

## French Calculation Schemes for Light Water Reactor Analysis

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This paper describes the recent code APOLLO2.5/CEA93.V6 currently implemented in the LWR calculation tools of CEA, Framatome-ANP and Electricité de France. The corresponding packages SAPHYR, SCIENCE.V2 and CASSIOPEE are presented. The recommended “CEA-97” reference scheme is detailed and some results of the Validation/Qualification work are enhanced. It is shown that the major design parameters are predicted within the required target accuracy in a wide experimental validation range : up to 4.8% w/o <sup>235</sup>U in UO<sub>2</sub> fuel and 13%Pu in MOX assemblies, for burnup ranging from 10 to 60 GWd/t.

**KEYWORDS:** *neutronics codes, APOLLO2, SCIENCE, CRONOS, CASSIOPEE, JEF2, PWR, calculation route*

### 1. Introduction

The recent code APOLLO2.5/CEA93.V6 developed by CEA [1] is a French versatile neutronics tool : it is used in the Cycle code package DARWIN [2], in the Criticality-Safety code package CRISTAL [3] and in the Reactor Physics code packages. In this paper we will mainly describe the Reactor code packages and emphasize the deterministic calculation routes.

The APOLLO2.5 assembly code is currently implemented in the modern PWR calculation tools of Framatome-ANP and Electricité de France, SCIENCE.V2 [4] and CASSIOPEE respectively. APOLLO2 is also extensively used at CEA for design studies of large Thermal Reactors (PWR, BWR, VVER, naval propulsion reactors, HCPWR, HTR, CANDU, Graphite-moderated reactors), as well as Irradiation reactors and Safety experimental reactors.

### 2. The APOLLO2.5/CEA93V6 neutronics tool

#### 2.1 APOLLO2 methodology

The APOLLO2 code performs direct or adjoint transport calculations with a fixed source or for a critical parameter. External iterations on the spatial distribution source and the eigenvalue are accelerated by Chebyshev method. Upscattering is accounted for by thermal iterations, which are accelerated through group-constant rebalancing factors together with a rest minimization technique.

A first solver corresponding to the solution of the integral transport equation by the Collision Probability method is implemented. 1D and 2D geometries are available; the XY solver works on a basic regular mesh, but allows for several levels of local mesh refinement and for elementary square or rectangular cells with sectorized internal circles. A recent improvement was brought by the TDT module which performs interface-current transport calculations of unstructured XY geometries [5]. The TDT module has been generalized to treat 3D geometries generated by axial translation of a 2D unstructured motif. The GUI Silene is used to create TDT geometries that are made out of homogeneous cells whose

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perimeters are composed by straight segments, arcs or circles.

The double-heterogeneity problem, encountered in HTR bundles and LWR Gd fuel rods, is handled through an independent treatment of each type of grain and the replacement of the stochastic medium by a homogeneous medium [6].

Recently, a Method Of Characteristics was developed with an efficient synthetic acceleration [7].

From the beginning, the integro-differential equation can be solved using a 1D or 2D discrete-ordinates module accelerated by the DSA technique [8]. A 2D linear-linear nodal  $S_N$  method, with Boundary Projection Acceleration, was added to this module. The multidimensional discrete ordinates code IDT, that uses nodal and characteristics methods for the discretization of the spatial variable on regular 2D and 3D Cartesian meshes, was developed and recently implemented in APOLLO2 [9].

Concerning resonance reaction rate calculation, a powerful space-dependent self-shielding based on the French “Background Matrix” method [10] is implemented; in Version 5 of APOLLO2, a more efficient quadrature technique for the homogeneous/heterogeneous equivalence is available, based on Probability Tables [11]. Furthermore, a model based on the subgroup method is also available [12].

The development of the APOLLO2.5 industrial code was achieved within Quality Assurance process. Therefore, a rigorous methodology of Verification/Validation/Qualification was developed and applied.

## 2.2 The Verification/Validation/Qualification process

The first step of this process verifies that numerical models and programming of each module are correct; this Verification is also based on the Test Machine which avoids non-regression in the new APOLLO2 Version.

The second step corresponds to the Validation of the APOLLO2 functionalities ( $P_{ij}$ , resonance self-shielding, fine flux, depletion, accurate SPH homogenization,  $S_n$ , etc.) as well as the ‘CEA-97’ reference calculation route. This Validation is based on the comparison of APOLLO2.5/CEA-97 calculation results against continuous-energy Monte Carlo TRIPOLI4 reference calculation. Both calculations use the same nuclear data JEF2.2. This Validation enables also the “calibration” of the recommended CEA-97 Reference route : the calculation bias is determined for each LWR design parameter. This validation process is automated through the MACH2 Machine.

The Qualification is the third step, corresponding to the comparison of the results of the global package (code + reference calculation route + nuclear data library, i.e APOLLO2.5/CEA-97/CEA93.V6) against experimental results from integral measurements :

- A first set of experiments characterised by their fundamental measurements are used to qualify the CEA93 nuclear data (processed from the JEF2.2 library) of the main isotopes : material bucklings, actinide fission rate ratios, conversion factors are measured in the Eole reactor [13] and capture cross sections of the main poisoning Fission Products are qualified through reactivity worth measurement of separated FP samples by an oscillation technique in various spectra at the central cell of the Minerve zero power reactor [14] [15].
- A second set of mock-up experiments are used to qualify the calculation of the whole LWR parameters; from this qualification process, based on several thousands of integral measurements; the total error of the APOLLO2.5 product is obtained for each design parameter, as well as the associated uncertainty [16].

## 2.3 The Reference “CEA-97” calculation scheme

The “CEA-97” Reference scheme was defined in order to meet the target accuracy for every LWR design parameter. In a second step, the “CEA-97” scheme was optimized to reach computing times acceptable for design calculations. For instance, the “CEA-97” scheme associated with the evolution of 17x17 UO<sub>2</sub> assemblies is able to reproduce <sup>239</sup>Pu build-up and pin-by-pin power within 1% accuracy (up to 70Gwd/t), in 15 mn CPU time on a COMPAQ SC232 computer (Alpha EV67 processor 667 MHz).

The optimized “CEA-97” scheme is then validated through the Validation Machine MACH2 of APOLLO2. We have to stress that this “CEA-97” scheme is used in the analysis of integral experiments, therefore it is the unique scheme calibrated for LWR design parameter calculation at CEA.

The APOLLO2.5/CEA93V6 product utilizes the CEA93 multigroup cross-section library (Version 6), processed by NJOY from the JEF2.2 evaluations. The “CEA-97” scheme recommends the use of the European X-MAS 172-group structure (99-group libraries are also available).

The recommendations for the flux calculation are the following :

- Spatial calculation for PWR assemblies is achieved using a UP1 accurate anisotropic interface current method. The inter-assembly water gap is integrated inside the peripheral rectangular cells
- With a view to reducing the calculation cost, a grouping of cells with similar flux within a unique ‘physical cell’ is recommended. In 17x17 UOX assemblies, it consists of 18 physical fuel cells, 2 physical “tube-guide” cells and one physical “instrumentation tube” cell [17]
- The fuel pellet is split into 4 rings (50%, 30%, 15% and 5% of the total volume of the pellet) in order to give a faithful representation of the resonant absorption of  $U_{238}$  inside the pin and of the actinide and fission product concentration profiles. This leads to the determination of 72 evolving media.
- MOX assembly depletion calculation is carried out with surrounding UOX assemblies [18].
- UOX assembly with  $UO_2$ - $Gd_2O_3$  rods are calculated without cell-grouping assumption.

The recommendations for the self-shielding pattern are the following :

- $U_{238}$ ,  $U_{235}$ ,  $U_{236}$ ,  $Pu_{239}$ ,  $Pu_{240}$ ,  $Pu_{241}$ ,  $Pu_{242}$ ,  $Am_{241}$  and Zr are self shielded. For Gd poison pins,  $^{155}Gd$ ,  $^{156}Gd$ ,  $^{157}Gd$  and  $^{158}Gd$  isotopes are self-shielded
- Self-shielding of the  $U_{238}$  large resonances are covered by the accurate model  $UP_1$ . The  $UP_0$  approximation, which considers an isotropic interface angular flux, is adequate to ensure the quality of the self-shielding results for the other isotopes
- Space-dependent self-shielding using the Background Matrix method: rim effect is accounted for by 4 concentric rings in each fuel rod
- 3 self-shielded pins are differentiated for  $U_{238}$  in order to adequately account for the differences in the Dancoff effect linked to guide-tube vicinity
- Doppler broadening is carried out through temperature-dependent effective cross sections. In order to handle crystalline binding in UOX fuel, an accurate effective temperature, which preserved  $^{238}U$  resonant capture rates, is recommended [19]. Radial temperature profile in the fuel pellet is also accounted for [17] [20].

The recommendations for the assembly depletion calculation are the following :

- Evolution steps : 0, 37, 75, 112.5, 150, 325, 500, 750, 1000, 1500, 2000, 2500, 3000, then constant step of 1000 MWd/ $t_m$
- If the LWR assembly contains  $UO_2$ - $Gd_2O_3$  rods, the evolution steps are more discretized. Each poison rod is divided into 11 evolving concentric zones. Thus, the assembly depletion calculation is carried out on approximately 210 evolving media.
- Self-shielding calculations are repeated at the following steps : 4, 8, 12, 24, 36, 48...GWd/ $t_m$
- The recommended depletion chain describes explicitly 20 Actinides ( $^{234}U \rightarrow ^{247}Cm$ ) and 85 Fission Products

The recommendations for cross-section collapsing and homogenisation are the following :

- Energy condensation from 172 groups down to the 20-group “universal mesh” [21]
- Cell by cell homogenisation
- Use of the equivalent homogenisation SPH which preserves reaction rates

The recommendations for core calculations are the following :

- Transport calculation in S8 quadrature (pin by pin pattern, 20 energy groups)
- Anisotropic scattering accounted for in P1 expansion

- Linear-linear nodal scheme: one mesh-point/cell is well suited for spatial discretization
- Specific calculation scheme based on cluster Pij calculation, followed by SPH equivalent homogenization, are proposed for core calculations including absorber pins [22] and control rod cluster [23].

## 2.4 The MACH2 Validation Machine

The Validation process is based on the benchmark concept. A simplified geometry, representative of the LWR calculation challenge, is defined in order to check the APOLLO2 deterministic route against reference calculation results, generally obtained from the TRIPOLI4 [24] 3D continuous-energy Monte Carlo code.

For example, the 4 first benchmarks in Table 1 corresponds to square pin-cell geometries to validate LWR lattice calculation for fresh UOX fuel, spent UOX, MOX and re-enriched reprocessed uranium respectively. In these 4 benchmarks, the PWR design parameter to validate (4<sup>th</sup> column in Table1) is the multiplication factor; the main capture and fission rates indicated in the 3<sup>rd</sup> column are validated on a 13-macrogroup output. This validation is automatically repeated in MACH2 for the various options of the APOLLO2 modules (validation of the functionalities given in Table1-2<sup>nd</sup> column), including the “CEA-97” scheme. Furthermore, phenomenological neutron balance is also carried out through a “six factor” breakdown of the  $K_{\infty}$  and printed out on the validation report, as shown in Table 2.

**Table 1** The PWR benchmarks in MACH2 for APOLLO2 validation

Benchmarks	Functionalities	Main Reaction rates	PWR parameters
UOX lattice (fresh fuel)	Pij, self-shielding	U235, U238	Keff
UOX lattice 40GWj/t	Pij, self-shielding	U235, U236, Np237, Pu, Am	Keff, reactivity loss with burnup
MOX 7%Pu lattice	Pij, self-shielding	U, Pu, Am241	Keff
URE reprocessed-U lattice	Pij, self-shielding	U236, U234	Keff
Evolution UOX	Evolution	Actinide concentrations vs Bu	fuel inventory, cycle length
UOX 17x17 assembly	Pij, self-shielding, Sn	abs.+fission radial distribution	pin-by-pin power map
MOX assembly + Mixed core	Pij, self-shielding, Sn	abs.+fission radial distribution	UOX/MOX interface, zoning, power
UO2-Gd2O3 burnable poison	Evolution	Concentration Gd, U235, Pu239	poison worth and reactivity loss vs Bu
B4C isolated absorber	Pij, Equivalence, Sn	absorber capt. rates, fission map	absorber worth, pin-by-pin power map
Stainless-steel rod	Pij, self-shielding, Sn	$\Delta\rho$ , Fe56, Ni58, Cr52, Mn55	absorber worth, pin-by-pin power map
UOX assembly - 24 B4C cluster	Pij, Equivalence, Sn	abs.+fission radial distribution	CRC worth, pin-by-pin power map
MOX assembly -24 B4C cluster	Pij, Equivalence, Sn	abs.+fission radial distribution	CRC worth, pin-by-pin power map

**Table 2** APOLLO2.5 validation report issued from MACH2 output



Les deux premiers résultats sont effectués avec le modèle d'autoportance WEST de l'échelle CEA-97 et le modèle de calcul de l'échelle de référence (M5, M5, M5, M5, M5, M5).

Les résultats obtenus et les comparaisons sont présentés dans le tableau 2.3.

**Tab. 2.3: Comparaison du bilan neutronique**

	Cyl. (pcm)	Rothx4 (pcm)	UP0 (pcm)	UP1 (pcm)	CEA-97 (pcm)	CEA-97 opt (pcm)	TRIPOLI4	$\sigma$ (pcm)
$\chi_{(n,2n)}$	39	39	39	39	38	38	1.00085	55
$\epsilon_{pair}$	-5	-5	-3	11	-52	-50	1.06777	8
$\epsilon_{impair}$	118	118	108	22	41	41	1.21502	24
$p$	-475	-475	-398	16	61	35	0.61597	24
$f$	328	328	269	158	74	75	0.88199	13
$\eta$	20	20	20	22	22	22	1.87120	10
$K_{\infty}$	55	55	66	302	217	194	1.31960	50

Le tableau 2.3 est illustré ci-dessous par le schéma de la cellule de combustible.

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## 2.5 The APOLLO2 Qualification

The calculation errors and their confidence intervals, reported in the APOLLO2.5/CEA93V6 Qualification Report [16], are used by CEA and EDF to define the Safety Factor to be adopted in PWR and Mixed-core design studies. These errors for fuel inventory prediction, obtained from numerous chemical assays in various French PWR UOX and MOX assemblies, are summarized in Table 3; recently, MOX qualification was extended to high burnups with Post Irradiation Experiments on Dampierre 4 and 5 cycles assemblies [25].

**Table 3** C/E comparison on major actinide isotopic ratios from P.I.E

Isotope	UOX 40GWd/t	UOX 60GWd/t	MOX 40GWd/t	MOX 60GWj/t
U235	$2.5 \pm 2.0$	$4.0 \pm 3.5$	$4.3 \pm 3$	$1.6 \pm 3$
U236	$-4.3 \pm 0.9$	$-4.1 \pm 0.6$	$-6.5 \pm 2$	$-7.1 \pm 2$
Np237	$-3.7 \pm 3.4$	$-3.8 \pm 3.2$	-	$-8.3 \pm 3$
Pu238	$-8.0 \pm 3.9$	$-7.4 \pm 3.7$	$-7.2 \pm 3$	$-2.0 \pm 3$
Pu239	$1.0 \pm 1.1$	$1.6 \pm 1.3$	$3.0 \pm 2$	$7.0 \pm 3$
Pu240	$-1.1 \pm 1.5$	$-0.4 \pm 1.1$	$1.5 \pm 2$	$3.2 \pm 2$
Pu241	$-2.6 \pm 1.8$	$-1.2 \pm 1.6$	$-1.8 \pm 2$	$3.0 \pm 3$
Pu242	$-8.0 \pm 3.4$	$-7.1 \pm 2.8$	$-5.6 \pm 2$	$-2.5 \pm 2$

The average of the C/E errors among the various integral experiments, mainly from EOLE critical experiment mock-ups, allowed the “calibration” of the APOLLO2.5/CEA93.V6/CEA-97 product, as well as the associated uncertainty, for the main PWR design parameters (Table 4). The qualification range extends up to 4.8% w/o U235 for UOX fuels, and up to 13%Pu for MOX fuels.

**Table 4** Average error, and associated uncertainty ( $1\sigma$ ), of the APOLLO2.5/CEA93 tool

PWR Parameter	UOX	MOX
Keff	$+ 270 \pm 150$ pcm	$+ 100 \pm 250$ pcm
Power Peak	$- 0.4 \pm 0.7$ %	$+ 1.3 \pm 1.5$ %
$\Delta\rho^{\text{cycle}}$	$+ 0.5 \pm 2$ %	-
$dK/dT_{\text{fuel}}$ (Doppler)	$+2 \pm 4$ %	$+11 \pm 4$ %
$dK/dT_{\text{mod}}$ T = 20°C-80°C	$- 0.0 \pm 0.3$ pcm/°C	$- 1.5 \pm 0.3$ pcm/°C
$dK/dT_{\text{mod}}$ T $\approx$ 300°C	$- 0.9 \pm 1.0$ pcm/°C	$+ 3.0 \pm 2.2$ pcm/°C
$dK/dC_B$ (boron coeff)	$+ 3 \pm 5$ %	$+ 0 \pm 3$ %
$\Delta K/\Delta V_{\text{mod}}$ (void coeff)	$+ 0 \pm 3$ %	$+ 2.0 \pm 2$ % (40-60% void) $+ 1.3 \pm 1$ % (100% void)
$\beta_{\text{eff}}$	$+ 2.4 \pm 1.6$ %	$+ 0.1 \pm 1.6$ %
Neutron Lifetime $\Lambda$	$+ 4 \pm 3$ %	$+ 6 \pm 3$ %
$\rho^{\text{Cluster}}$ (24 B <sub>4</sub> C or Ag-In-Cd)	$+ 1 \pm 1$ %	$+ 5 \pm 3$ %
Pyrex 24 SiO <sub>2</sub> -B <sub>2</sub> O <sub>3</sub> $\rho_{\text{initial}}$	$+ 2.7 \pm 1.5$ %	-
UO <sub>2</sub> -Gd <sub>2</sub> O <sub>3</sub> $\rho_{\text{initial}}$	$+ 0.2 \pm 0.6$ %	$+ 1 \pm 4$ %
UO <sub>2</sub> -Gd <sub>2</sub> O <sub>3</sub> $\rho(\text{BU})$	$+ 0 \pm 2$ %	-
Reflector Saving	$- 1.4 \pm 2$ %	$+3.5 \pm 2$ %

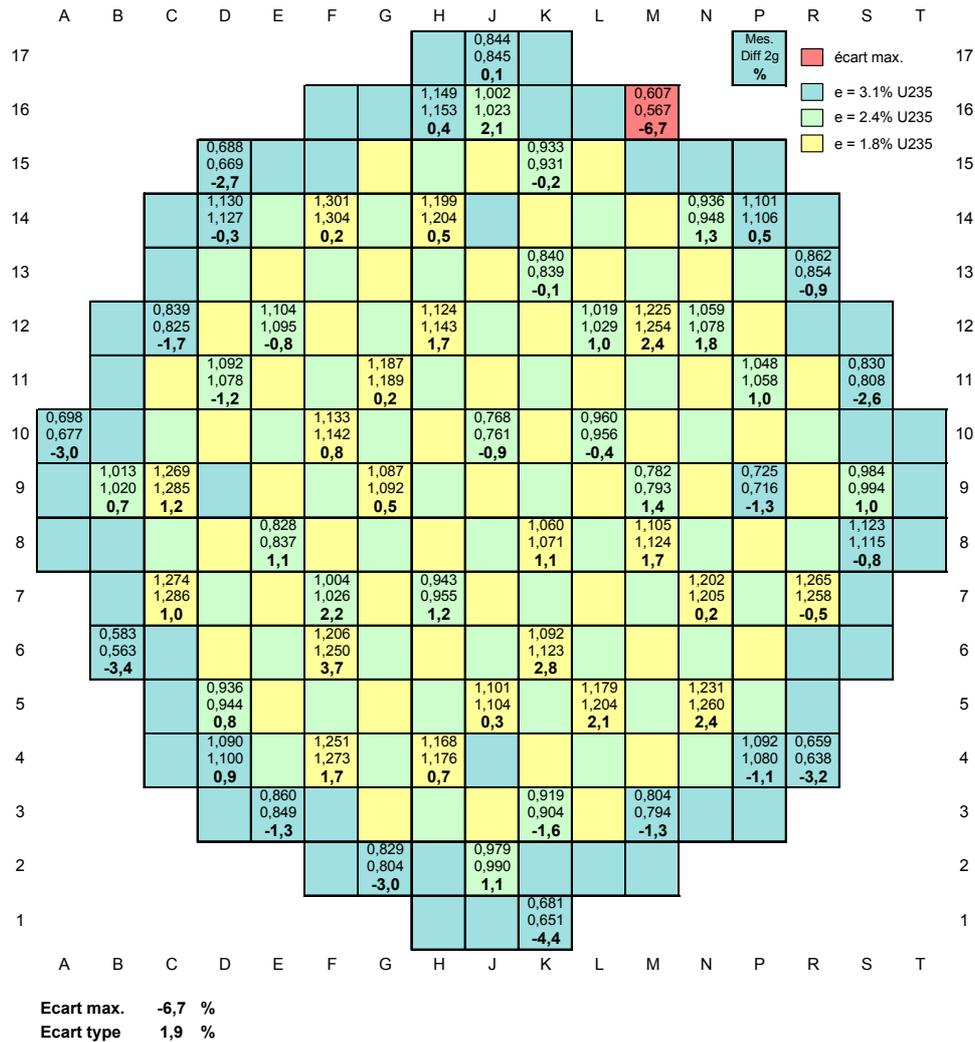
### 3. The CEA calculation scheme : the APOLLO2-CRONOS package

The collapsed and homogenized cross-sections resulting from APOLLO2 transport depletion calculations (SAPHYB libraries) are automatically handled by the CEA 3D-deterministic code CRONOS2 [26] for core calculations. APOLLO2, CRONOS2 and the FLICA4 thermalhydraulics code belongs to the SAPHYR package [27] devoted to reactor calculations and safety analysis. SAPHYR is based on a modular structure that allows a great flexibility of use. A specific user oriented language and a shared numerical toolbox have been developed to chain the various computation modules.

The satisfactory APOLLO2.5 results demonstrated in the qualification studies were globally confirmed by the follow-up of French PWRs, particularly for the 900Mwe Tricastin3 and the N4-1450Mwe Chooz reactors. The CRONOS2.4 core calculations were performed using the Diffusion operator in two energy groups (cut-off energy  $E_c = 0.625$  eV); 3D homogenized assembly pattern was implemented, based on equivalent homogenisation using Selengut normalisation. Finite Element Method was chosen with 2x2 meshes per assembly (parabolic in X and Y, linear in Z). Cross section sets for the axial and radial reflectors were obtained through the MDTBE method which preserves reference MC albedos [28]. A careful attention was paid to the analysis of Start-up experiments at BOC. Calculation-Experiment comparison on the reactivity worth of the various CRC groups is presented in Table 5. The activity maps from the 60 in-core detectors (miniature U235 fission chamber in the central thimble) are compared to the CRONOS results on Figure 1.

**Table 5** Integral reactivity worth of the various CRCs in the Chooz N4-1450Mwe PWR

CRC configuration	Measurement	AP2-CRONOS2	Calc - Meas.	C/M bias
Inserted group	pcm	pcm	(C-M) pcm	(C-M)/M %
X1	239	236	-3	-1.3
X2	457	454	-3	-0.7
SD	637	646	9	1.4
X3	738	733	-5	-0.7
X4	905	901	-4	-0.4
SB	881	901	20	2.3
SC	945	929	-16	-1.7
X5	992	1054	62	6.3
SA	1166	1149	-17	-1.5



**Fig.1** C/E comparison on BOC In-core Measurements (Chooz PWR 1450Mwe)

#### 4. The EDF calculation scheme : the CASSIOPEE package

EDF is currently qualifying a new core calculation chain, CASSIOPEE, which exploitation will start in 2005. It includes two main components :

- the GAB package, which aims to generate the neutronic libraries of assembly cross-sections using the APOLLO2 code ;
- the COCCINELLE core calculation code, which solves the diffusion equation for two energy groups on homogeneous assemblies.

This chain is qualified for a large domain which covers the field of operation of French nuclear power plants, thanks to critical experiments (UOX and MOX configurations in the EPICURE program of the EOLE facility or MOX configuration in the VENUS facility) and the experience feedback from EDF's PWR plants (900 MWe, 1300 MWe and 1450 MWe).

The GAB package ("Library Automatic Generator program") has been developed by EDF to perform lattice physics calculations on a user-friendly platform. It provides two main ways to create studies :

- a graphical user interface, based on a technological database containing information such as fuel composition, assembly geometry, fuel and coolant temperatures. With this interface, a user can build a library by selecting only few parameters. This interface is mainly used for industrial studies.

- an interactive text interface : a user can build a library or execute a graph of calculation dependencies of his choice for particular assemblies with his own data. The fine description of new assemblies for conception and R&D studies can be processed.

GAB offers the capability to generate cross sections libraries for all types of assemblies used in EDF PWRs: UOX as well as MOX assemblies, with or without burnable poisons, with or without inserted control rods, possibly taking into account corrections due to moderator density evolution in space and time or due to delayed neutrons.

GAB implements the industrial calculation scheme by executing about 800 calculations.

It first generates the space and energy homogenized cross sections. For each type of assembly, considered in an infinite medium and in operation conditions, and supposed to be critical, a depletion calculation is performed using a heterogeneous transport Pij-multicell option within the CEA code APOLLO2, associated with the 99-group energy cross sections library CEA 93 release 6. A simplified geometry with only a few cells (in which the calculated neutronic flux is the same) is used for this calculation, but each pin is split in different regions for the flux calculation. In order to be consistent with the Selengut homogenisation method, calculations are performed using the ROTH formalism.

Once the APOLLO2 depletion calculation has been completed, cross sections are homogenized in energy and in space, but still cannot be used directly: they must be corrected for the homogenisation and diffusion approximations. This “equivalence” is done by HERMES, one of the GAB components, which aims to evaluate the “equivalence” factors, so calculated as to render the diffusion and transport modes equivalent. It is based on the conservation of three values between the transport and the diffusion calculation: reaction rates, neutron flux at the cell, and migration area. The equivalence corrected cross sections can then be directly used for a pin by pin diffusion core calculation. However, as current calculations are performed using a homogeneous diffusion method, it is necessary to homogenize the cross sections on the whole assembly. JONAS is dedicated to this step: the cross sections are weighted with the flux derived from the pin by pin diffusion values obtained for the assembly, and then normalized with respect to the flux at the edge of the assembly. This normalization preserves assembly in-going and out-going fluxes and avoids power distribution artificial discontinuities at assembly interfaces, which is one of the strength of this scheme.

Afterwards, the radial power distribution within the assembly can be determined, in order to be used for power reconstruction by factorisation with the macroscopic fluxes derived from homogeneous diffusion core calculations. MOX assembly fine power structure is calculated on a special pattern including UOX assemblies to improve the flux calculation on the MOX/UOX interface.

At last, GAB supplies the coefficients for the analytic feedback model implemented in the 3D core calculation code COCCINELLE, which allows to performed core calculations in all kinds of thermal-hydraulic situations.

Notice that the GAB package uses an independent data model: when calculations are processed, it translates user data into the data model of each computer code (i.e. APOLLO2, HERMES, JONAS) and dispatches jobs on several computers, then brings results back, which can be post-processed by users, or directly used for core calculations with the 2D-3D code COCCINELLE.

COCCINELLE is used for the basic designs as well as for the refuelling studies. It allows to check safety assessment of each loading pattern, thanks to an application called NACRE (which is also designed to complete the full information the operator needs). It solves the diffusion equation for two energy groups with the nodal method for pin by pin geometry or homogeneous assembly with reconstruction by factorisation of the pin power.

The user can compute steady-state calculations with fixed or critical Boron concentration, as well as transient scenarios for accident studies or poisoning of the core with Xenon or Samarium. Neutron sources can also be simulated. The code is used for depletion (including stretch-out), and rod-worth evaluations.

Its high adaptability to operational and accidental calculations is based on a 1D thermal-hydraulics module and a fuel model, to deal with heat-exchanges between the moderator (light water) and the fuel, and within the fuel (pellet, gap and clad) by means of qualified correlations, as well as on the analytic feedback model which allows to perform calculations in extreme conditions. This feedback model takes into account Doppler effect, boron concentration and water density for the fast group, and water temperature, water density, boron and xenon concentration for the thermal group, by the means of the coefficients determined with APOLLO2.

To deal with accidental simulations, such as SLB (Steam Line Break) and Boron dilution, in which 3D thermal-hydraulics effects are major, COCCINELLE can be coupled with the THYC (3D two-phase thermal-hydraulics EDF code) or the CATHARE code.

## **5. The Framatome-ANP S.A.S calculation scheme : the SCIENCE package**

The Framatome-ANP S.A.S. package SCIENCE has been fully operational for nuclear design since 1997 and calculation results have demonstrated the high accuracy of the physical models.

SCIENCE's user accesses computer codes through the friendly graphical user interface COPILOTE which manages all engineer tasks needed for calculation: computations, chaining, data input, job submittal, execution monitoring,...

Main components are the APOLLO2-F code for assembly calculations, the SMART advanced nodal code for 3D core calculations and the SQUALE code for flux map processing. All of these codes have the same modular architecture allowing easy management of data structures, using "objects" and easy handling of various calculation schemes.

APOLLO2-F is the Framatome-ANP S.A.S. version of the APOLLO2 code. In the present SCIENCE V2 industrial scheme, it is used with the CEA93 99 neutron-energy group library supplied by CEA, and based on the JEF2.2 evaluation. Neutron transport over the PWR assembly is thus modelled with APOLLO2-F, using the following main features:

- in a first step a 99-group multicell Pij heterogeneous assembly calculation is performed, with one cell per type of rod and the actual geometry for each cell; fuel pellets are divided into 5 rings- a heterogeneous transport /homogeneous transport equivalence is then realised, leading to 6 groups collapsed homogeneous cross-sections for the assembly,
- the flux calculation is then performed with this 6 groups structure, using the Sn method to solve the 2D transport problem over the assembly, where each fuel cell has been homogenized with its surrounding moderator media,
- finally, the Sn flux is used to deplete the fuel while preserving the "ring-by-ring" depletion effect, keeping in memory the 5 rings structure of the first step above.

The SMART code, the core simulator developed by Framatome-ANP S.A.S., is a 3D nodal code, which reads the cross-sections generated by APOLLO2-F, and uses a sophisticated cross-section and feedback model, based on multi-parametrized tables, to solve the 3D diffusion version of the Boltzmann equation. Special care has been given for depletion modelling in SMART: microscopic depletion is performed, associated with extended depletion chains, with 28 isotopes and 2 new macro-isotopes, equivalent to 4 fission products each. In particular, this allows model 90% of the reactivity effect during plant shutdown. Also, the latest versions of SMART benefit of a state of the art thermal model for fuel rod temperatures using the Framatome-ANP S.A.S. thermo-mechanical code COPERNIC, which copes with rim effect and high burnup fuels.

In addition to physical improvements, new functions developed for accident analyses are now fully integrated into SCIENCE-V2: 3D kinetic calculations, coupling with open channel thermal-hydraulics core model and with plant simulation (coupling of SMART and FLICA codes).

An example of physical performances of the APOLLO2-F code as used by Framatome-ANP is given

in Table 6, where one can find the values of the control rod cluster worth, as calculated by APOLLO2-F and compared with measured control rod worth (Silver-Indium-Cadmium and Boron Carbide clusters in EPICURE experiments).

**Table 6** SCIENCE-V2 calculation of control rod cluster worth in the EPICURE experiment

EPICURE Configurations	Control rod cluster	SCIENCE V2 C/M-1 (%)	Measurement uncertainty ( $1\sigma$ )
UOX: UH1.4	24 AIC	1.7%	2.5%
	24 B4C	0.3%	2.4%
MOX: UMZONE	24AIC	-0.9%	1.4%
	24 B4C	2.4%	1.8%
<b>Mean value</b>		<b>0.9%</b>	

## 6. Conclusion

Thanks to a continuous effort in development and validation/qualification, the current APOLLO2.5/CEA93V6 product has become an outstanding tool for diversified neutronics applications, from sophisticated R&D studies requiring state-of-art methods to routine industrial calculations. In LWR studies particularly, with its reference scheme "CEA-97" and using the stored APROC procedural libraries corresponding to the recommended code options, the most part of design parameters are predicted within the required target accuracy. In the near future, the calculation of high burnup fuel inventory would be improved thanks to the use of a new APOLLO2 library CEA2003 [29], processed from the recent European File JEFF3. The next generation tool, i.e the DESCARTES neutronics code, will involve both lattice and core solvers using deterministic and Monte Carlo methods, with an increased level of flexibility and conviviality.

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