An algebraic model of relativistic scattering

When the Hamiltonian *H* of a quantum-mechanical system is a function of a Casimir invariant of a non-compact Lie group, *G*, the *S* matrix can be worked out analytically from an intertwining relation between Weyl-equivalent representations of *G*. Furthermore, if the system is relativistic, the *S* matrix has definite properties under transformations of the Poincaré group. The two requirements can be met in the approach to relativistic dynamics proposed by Bakamjian and Thomas by expressing the interacting mass operator *M* in terms of a quadratic Casimir invariant of *G*. A simple example is provided by the Coulomb interaction between two relativistic spinless particles, where *G* is identified with *SO(3,1)*. The scattering amplitude is obtained by intertwining two Weyl-equivalent representations $(\tau,0)$ and $(-\tau,0)$ belonging to the principal series, with $-\infty < \tau < +\infty$. If the two bosons are identical, the properly symmetrized scattering amplitude yields the well-known Mott formula for the elastic scattering cross section [A.1].

Overcritical *PT*-symmetric square well in the one-dimensional Dirac equation

When the non-Hermitian Hamiltonian *H* of a quantum-mechanical system commutes with the product *PT* of parity *P* and time reversal *T* and the bound-state eigenfunctions are eigenfunctions of *PT* , the corresponding eigenvalues of *H* are real and the system exhibits an exact *PT* symmetry. By increasing the strength of the imaginary part of *H*, some or all eigenfunctions may no longer be eigenfunctions of *PT*, and the corresponding eigenvalues turn into complex conjugate pairs: the *PT* symmetry is thus spontaneously broken.

An additional effect of spontaneously broken *PT* symmetry can be seen in a relativistic system obeying the Dirac equation with the time component of a vector potential. Consider the Hermitian case when the depth of the potential well becomes larger than the threshold of particle-antiparticle pair production: the potential becomes overcritical with respect to spontaneous pair production. The signature of overcriticality in one-dimensional systems is given by transmission resonances at negative energies inside the potential well, interpreted as bound states that merge with the negative-energy continuum of scattering states. If the potential well is *PT*-symmetric, overcriticality effects can be damped by increasing the imaginary strength of the well. While bound state energies become complex above some critical value of the imaginary strength, transmission resonances at negative energies inside the well become weaker and weaker, but do not disappear even at large imaginary strength [A.2].

.Non-local *PT*-symmetric potentials in the one-dimensional Dirac equation

A peculiarity of non-local *PT*-symmetric potentials is that they do not satisfy the intertwining relation $TH = H^{\dagger}T$, where $H^{\dagger}$ is the Hermitian conjugate of *H*. As a consequence, the transmission coefficients for progressive and regressive waves ($T_{L\rightarrow R}$ and $T_{R\rightarrow L}$, respectively) are different, since one can prove that they have the same modulus and different phase. The reflection coefficients $R_{L\rightarrow R}$ and $R_{R\rightarrow L}$ have different modulus and the same phase, as in the case of local potentials. Unitarity is broken in both cases.

If the non-local *PT*-symmetric potential has a separable kernel of the form:

$$K(x,y) = g(x)e^{iax}h(y)e^{iby} ,$$

with *g* and *h* even real functions of their arguments, and *a* and *b* real constants, the one-dimensional Dirac equation can be solved analytically by means of the Green function method, and the properties of scattering and bound-state wave functions can be described in full detail. This has been done for a scalar-plus-vector mixture of one-dimensional Yamaguchi potentials, with:

$$g(x) = e^{-c|x|} \, , \; h(y) = e^{-d|y|} \, ,$$

in which *c* and *d* are positive constants. The three-dimensional Yamaguchi potential was originally proposed for the description of bound and scattering states of the proton-neutron system.

The wave functions and their non-relativistic limits turn out to be particularly simple when the scalar and vector strengths are either equal, or opposite, $c_V = \pm c_S$ [A.3], thus providing the one-dimensional equivalent of three-dimensional spin and pseudo-spin symmetry. The latter corresponds to $c_V = - c_S$, and is observed in the spectra of heavy nuclei.

Nuclear Structure Theory

Dynamic chirality in the interacting boson-fermion-fermion model

Doublets of $\Delta I = 1$ bands almost degenerate in energy have been observed in odd-odd nuclei in the $A \sim 105$, $A \sim 130$ and $A \sim 190$ mass regions. They have been interpreted as chiral doublets in a geometrical model where a triaxial even-even core is coupled to a high-*j* particle-like proton and a high-*j* hole-like neutron (or vice versa) and the angular momenta of the core, the odd proton and the odd neutron form a mutually orthogonal right-handed or left-handed triplet in the intrinsic reference frame. This static picture of chirality is not present in the interacting boson-fermion-fermion model (IBFFM) of odd-odd nuclei, where the even-even cores in the above mentioned mass regions are not statically triaxial, but rather soft with respect to γ vibrations, and the yrast and yrare bands forming the doublets in odd-odd nuclei have a different dynamical structure.

As a consequence, the almost degenerate energies of the levels of same angular momentum are reproduced, but the *E2* and *M1* transitions in the two bands are different, at variance with the predictions of static chirality models, but in reasonable agreement with experimental data. Nonetheless, careful choice of IBFFM parameters permit the generation of dynamic chiral configurations, playing a significant but never dominant role in the pattern of electromagnetic transitions in the doublet.

Figure 1 shows two typical behaviours of *E2* and *M1* transitions in the yrast and yrare bands of an odd-odd nucleus within the $A \sim 130$ mass region, corresponding to an achiral configuration (case A) and a dynamic chiral configuration (case B). One observes in the latter case particular the marked odd-even staggering of *B(M1)* values in both bands [A.4].

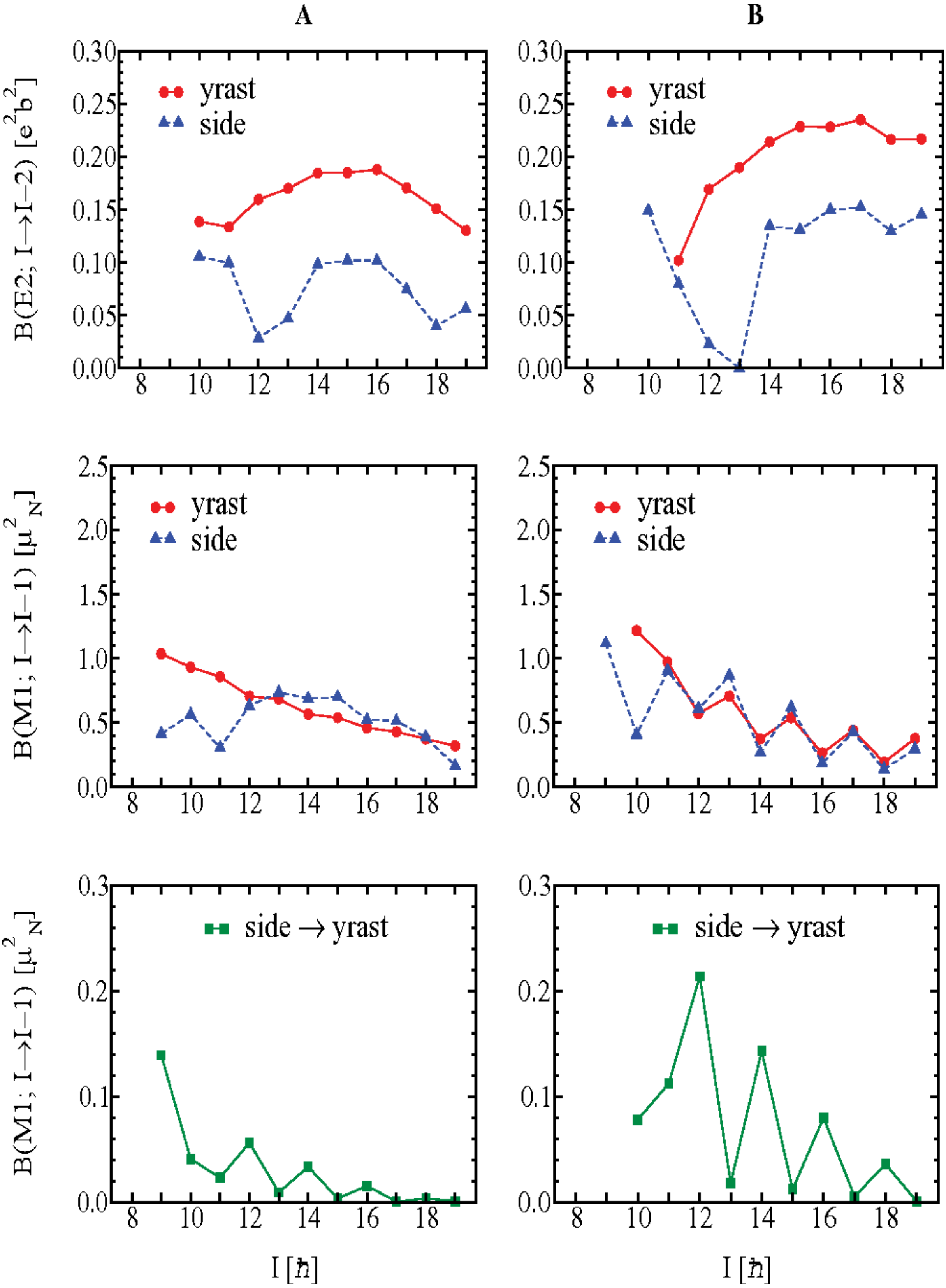

Fig.1. Calculated *B(E2)* and *B(M1)* values for intra-band and inter-band transitions of yrast and yrare bands of an odd-odd nucleus within the *A ~ 130* mass region. Case A (left panels): achiral configuration; case B (right panels): dynamic chiral configuration..

Nuclear Reaction Theory and Experiments

Measurements of Neutron Cross Sections at the n_TOF Facility, CERN

Publication of experimental results obtained in the 2002-04 campaign at the n_TOF facility, CERN, continued in 2008 with definitive values of neutron capture cross sections of ^{90}Zr [A.5] and ^{91}Zr [A.6]. The neutron capture cross sections of *Zr* isotopes have important applications in nuclear astrophysics and reactor design. In particular, as a consequence of the small capture cross section, the neutron-magic ^{90}Zr nucleus is one of the key isotopes for the stellar *s*-process, acting as a bottle-neck in the neutron capture chain betwen the *Fe* seed and the heavier isotopes. The *(n,γ)* cross section has been measured at the n_TOF facility at energies up to 70 keV, where 45 resonances have been observed, 10 of them for the first time, thanks to the high resolution and low backgrounds of n_TOF. Furthermore, the accuracy of the Maxwellian averaged cross section for *s*-process calculations has been improved by more than a factor of 2 [A.5].

Consider the *s*-process path: ^{91}Zr follows the neutron-magic ^{90}Zr and belongs to the critical mass region around $A = 90$. Massive stars in which the *s*-process takes place during the pre-supernova evolution, contribute only to the *s* abundances below $A = 90$. The *s* abundances from *Zr* to *Bi* constitute the main *s* component and are produced in low mass asymptotic giant branch stars. *Zr* assumes a crucial role situated at the matching points of both components. The $^{91}Zr(n,\gamma)$ cross section has been measured at n_TOF for energies up to 26 keV, where accurate data for 157 resonances have ben obtained – 33 resonances are either absent from the main databases or have been observed for the first time. Strength functions S_0 and S_1, as well as average *s*- and *p*-wave resonance spacings D_0 and D_1 have been extracted from resonance fits. The deduced Maxwellian averaged cross section (MACS) is in good agreement with values in the literature [A.6]. Fig. 2 shows the temperature dependence of the MACS deduced from n_TOF measurements of ^{91}Zr in comparison with a previous compilation.

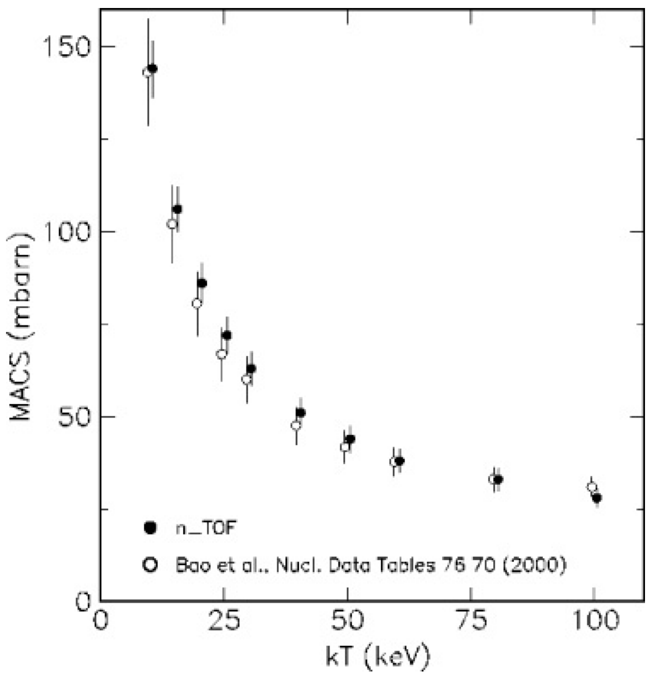

Fig. 2 Temperature dependence of the Maxwellian averaged cross section of ^{91}Zr.

Partial results on neutron capture by other isotopes have been presented at various conferences, with particular reference to ^{206}Pb [A.7], $^{186,187,188}Os$ [A.8], $^{92,93,94,96}Zr$ [C.1], ^{197}Au [C.2].

Nuclear Data Processing and Validation

Work on nuclear data processing and validation has been mainly devoted to the continuation of generation, testing and reporting of fine-group coupled neutron and photon cross-section libraries and broad-group-derived cross-section libraries for nuclear fission applications. VITAMIN-B6 (199 n + 42 γ) American library energy group structure was adopted for the fine-group libraries, while the BUGLE-96 (47 n + 20 γ) American library group structure was assumed for the broad-group libraries. The resulting cross-section libraries are based on the most recently released OECD/NEA Data Bank (JEFF-3.1), American (ENDF/B-VII.0) and Japanese (JENDL-3.3) evaluated nuclear data libraries. Libraries in the VITAMIN-B6 group structure are based on the Bondarenko (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects, and were produced in the AMPX and MATXS formats. BUGLE-96 group structure libraries were generated in the FIDO-ANISN format, through collapsing from the fine-group libraries in AMPX format with proper problem-dependent cross-section self-shielding. These working libraries are mainly dedicated to LWR shielding and structural component (e.g. LWR pressure vessel and internals) dosimetry [C.3], but can also be applied to dosimetry analyses in support of BNCT (Boron Neutron Capture Therapy) medical activities.

Consider the JEFF-3.1 libraries: work on the VITJEFF31.BOLIB fine-group library in AMPX format was completed with the compilation of a comprehensive user's manual [R.1]. The VITJEFF31.BOLIB package was then transferred under contract to OECD/NEA Data Bank for free distribution, and assumed the denomination NEA-1810 ZZ VITJEFF31.BOLIB. A broad-group library in FIDO-ANISN format, derived from VITJEFF31.BOLIB and named BUGJEFF31.BOLIB, was tested on the VENUS-3 neutron shielding benchmark, dedicated specifically to the improvement of the accuracy of dosimetry calculations in the PWR internals. A massive validation study of the fine-group library MATJEFF31.BOLIB in MATXS format was performed with transport codes on the same set of criticality safety benchmark experiments used for the VITJEFF31.BOLIB library validation: about 90 critical experiments with thermal, intermediate and fast neutron fission spectrum. The transport calculations were performed with the ONEDANT one-dimensional (1D) discrete-ordinates transport code of the American DANTSYS system of deterministic codes. Self-shielded working libraries were generated with the TRANSX-2.15 code which performed the interpolation of the cross-section self-shielding factors and the format conversion of the cross sections.

As for the ENDF/B-VII.0 libraries, testing of the VITENDF70.BOLIB and MATENDF70.BOLIB libraries in AMPX and MATXS format, respectively, was completed on the same set of criticality benchmark experiments cited previously. Both the discrete ordinates transport codes XSDRNPM (1D module of the SCAMPI American data processing system) and DORT (2D module of the DOORS American system) were used in the validation of VITENDF70.BOLIB, while the ONEDANT code was used to test MATENDF70.BOLIB. The calculated k-effective (k-eff) results were also compared with the corresponding results obtained by means of the MCNP-4C code, which used a previously prepared ENDF/B-VII.0 continuous-energy library in ACE format.

With regard to fine-group libraries in the VITAMIN-B6 group structure based on the Japanese JENDL-3.3 library of evaluated nuclear data, the data processing and validation of the new libraries VITJENDL33.BOLIB in AMPX format and MATJENDL33.BOLIB in MATXS format were completed. They were generated through an ENEA-Bologna modified version of the NJOY-99.160 American nuclear data processing system, used previously to generate the fine group libraries VITJEFF31.BOLIB, MATJEFF31.BOLIB, VITENDF70.BOLIB and MATENDF70.BOLIB. This modified version contains an ENEA-Bologna revised patch for the GROUPR module dedicated to extend the group-wise data processing capability to the evaluated data files, e.g. 69 JEFF-3.1 nuclear data files, including non-Cartesian interpolation schemes for secondary neutron energy distributions. VITJENDL33.BOLIB and MATJENDL33.BOLIB were tested on the same set of criticality safety benchmark experiments used for the validation of other similar libraries. We stress that the JENDL-3.3 library of evaluated nuclear data does not include the thermal scattering law data for bound nuclides, nor photo-atomic data. These important types of data were taken from the ENDF/B-VII.0 evaluated nuclear data library. Finally, the new broad-group BUGJENDL33.BOLIB library in FIDO-ANISN format was obtained through proper collapsing from the VITJENDL33.BOLIB library in AMPX format.

Collapsing was performed by means of the data processing package designated "ENEA-Bologna 2007 Revision of SCAMPI". This package was transferred to OECD/NEA Data Bank, in parallel with the release of the NEA-1810 ZZ VITJEFF31.BOLIB library, to permit further potential data processing dedicated to the new libraries based on JEFF-3.1, ENDF/B-VII.0 and JENDL-3.3. A new updated and corrected version of the AMPX/SCAMPI system has been released by OECD/NEA Data Bank with the designation PSR-0352/05 SCAMPI, and was necessary to translate the fine-group cross sections in the AMPX format and to collapse these data for the generation of self-shielded cross sections of broad-group working libraries in FIDO-ANISN format.

All these activities were performed with fundamental contributions by a specialist in nuclear data processing, formerly at the Institute of Physics and Power Engineering of Obninsk (IPPE-Obninsk, Russian Federation).

The horizontal and vertical sections of the geometrical model of the VENUS-3 experiment are reported in Figs. 3 and 4. The Calculated/Experimental (C/E) results for the dosimeter equivalent fission fluxes are reported in Figs. 5, 6 and 7, respectively for the *In-115(n,n')*, *Ni-58(n,p)* and *Al-27(n,α)* dosimeters.

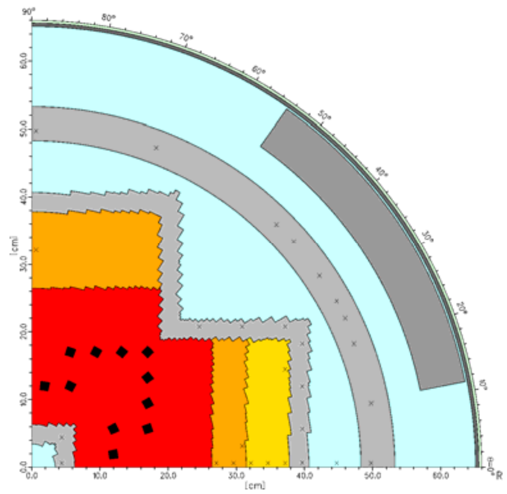

Fig. 3 VENUS-3 horizontal section at Z = 114.50 cm, dosimeter locations « x », TORT-3.2 (R,Θ,Z).

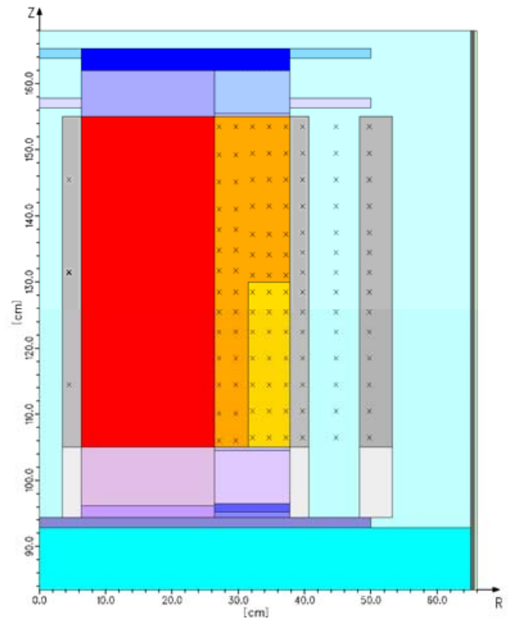

Fig. 4 VENUS-3 vertical section at Θ = 0˚, dosimeter locations « x », TORT-3.2 (R,Θ,Z).

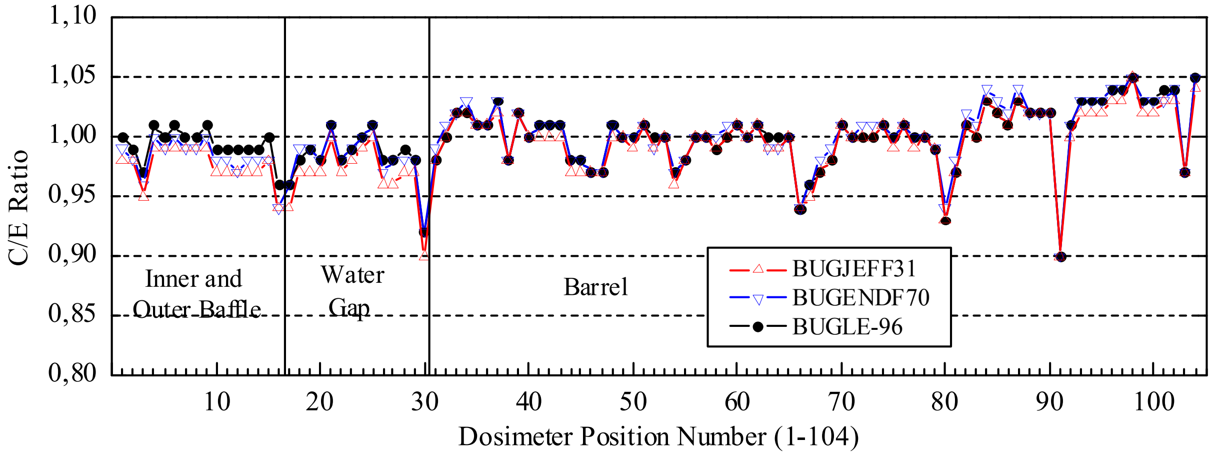

Fig. 5. VENUS-3: In-115(n,n') equivalent fission flux ratios (Calculated/Experimental).

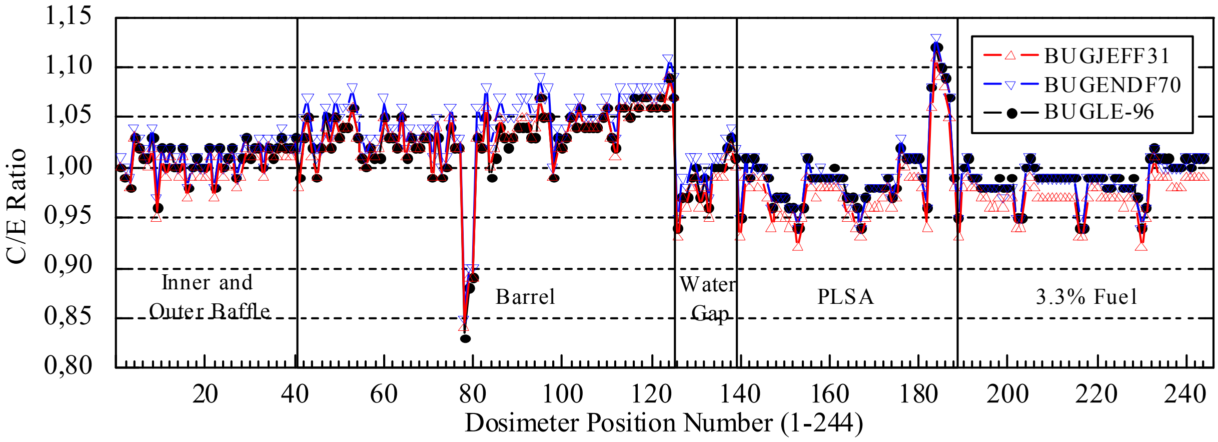

Fig. 6. VENUS-3: Ni-58(n,p) equivalent fission flux ratios (Calculated/Experimental).

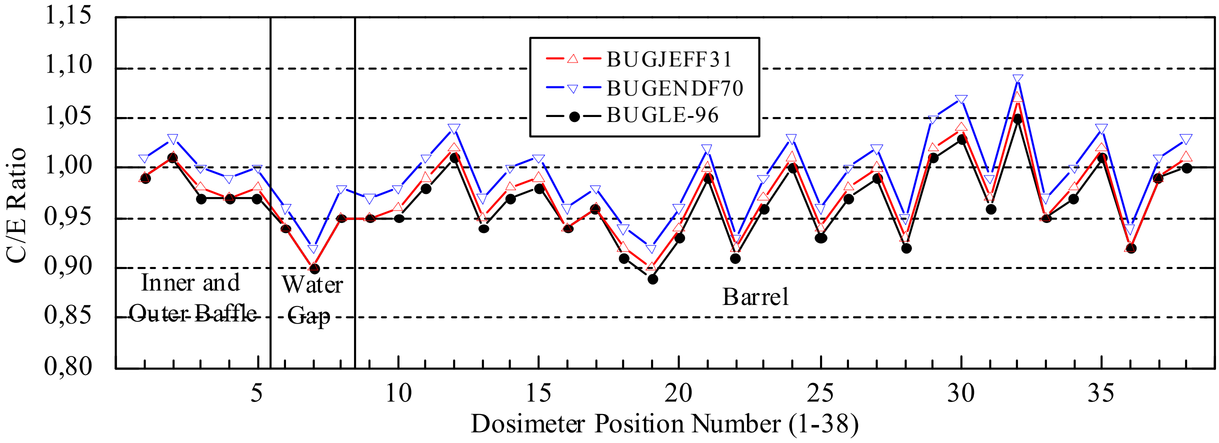

Fig. 7. VENUS-3: Al-27(n,α) equivalent fission flux ratios (Calculated/Experimental).

Computer Code Development

ADEFTA Version 4.1 (ADEFTA-4.1) was released in 2008 and transferred to OECD/NEA Data Bank. ADEFTA is a script file for any UNIX/Linux platform that uses only Bourne shell commands and the "awk" UNIX-Linux utility in order to calculate the atomic densities related to any compositional model for transport analysis [R.2]. ADEFTA is designed to address the needs of users of the GIP cross-section handling code and the American MCNP Monte-Carlo code.

GIP is included in the American DOORS package of deterministic codes and prepares the macroscopic cross sections for the two-dimensional DORT and three-dimensional TORT transport codes included in the DOORS package. Changes within ADEFTA-4.1 extend the previous version considerably beyond the provision of only an input file for GIP.

BOT3P Version 5.3 (BOT3P-5.3) was released in 2008, and transferred to the OECD/NEA Data Bank. This package is a set of standard FORTRAN 77 language codes developed by the ENEA Nuclear Data Group from August 1997 onwards, and is designed to run on Linux/UNIX platforms [R.3]. BOT3P Version 1.0 was originally conceived as a set of standard FORTRAN 77 language programs in order to give users of the DORT and TORT deterministic transport codes some useful diagnostic tools to prepare and check their input data files for both Cartesian and cylindrical geometries, including mesh grid generation modules, graphical display and utility programs for post-processing applications. Later versions extended the possibility to produce the geometrical, material distribution and fixed neutron source data to other deterministic transport codes such as TWODANT and THREEDANT (both included in the American DANTSYS package of deterministic codes), PARTISN (updated parallel version of DANTSYS), the SUSD3D sensitivity code (distributed by the OECD/NEA Data Bank), and potentially any transport code through BOT3P binary output files that can be very easily interfaced. For example, see the Russian two- and three-dimensional discrete-ordinate neutron, photon and charged-particle transport codes KASKAD-S-2.5 and KATRIN-2.0. BOT3P allows users to model X-Y, X-Z, Y-Z, R-Θ and R-Z geometries in two dimensions, and X-Y-Z and R-Θ-Z geometries in three dimensions. ENEA staff used BOT3P in 2008 to generate the R-Θ-Z geometrical models in the IRIS (International Reactor Innovative and Secure) preliminary shielding analysis of the vessel by deterministic methods.

The IRIS application involved some important additions to BOT3P that are now included in Version 5.3, such as more flexibility in the fixed neutron source management and enhanced performance as a post-processor of the TORT code.

BOT3P has undergone world-wide distribution (OECD/NEA Data Bank received 137 dispatch requests of the different versions up to February 2009), and is currently used by important companies such as Westinghouse Electric Company.

Publications 2008

Articles

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[A.3] F. Cannata and A. Ventura, *Non-local PT-symmetric potentials in the one dimensional Dirac equation*, J. Phys. A: Math. Theor. **41**, 505305: 1-21 (2008).

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[C.3] M. Pescarini, V. Sinitsa and R. Orsi, *Generation and Preliminary Testing of ENEA-Bologna BUGLE-Type Group Libraries Based on JEFF-3.1 and ENDF/B-VII.0 Nuclear Data for LWR Shielding and Pressure Vessel Dosimetry,* Proceedings of the International Conference on the Physics of Reactors "Nuclear Power: A Sustainable Resource", Interlaken, Switzerland, September 14-19, 2008 - Internal Technical Report ENEA/FPN-P9H6-012 (2008).

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