CRISTAL V1: CRITICALITY PACKAGE FOR BURNUP CREDIT CALCULATION

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ABSTRACT

Since long years, IRSN, COGEMA and CEA are pursuing a joint project to develop and to validate the new CRISTAL package, created to improve the criticality safety studies including the burnup credit.

The first part of this paper is a presentation of new features and innovations of the V1version of the CRISTAL package. The second part is devoted to illustrate the new possibilities and to describe, through some applications, calculation processes (multi-cell calculations for fuel pins arrays and burnup credit configuration where axial burnup profile, actinides and fissions products are taking into account).

Key Words: criticality package, burnup credit, Monte Carlo method

1 INTRODUCTION

The CRISTAL V1 package was developed as an easy-to-use system using data libraries (based on JEF 2.2 evaluation), well established computer codes (APOLLO2.5, MORET 4.B and TRIPOLI-4.3) and including a Graphical User Interface (GUI) with the data generator CIGALES and the graphical editor EGM. Otherwise, a pre- and post-processing toolbox developed for the MORET 4 computer code is provided to CRISTAL users. For the criticality calculations using burnup credit, a coupling is available between the tools dedicated to nuclide material depletion calculations (DARWIN package and CESAR computer code) and the package dedicated to k_{eff} determination (CRISTAL). Starting from the previous version (CRISTAL V0), CRISTAL V1 has several important new features like multi-cell calculation possibilities, new geometry and array options in MORET 4.

2 CRISTAL V1 PACKAGE DESCRIPTION

2.1 Functional architecture

The functional architecture of the CRISTAL V1 package, described in figure 1, specifies two routes for the k_{eff} determination: the "standard" route and the "reference" route.

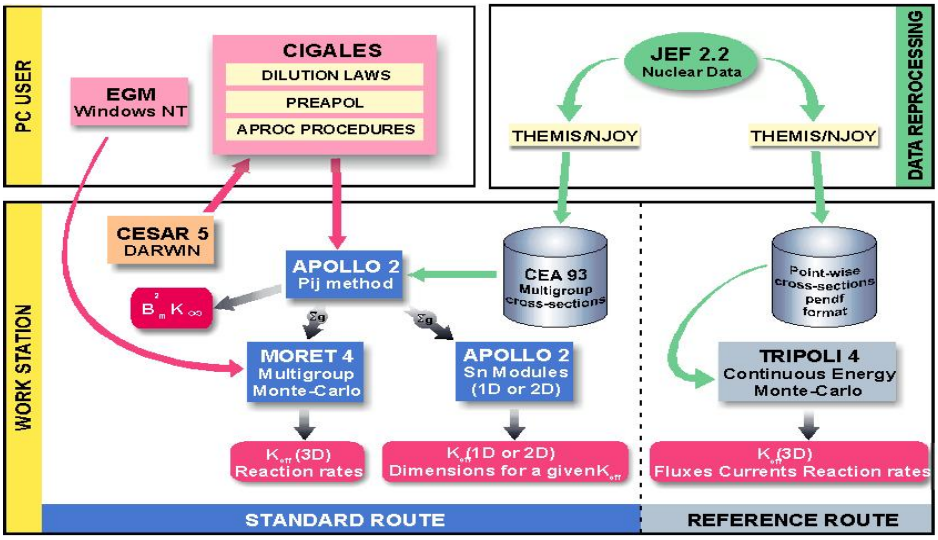

Figure 1. Functional architecture of the CRISTAL V1 package.

The "standard" route with the multi-group cross-sections formulation allows realizing:

- probabilistic calculations with "APOLLO2 - MORET 4",

- deterministic calculations with the Sn modules of APOLLO2 (1D or 2D geometry) or for the standard worth at one dimension.

The "standard" route, managed by the Graphical User Interface (GUI), integrates the know-how of criticality engineers. The linking of different codes is done according to procedures adapted to each configuration integrating recommendations related to calculation schemes.

The "reference" route is to use a minimum of physical approximations in modeling for the k_{eff} determination. Calculations are done with the continuous-energy Monte Carlo code TRIPOLI-4.

2.2 Libraries

2.2.1 CEA93.V6 Neutron Library

The CEA93.V6 library was obtained by processing JEF2 European File data [1] with the NJOY [2] system and has no cross-section adjustment. This library includes isotopic microscopic cross-sections, pre-tabulated isotopic reaction rates for self-shielding calculations and complementary isotopic data. For each isotope, the library contains total, radioactive capture and

transport-corrected multigroup cross-sections, as well as multigroup transfer matrices. For a fissile isotope, it also includes the multigroup fission cross-sections and the fission spectrum. A special “excess” multigroup cross-section is also included to account for neutron multiplication via (n, 2n) and (n, 3n) reactions. This library, available for users in two standard multigroup formats (the 99-group energy mesh and the Xmas 172-group structure), contains data for 279 isotopes and self-shielding data for 56 resonant isotopes.

For the needs of CRISTAL V1 package, the CEA93.V6 library was extended to integrate essential nuclides for the criticality calculations (e.g. chlorine, calcium, zinc and tin) and multigroup transfer cross-sections at Legendre order 9 for Uranium, Plutonium and Americium isotopes.

2.2.2 Procedures libraries

The APOLLO2 code is a part of the SAPHYR package [3]. It was designed as a modular structure consisting of a predefined set of operators (functions) and a predefined set of objects (data). Indeed, APOLLO2 has been conceived as a toolbox in which users can pick up the physics and the operator they need to solve their specific problems. Physical, numerical and structural functions are built into modules that perform a specific task (geometry, self-shielding, flux solver …) and that can be viewed as operators that act on input objects to create output objects. The GIBIANE macro language is used to dynamically chain the operators at run time, defining thus a particular calculation scheme fit to specific user’s goals. Thus, it makes possible to draw up procedures, called APROC, including recommended calculation schemes that allow, for each situation, the selection of the optimum sequence of calculation options.

A specific APROC_CRISTAL library was developed for the CRISTAL V1 package for the description of geometry, self-shielding, multi-cell and Sn calculations.

2.3 Neutron transport computation codes

2.3.1 APOLLO2 computer code

The neutron and gamma multigroup transport lattice code APOLLO2 is developed since 1983 by CEA in a joint development effort with Electricité de France and Framatome-Anp. It allows assembly transport computations using various flux solvers: Collision Probability method, Discrete Ordinates method and more recently Characteristics method [4]. It is used in CRISTAL, but also in the DARWIN Cycle code package and in the Reactor Physics code packages [5].

An a priori ineluctable step is the calculation of equivalent multigroup self-shielded cross-section for resonant isotopes whose cross-sections exhibit large variations within the relatively large energy groups. Recently, improvements in APOLLO2 hope to take into account resonant mixture [6]. Also, one of the main purposes of the code is to provide parameterized cross-section data for subsequent homogenized, coarse-group whole-core diffusion or transport calculations. Leakage models can be invoked to represent equilibrium core assembly conditions and the resulting multigroup flux can be used to produce homogenized and collapsed cross-section by either direct flux weighting or via equivalence theory. A burnup model allows for the calculation of isotope depletion and production, and for the calculation of core equilibrium fluxes at different burnup stages that can then be used in the production of the parameterized coarse-mesh library.

APOLLO2 works with an arbitrary number of regions, groups, isotopes and burnup zones. The operator and data structures have been designed for optimal calculation performances in the 100-group range, but reference calculations using a very fine energy mesh can be performed.

In the CRISTAL V1 package, the main functionalities of the APOLLO2.5 code used are:

- the self-shielding module,

- the collision probability method (Pij method) for flux calculations,

- the collapsing and homogenization of the cross-sections,

- the discrete ordinates method for Sn calculations.

The APOLLO2.5 computer code allows preparing homogenized and self-shielded macroscopic cross-sections for MORET 4 and Sn calculations.

2.3.2 MORET 4 computer code

The MORET 4 code [7] is a three dimensional multigroup Monte Carlo code which calculates the effective multiplication factor (k_{eff}) whatever is the complexity of configuration, as well as reaction rates in the different volumes of the geometry and the neutron leakages.

The MORET 4 code is a modular code, well suited for requirements of criticality surveys performed for fuel cycle facilities and plants and for fissile material transport packaging.

Recent developments and improvements of the previous version of MORET have led to include the new version MORET 4.B in the CRISTAL V1 package. The new features concern:

- the modernization of the geometry with regard to the previous version. A modular geometry structure allows constructing complex geometries using particular zones, called units,

- the new geometry structure enables the description of arrays in arrays and hexagonal arrays,

- the implementation of perturbation algorithms based on the correlated sampling method,

- the source distribution convergence,

- the statistical detection of stationarity,

- the unbiased variance estimation.

Moreover, the MORET 4.B version is connected with post-processing tools to help users to analyze the simulation results.

2.3.3 TRIPOLI-4 computer code

The TRIPOLI-4 parallelized code [8], developed by CEA/DEN, is a three-dimensional, continuous energy, particle transport calculation code (neutrons and gamma), based on the Monte Carlo method. The TRIPOLI-4.3 code is the “reference” route of CRISTAL V1. This code allows to describe complex configuration both by combinatorial or/and surfacic geometries. This code has also repetitive pattern functionalities: arrays and arrays in arrays. Perturbation calculations can be performed with the correlated sampling method implemented into TRIPOLI-4. Then TRIPOLI-4 determines the k_{eff} as well as the neutron flux, reaction rates and fission

rates, neutron leakage, for example. It is possible to carry out criticality calculations with different nuclear data evaluations in ENDF/B format as JEF-2, ENDF/B6, JEFF-3, JENDL-3 …

2.4 Pre and post-processing tools

The main aim of the different tools provided with the package is to offer users a high level of user-friendliness and to assist them in the input setup and execution of the "standard" route of the CRISTAL V1 package.

Two sets of tools are offered to users to help them:

- the first one comes with CRISTAL and contains the CIGALES code (a data generator for materials multigroup self-shielded cross-sections) and the EGM 3D graphic editor used to visualize MORET 4A geometry,

- the second, dedicated to MORET 4 computer code, has been recently developed and gathers through a unique interface (SYCOMORE) all tools related to MORET 4 code. The main tools available in this interface are: a data editor which displays automatically the MORET geometry (EJM), a post-processing toolbox (OPOSSUM) and a characterization tool to assist code bias estimation (MACSENS).

2.4.1 SYCOMORE System

The SYCOMORE system [9] comprises three main modules: EJM, OPOSSUM and MACSENS modules.

The EJM module is a useful and powerful editor to display automatically the MORET 4 geometry model. EJM in the editor part allows users to view the components of their geometry model as it is constructed. This tool is developed with JAVA 2 to ensure the portability in different environments (Windows, Unix and Linux).

2.4.2 CIGALES computer code

The CIGALES Version 3.0 computer code [9] provides input menus and context-sensitive help to guide users through the set up of their input. CIGALES V3 is used to calculate isotopic compositions by means of dilution laws for the fissile materials [10] and predefined materials (such as steel and concrete) for the others, and to provide automatically data files for the APOLLO2.5 code:

- for cell and multi-cell calculations for arrays with Pij method of APOLLO2.5 code,

- for the calculation of the effective multiplication factor k_{eff} (1D or 2D calculations) with Sn method,

- for calculation of standard worth with Sn method.

Moreover, the CIGALES computation code allows using in APOLLO2.5 the isotopic data issued from depletion codes (DARWIN package [11] and CESAR code [12]). The DARWIN package and the CESAR code upstream of the application of the CRISTAL package are used to calculate changes in the physical parameters such as abundance of each nuclide, taking into account the detailed history of the fuel assembly (in the reactor and during cooling) for the fuel cycle of any reactor type (PWR, BWR…).

The CRISTAL V1 package, devoted to perform automatized criticality calculations using burnup credit, contains an interface coupled with the depletion code and designed to issue automatically data files for the criticality calculations. This interface takes into account:

- correction factors (of actinides and fission products concentrations) determined by the validation of the depletion calculations and by the validation of cross-sections,

- the axial profile of burnup and the number of axial zones chosen.

The CIGALES computation code, developed with Visual Basic 6.0, is available on Windows NT environment. Input data are provided in an interactive way, using the arborescent structure of panels with predefined fields.

2.4.3 EGM Graphic Editor

The EGM 3D graphic editor [13] allows to model graphically and interactively 3D complicated configurations. The user draws the configuration with different menu bars, popup menus and icons. EGM is an application based on CAS.CADE Object Libraries using geometric primitives and topological operations (intersection, union, …) to apply to the 3D geometry. This functionality will be added to the EJM tool in the future which will replace EGM.

2.4.4 MACSENS characterization system

Accurate predictive estimation of the effective multiplication factor k_{eff} and associated errors determination are essential for users of neutronic code systems like CRISTAL V1 package. The MACSENS characterization system [14] allows reaching these two objectives and is assigned:

- to locate a criticality calculation among a group of similar experiments whose bias are known. The critical experiments have been calculated with the CRISTAL V1 package to obtain “calculation-experiment” deviation,

- to determine an estimation of the overall bias of the CRISTAL V1 package for the particular situation studied.

2.5 Validation Database of CRISTAL V1 Package

The experiments of the CRISTAL V1 validation base have been selected to have an extensive representation of media and geometries encountered in the nuclear fuel cycle. The validation database of CRISTAL V1 package contains 2132 experimental configurations with:

- the CRISTAL V0 update database (516 experiments),

- experiments involving slabs, arrays of UO_2 and MOX fuel rods, fuel-pin lattices in nitrate solutions, uranyl nitrate solutions, mixed plutonium and uranium nitrate solutions, uranium nitrate solutions, uranium metal and plutonium metal, uranium powders,

- experimental programs dedicated to Burnup Credit (programs carried out in criticality laboratory at Valduc and experimental programs carried out at Cadarache by the CEA).

As shown in Table 1, the validation database is presented by medium type: solutions, interactions, ^{233}U (solutions), powders, arrays, dissolvers, metallic systems.

Table I. CRISTAL V1 Validation Base - Selected experiments

Classes	No of Series	No of Cases
Solutions	62	484
Interactions	24	279
^{233}U (solutions)	6	43
Powders	8	191
Arrays	81	925
Dissolvers	7	81
Metals	72	129
Total	**260**	**2132**

The experimental data are taken from:

- the handbook of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [15],

- the experiments performed by IRSN in the Valduc facility, partially with the financial support of COGEMA company,

- the experiments performed by CEA in Cadarache facilities (Minerve and Eole facilities).

These experiments are used for the validation of the “standard” route [16, 17] (APOLLO 2 - MORET 4 and APOLLO2 Sn) and the “reference” route TRIPOLI 4 [18] with the following repartition as showed in the Table II.

Table II. Selected CRISTAL V1 Validation - Experiments by route

	“Standard” Route		**“Reference” Route**
Classes	**A2 - M4**	**A2 Sn**	**T4**
Solutions	426	346	265
Interactions	272	13	180
^{233}U (Solutions)	43	0	6
Powders	184	92	144
Arrays	827	279	204
Dissolvers	81	6	14
Metals	93	118	59
Total	**1926**	**854**	**872**

A2 - M4 = “Standard” route with APOLLO2 - MORET 4 calculations / A2 Sn = “Standard” route with APOLLO2 Sn calculations / T4 = “Reference” route with TRIPOLI-4 calculations.

3 CRISTAL V1 PACKAGE APPLICATIONS

3.1 APOLLO2 Sn calculation

This application is devoted to illustrate the possibilities of the CRISTAL V1 package for multi-cell calculations for spent fuel arrays in a storage pool. Neutron transport calculation of the system is performed using the Sn modules of the APOLLO2 computer code. These modules performed the 2D criticality calculation that provides the neutron fluxes that are used to determine the k_{eff}. The figure 2 shows the multi-cell geometry for APOLLO2 calculation and the figure 3 is a horizontal cross-section of the 2D representation of storage of spent UOX fuel assemblies.

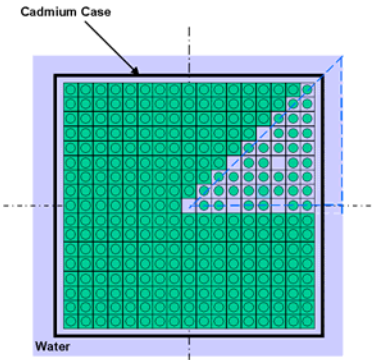

Figure 2. Multi-cell geometry for APOLLO2 calculation

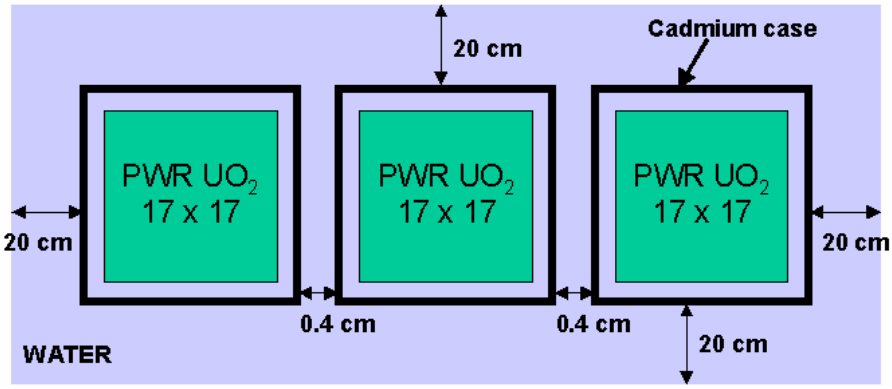

Figure 3. Horizontal cross-section of the 2D representation of a storage of spent fuel assemblies

3.2 TRIPOLI-4 3D continuous energy Monte Carlo calculation

Neutron transport calculation of the system is performed using the reference code TRIPOLI-4. The 3D criticality calculation provides the neutron fluxes and determines the k_{eff}. The figure 4 is a horizontal cross-section of the 3D representation of storage of spent UOX fuel assemblies. This 3D geometry is generated by using the repetitive pattern functionality of TRIPOLI-4 : arrays and arrays in arrays.

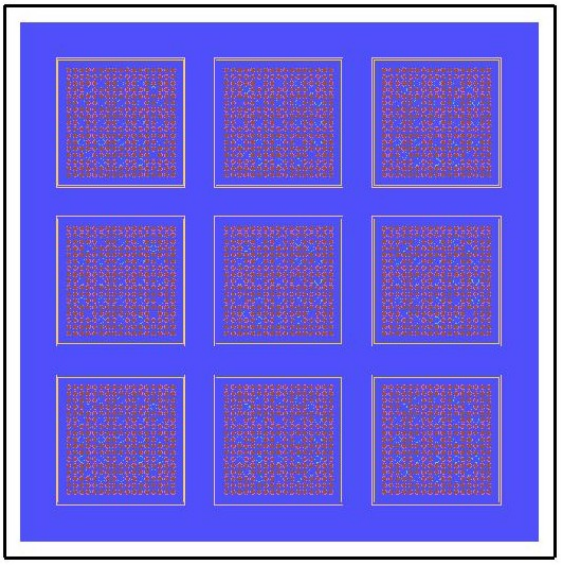

Figure 4. TRIPOLI-4 horizontal cut of the 3D representation of a storage of spent fuel assemblies

3.3 Burnup credit calculation

The CRISTAL V1 package performs criticality calculations for systems using burnup credit (see figure 5). This package is linked with CESAR which performs depletion calculations of each spatially varying burnup region with an axial specified burnup profile. The inventory calculation is then used to generate resonance self-shielded cross-sections for each burnup-dependent fuel region with the APOLLO2 computer code. Finally, a MORET 4 criticality calculation is performed using the spatially varying cross-sections to determine the neutron multiplication factor for the system. A lot of the spent fuel actinide or fission product isotopes may be included in the criticality calculation.

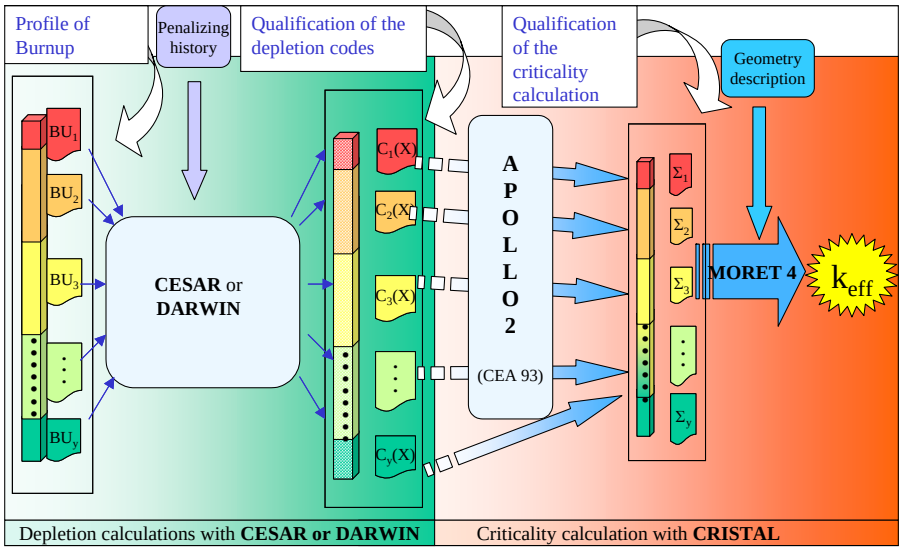

Figure 5. Process to take Burnup Credit into account in a criticality calculation with CRISTAL V1

3.3.1 Link with the CESAR code

The figure 6 shows the panel used to read the concentrations issued from a CESAR calculation, to select actinides and fission products and to provide the axial burnup profile. The user may specify the number of axial zones and the post-irradiation cooling time. Isotopic correction factors may be input to adjust the calculated isotopic inventories to account for known bias and/or uncertainties associated with the depletion calculations. The actinides used in the calculations are: ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am and ^{237}Np. The fission products used for the calculations are: ^{103}Rh, ^{133}Cs, ^{143}Nd, ^{149}Sm, ^{152}Sm, ^{155}Gd, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{109}Ag, ^{145}Nd, ^{147}Sm, ^{150}Sm, ^{151}Sm and ^{153}Eu. This group of 15 fission products accounts for around 80 % of the reactivity loss produced by all fission products.

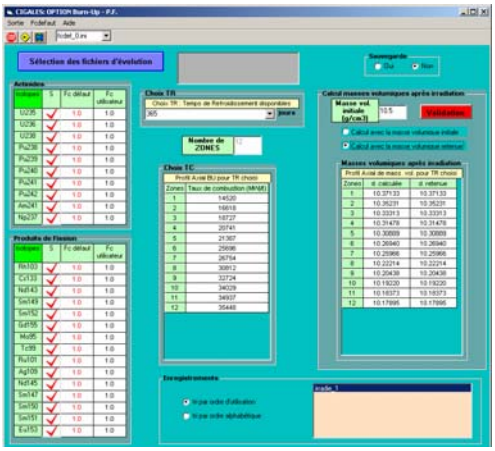

Figure 6. Burnup Credit Panel in CIGALES V3

3.3.2 Description of application

The application concerns an interim storage of 9-cavities-baskets in which assemblies stand higher than the borated internal structures. The axial burnup profile is discretized in 12 different zones. Two examples of graphical cut from MORET 4 outputs are given in figures 7 et 8.

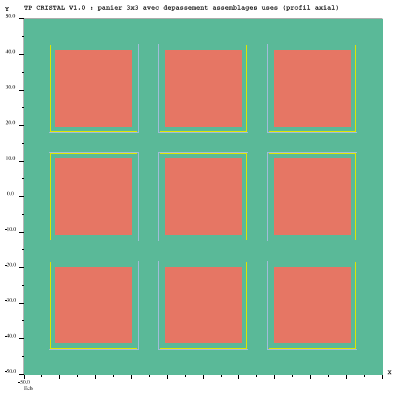

Figure 7. Horizontal cut

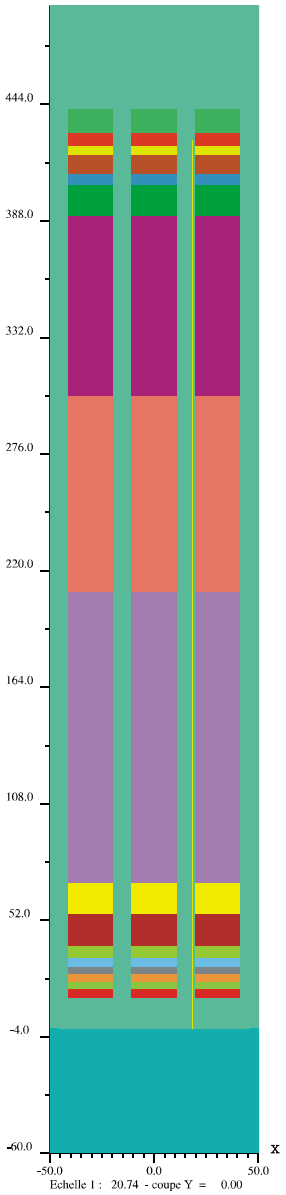

Figure 8. Axial cut

4 CUSTOMER SERVICES

The CRISTAL V1 package comprises also Customer Services to take into account the expectations of customers. The recent developments cover a range of areas of activity like documentation, maintenance and training courses.

The Internet, including a password-protected customer area, is used for distribution of software and access of technical documentation. A help-desk system is adopted to enhance the tracking and reporting of customer enquiries. An extension of the standard system platforms is supported to cover PC Windows and Linux, in addition to various Unix workstations. Concerning the activity of maintenance, a specific tool (ODICE), available on the Internet protected customer area, has been developed to record user's technical requests and to constitute a database. The whole technical answers, given by the developers, can be consulted by the CRISTAL users.

5 CONCLUSIONS

This paper has summarized the current status of the CRISTAL V1 package, outlining new features and innovations and has presented applications to show the calculation process. The CRISTAL V1 package contains many new capabilities for criticality studies including Burnup Credit effect. The development of the CRISTAL package over the next years is envisaged to include improvements to new tools and libraries (JEF 3 evaluation), extensions of the validation database and future needs of customers.

6 ACKNOWLEDGMENTS

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7 REFERENCES

[1] C. Nordborg, M. Salvatores, "Status of the JEF Evaluated Data Library," *Proc. Int. Conf. Specialists,* Jackson Hole, Wyoming (USA), September 1998.

[2] R.E. MacFarlane et al., "NJOY, A Code System for Producing Point wise and multigroup Neutron and photon Cross-sections from ENDF/B Evaluated Nuclear data," LA-UR 89-2057, LANL, USA (1994).

[3] R. Sanchez, C. Fedon-Magnaud, J.J. Lautard, D. Caruge et alter, "SAPHYR : A Code System from Reactor Design to Reference Calculations," *International Conference on Supercomputing in Nuclear Applications,* Paris, France, September 2003.

[4] S. Santandrea, R. Sanchez, "Analysis and improvements of the DPN acceleration technique for the method of characteristics in unstructured meshes," *Annals of Nuclear Energy 32,* 163-193, (2005).

[5] A. Santamarina, C. Collignon, Ch. Garat, "French calculation schemes for Light Water Reactor Analysis," *PHYSOR 2004,* Chicago, April 24-29, 2004 (USA).

[6] M. Coste-Delclaux, S. Mengelle, "New resonant mixture self-shielding treatment in the APOLLO2 code," *PHYSOR 2004*, Chicago, (USA), April 2004

[7] O. Jacquet et al., "MORET: Version 4.B, a Multigroup Monte Carlo Criticality Code Package," *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, 2003.

[8] J.P. Both, H. Derriennic, B. Morillon, J.C. Nimal, "A Survey of TRIPOLI-4", Proceedings of the 8th International Conference on Radiation Shielding, Arlington, Texas, USA, 24-28 avril 1994, pp. 373-380 ; J. P. Both, Y.K. Lee, A. Mazzolo, O. Petit, Y. Pénéliau, B. Roesslinger, M. Soldevila, TRIPOLI-4 - "A Three Dimensional Polykinetic Particle Transport Monte Carlo Code, SNA'2003", Paris September 2003.

[9] L. Heulers et al., "The Graphical User Interface for CRISTAL V1," *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).

[10] N. Leclaire et al., "Isopiestic Density Law of actinides Nitrates applied to Criticality Calculations," *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).

[11] A. Tsilanizara, C. M. Diop *et al*., "DARWIN: an Evolution Code System for a Large Range of Application," *J. Nucl. Sci. Technol.*, Supplement 1, pp 845-849 (2003).

[12] M. Sansom et al., "CESAR: a Simplified Evolution Code for Reprocessing Applications," *Proceedings of Meeting on Recycling, Conditioning and Disposal RECOD* 98, Nice, France, September 25-28, (1998).

[13] E. Létang, G. Courtois, J.M. Gomit, "The Graphical User Interface for the CRISTAL Package," *Proceedings of Meeting on Nuclear Criticality Safety*, Versailles, France, September 20-24, (1999).

[14] F. Fernex, Y. Richet, "A new MORET tool to assist Code Bias Estimation," *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).

[15] OECD Nuclear Energy Agency, "International Handbook of Evaluated Criticality Safety Benchmark Experiments", NEA/NSC DO(95)03, 2004.

[16] I. Duhamel et al., "Experimental Validation of the APOLLO2-MORET 4 Standard Route of the French CRISTAL V1 Package," *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).

[17] C. Venard et al., "Contribution of the Experimental Validation of the French Criticality-Safety Package CRISTAL V1: APOLLO2 Sn Route", *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).

[18] Y.K. Lee et al., "CRISTAL, Criticality Safety Package Validation: TRIPOLI-4 Monte Carlo Code, JEF2.2 Library and ICSBEP Experiments," *Proceedings of Meeting on Nuclear Criticality Safety*, Versailles, France, September 20-24, (1999) ; E. Gagnier, Y.K. Lee, L. Aguiar, N. Vedrenne, "Validation of the 3D TRIPOLI-4.3 Monte Carlo Code for metallic fissile media configurations with JEF2.2 and ENDF/B6 evaluations", *Proceedings of Meeting on Nuclear Criticality Safety*, Tokai Mura, Japan, October 20-24, (2003).