

## THE SAPHYR SYSTEM: AN OVERVIEW

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### ABSTRACT

The multi code system SAPHYR has been developed by the (French) Commissariat à l'Energie Atomique (CEA) for reactor analysis and studies. This package, whose main components are APOLLO2 [1], CRONOS2 [2] and FLICA4 [3] (Figure 1), includes codes for neutronic and thermal hydraulics core calculation. The SAPHYR code system is used to study various types of reactors, from PWRs and BWRs, to experimental reactors, from spatial power reactor designs to VVERs, from RBMKs to naval propulsion systems. FRAMATOME-ANP has already integrated APOLLO2 and FLICA4 as part of its reactor calculation package SCIENCE and Electricité de France is integrating APOLLO2 in its newest calculation scheme.

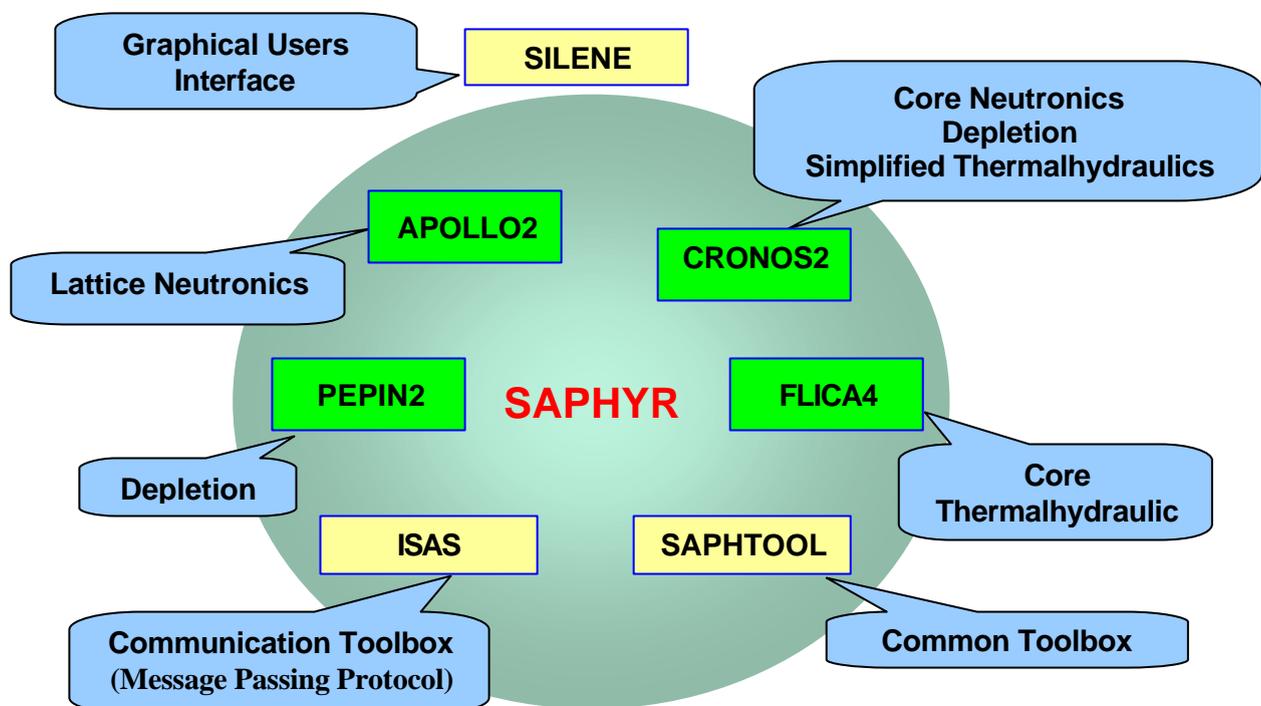


Figure 1. The SAPHYR code System

## 1 INTRODUCTION

The purpose of reactor core neutronic studies is to predict the phenomena likely to occur when the number of neutrons in the fissile and non-fissile material in the core changes. The amount of energy released by fission, neutron capture and radioactive decay can therefore be determined. Neutronics makes use of well-known equations, such as Boltzmann's equation for particle transport and Bateman's equation for fuel modifications. They model physical phenomena perfectly and can be solved theoretically with great accuracy. However, reactor cores are extremely heterogeneous, the variations in the energy released by the cross-sections are highly complex and there is such a high degree of dependency between neutronic and thermal hydraulic phenomena that current calculation tools are unable to produce solutions using a direct method.

Therefore, a multi-scale method involving three steps is used at present:

- Step 1: Multigroup cross-sections libraries are obtained from international evaluations (such as ENDF or JEF2). Data processing is performed using NJOY or THEMIS codes. During this step, self-shielding and Doppler parameters are computed. Cross-sections libraries obtained may be dependent on the energy spectrum used at this stage (about 100 groups).
- Step 2: A lattice code is used to solve a small highly heterogeneous domain (such as a fuel assembly or part of one). Multigroup cross-sections are computed by taking into account the self-shielding phenomena. This step is processed by the multigroup transport code APOLLO2. The cross-sections are then homogenized in space, collapsed in energy and stored in a neutronic library. The homogenization process is either performed on the assembly as a whole, or on the pin cell level.
- Step 3: CRONOS2 uses the fuel assembly libraries to solve the problem for the entire core. The reflector is modeled using a specific equivalence method in order to preserve the albedos. Thermal hydraulics feedback effects can be modeled either with simplified models within CRONOS2, or by coupling the Thermal hydraulics code FLICA4. Microscopic and macroscopic depletion is performed with internal modules.

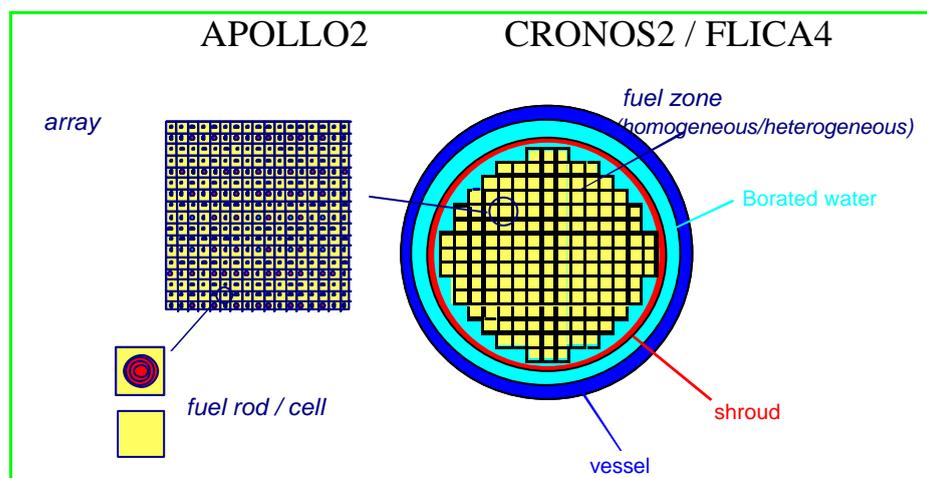


Figure 2. Stages in the PWR calculation system

This 3-stage approach is widely used for power reactors and constitutes a powerful calculation system for pressurized (Figure 2) and boiling water reactors, with rectangular and hexagonal fuel arrangements, gas-cooled, graphite-moderated reactors, fast reactors, naval propulsion reactors and certain experimental and research reactors.

This paper comprises three parts. In the first one, we give a brief review of the dedicated improved code structure common to all the codes included in SAPHYR code system. The second part is devoted to a more detailed description of the physical modeling and advanced numerical methods used in the APOLLO2 and CRONOS2 codes. To illustrate the potential of the actual version of SAPHYR, in the last part we present some recent studies using coupled neutronic/thermal hydraulic calculations.

## 2 SOFTWARE SUPPORT PACKAGE

One of the main aims of the code designers was that SAPHYR should be able to perform reference calculations, with the maximum precision allowed by the available computers, as well as industrial and project routine calculations that would run faster and would require less precision.

They also wanted to have a code structure that would allow an easy implementation of new methods and models with the benefit of all the possibilities already available in the codes.

For those two reasons, the SAPHYR codes were designed with a fully modular structure, consisting of a predefined set of operators (functions) and a predefined set of objects (data). Indeed, SAPHYR 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, etc.) and that can be viewed as operators that act on input objects to create output objects.

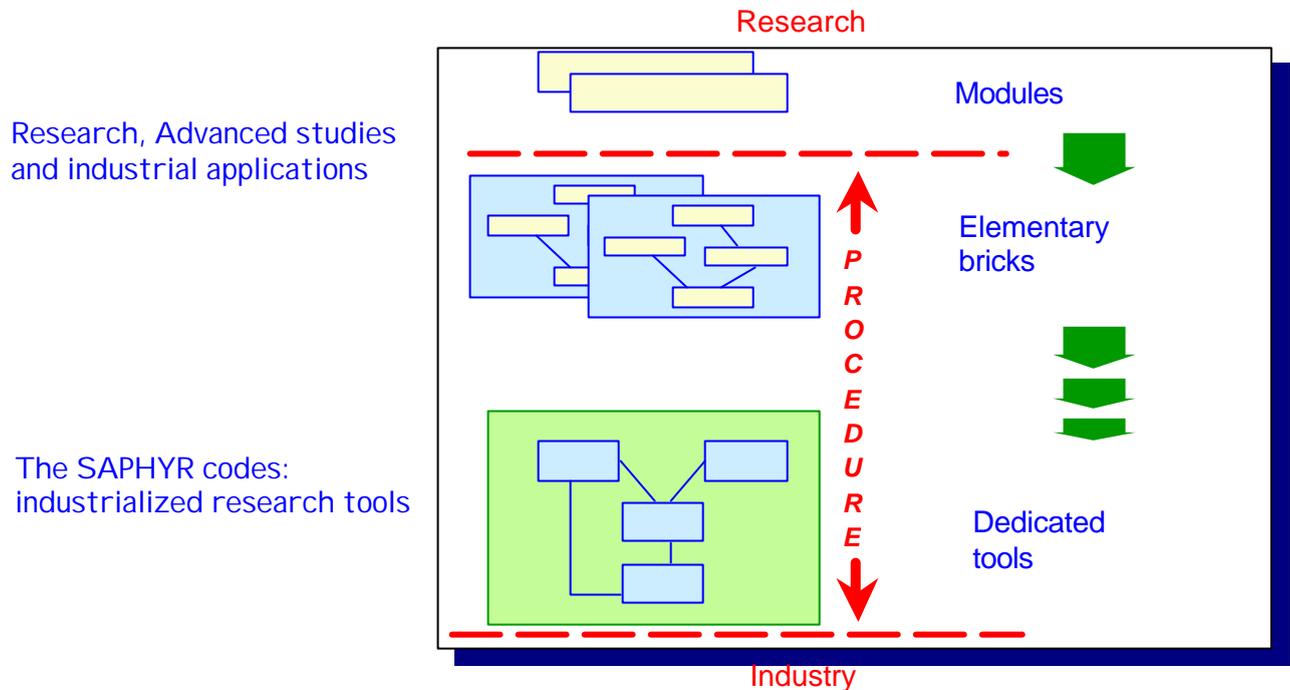


Figure 3. The modular structure

The GIBIANE macro language is used to dynamically link the operators at run time, defining thus a particular calculation scheme to fit specific users' goals (Figure 3). The implementation was made possible by the use of an extension of FORTRAN 77 developed in the early 80s by the CEA, the ESOPE-GEMAT software package, that allows for data structuration, dynamic memory allocation (DMA). At that time, such functionalities were not available in conventional computer languages, especially not the DMA, or the garbage collector. Both GIBIANE and ESOPE-GEMAT can be translated into standard FORTRAN77 code source to ease the implementation of the SAPHYR codes on various platforms.

SILENE, a JAVA based GUI [4] has been developed to ease the description and treatment of complex geometries, especially unstructured meshes. The latest version of SILENE provides pre and post treatment for APOLLO2 and the Monte Carlo code TRIPOLI4.

The self-descriptive, general purpose, parameterized output library SAPHYB contains not only macroscopic and microscopic cross-section data resulting from space - energy homogenization by APOLLO2, but also fluxes, kinetic parameters and much more. The SAPHYB library is used for applications such as pin-by-pin or homogeneous whole-core CRONOS2 calculations and PEPIN2 depletion calculations.

The ISAS code is a message passing protocol based on PVM. It allows users to create data flow networks for scientific computations by passing data between modules of slave codes. This system allows coupling different codes of the SAPHYR system, like CRONOS2 and FLICA4, which normally run on standalone mode.

The SAPHYR codes are being developed under the control of the ACROPOLE software workshop. This tool manages source files with conflict resolution. It also enables the code to be launched from a graphical interface. Today the SAPHYR codes run on all kinds of computers from CRAY (C90 or MPP) to personal computers (PC under Solaris) or workstations of all brands (Sun/Solaris, IBM/AIX, HP/HP-UX, SGI/IRIX, DEC Alpha/OSF1, VPP Fujitsu, etc.). Code development is done under strict quality control.

### **3 PHYSICAL MODELS AND ADVANCED NUMERICAL METHODS**

#### **3.1 THE APOLLO2 CODE**

The neutron and gamma multigroup transport cell code APOLLO2 was previously presented [1]. APOLLO2 works with an arbitrary number of regions, groups, isotopes and burnup zones. The operators and data structures have been designed to optimal calculation performances in the 100-group range. The main functions, shown on Figure 4, are reviewed next.

##### **3.1.1 The multigroup isotopic library**

The CEA93 library is based on the JEF2 evaluation. The processing is done with the same options and precisions than the ones used to prepare libraries for Monte Carlo calculations, allowing thus for unbiased calculations and validation with TRIPOLI4 [5]. This library is available to the user in two standard multigroup formats: the traditional 99-group energy mesh and the Xmas 172-group structure [6]. Transfer cross-sections for some specific 'isotopes,' such as lead or light water, have been developed up to  $P_5$  order of anisotropies. Information has enriched the CEA93 libraries. Among these one finds  $(n, \alpha)$  and  $(n, p)$  reaction cross-section data; and delayed neutron data are included in the

library so that APOLLO2 can calculate the effective fraction of delayed neutrons,  $\beta_{\text{eff}}$  and pass it to the core code CRONOS2 to perform kinetic calculations. Various depletion chains are associated with the CEA93 library. The CEA93 does not require any cross-section adjustments. Recently, gamma cross-sections have been introduced in order to treat coupled neutron-gamma phenomena.

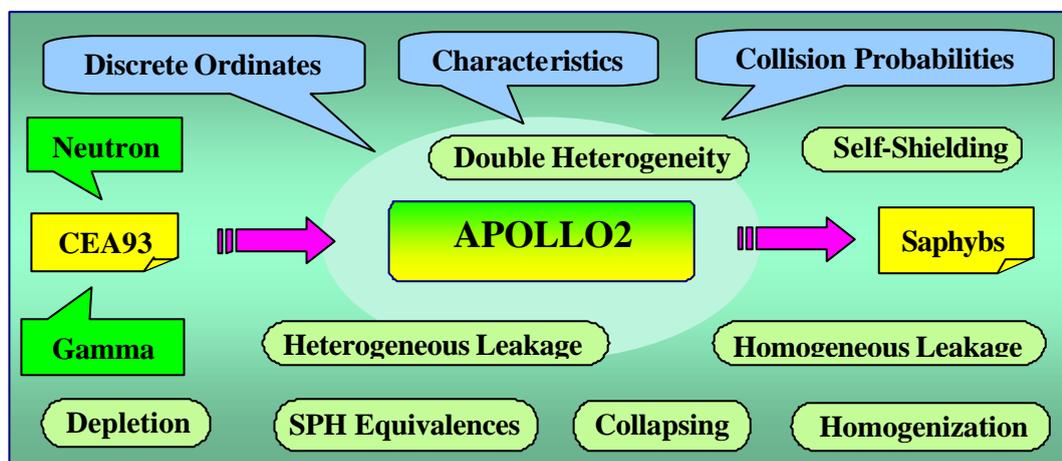


Figure 4. APOLLO2 functionalities

### 3.1.2 Self-shielding

In order to provide better stability and enhanced accuracy, a continuous effort has been put into the improvement and development of self-shielding methods. The main directions of research are improvement of the existing methodology, development of new models and elaboration of fine-multigroup reference calculations. Quadrature formulas based on probability tables (PT) have been introduced. These tables are computed with CALENDF's formalism for total cross-sections and their partial cross-sections by preserving group moments of positive and negative powers. Group collapsing can be readily performed. Two robust models (ST and TR models) for resonant slowing down have been developed [7]. These models share two common assumptions: scattering is isotropic in the center-of-mass reference frame and the nuclei are heavy. By making the assumption that isotopic cross-section behavior is similar at different temperatures, one can construct a probability table that describes region interactions from individual single-temperature PTs, and use them to compute accurate temperature-dependent multigroup self-shielded cross-sections. Extensive comparisons with Monte Carlo results have allowed determining the accuracy of the models.

Recently, a linear interpolation scheme has been used to reconstruct fine-multigroup microscopic cross-sections, allowing thus for thousand-of-group assembly calculations [8].

### 3.1.3 Cross-section collapsing and homogenization

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-sections by either direct flux weighting or via equivalence theory (SPH formalism) [9].

### 3.1.4 Burnup

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.

### 3.1.5 Leakage models

The homogeneous leakage model proves to be insufficient in cases of strong leakage or anisotropy, such as those involving accident analysis of partially or totally voided assemblies. The  $P_1$ -corrected heterogeneous leakage TIBERE model [10] has been developed by introducing adequate approximations in  $B_1$  heterogeneous leakage theory. Unlike the homogeneous leakage model, TIBERE yields more realistic region-dependent directional leakage coefficients.

### 3.1.6 Transport solvers

Transport solvers, based on the classical collision probability method have, for many years, been implemented in APOLLO2. The transport solver (TDT) introduced in APOLLO2 code [11], provides an interface-current method with the ability of treating unstructured 2D meshes and the 3D geometries axially generated from these meshes. The TDT solver is based on the method of characteristics. The discrete ordinates IDT solver [12] allows to treat 2D and 3D Cartesian regular geometries with nodal and characteristics approximations. Powerful DSA acceleration techniques have been introduced in IDT [13,14,15].

## 3.2 THE CRONOS2 CODE

The CRONOS2 code [2] has been designed to provide all the computational means needed for diffusion and transport core calculations, including design, fuel management, follow up and accidents. CRONOS2 most outstanding are shown in Figure 5.

It allows steady state, kinetic and transient multigroup calculations of power distribution taking into account the thermal-hydraulic feedback effects, including sensitivity analysis thanks to the generalized perturbation theory. There is a large range of processing possibilities as regards both cross-sections and geometry types. The code also includes a number of graphical tools for pre and post processing. All this can be done without any limitation on any parameter (energy groups, meshes...).

### 3.2.1 Cross-sections processing

Once the various modeling steps required before CRONOS2 core calculation have been completed, the homogeneous, isotopic multigroup neutron data are stored in a cross-section library. The cross-sections are parameterized to make allowance for the variation in spectrum resulting from burnup and temperature effects when energy homogenization is being carried out. The user is free to select whichever type of parameterization is desired. Cross-sections at the operating point are computed by a linear interpolation between the points that are closest to each other in the library. This simple and general method allows a wide range of applications. Using the finite element approach, the method can be refined by representing the parameters by polynomial approximation within each mesh of the calculation.

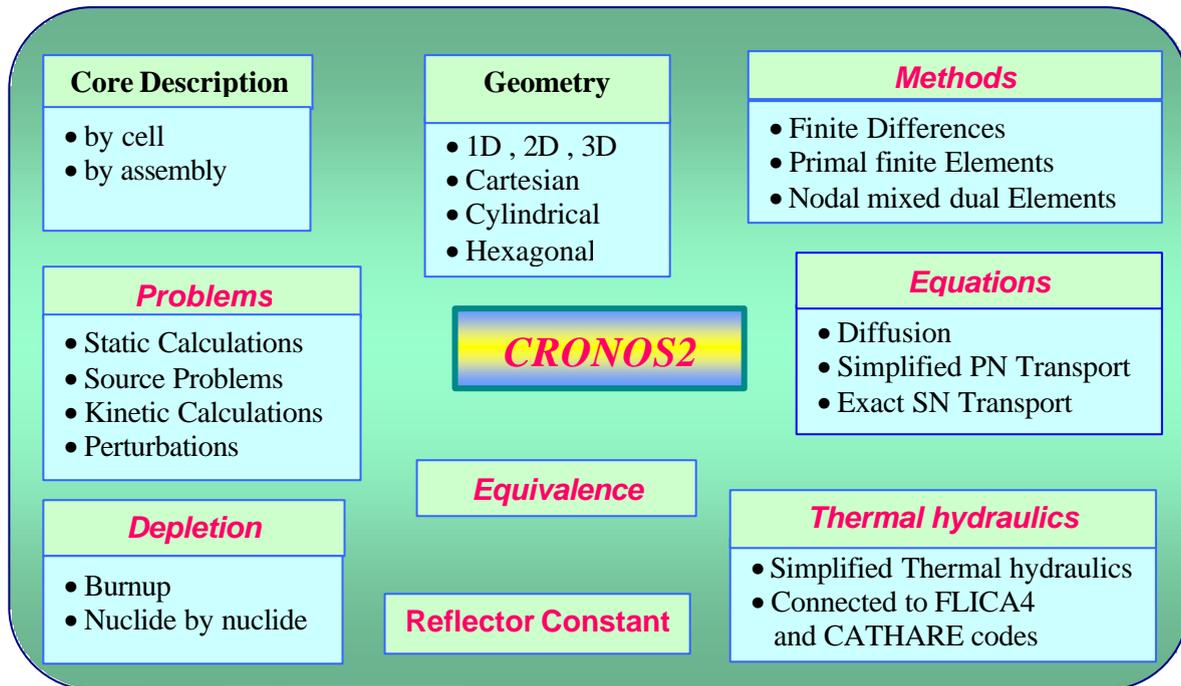


Figure 5. CRONOS2 functionalities

### 3.2.2 Static calculations

Static calculations are used to study reactor behavior in normal operating conditions and carry out fuel management studies. Assembly or pin homogenized calculations can be performed. Pin-by-pin calculations are intended to give further information on the local power peak, without having to apply fine flux reconstruction models.

The CRONOS2 code is able to solve the diffusion and the transport equations. This last equation is required for situations where the high flux anisotropy is such that diffusion approximation is insufficient. The two main flux solvers in CRONOS2 are:

- The PRIAM solver: it is based on finite element approximation (FEM) in space, and the  $S_N$  approximation in angle. This approach offers a high degree of flexibility when defining the geometry: rectangular, hexagonal or cylindrical, and more recently geometry based on triangular and isoparametric elements [14]. Various boundary conditions (reflection, symmetry, periodicity, translation, albedos) are available. Thanks to this method, CRONOS2 was one of the first codes in the world to solve the 3D pin-by-pin transport equation [16].
- The MINOS solver: it is a powerful nodal method [17] for dealing with structured geometries. It differs from conventional nodal methods in that it has a rigorously FEM mathematical basis. The main advantages of this method are that the system is conventional in terms of the neutron balance and it can be used to process singularity equations at the mesh interfaces. Transport calculations can be carried out on a routine basis due to the extension of the solver to the simplified transport equation ( $SP_N$ ) [18]. It has been possible to carry out an entire PWR transport calculation cycle that has reduced by a half the gap between calculation and measurement, and supplied further information on control rod worth [19].

### 3.2.3 Kinetic calculations

Three-dimensional fast kinetic calculations are required for studying accident situations such as main steam line break or control rod ejection. When the time variable and delayed neutrons are taken into account, the systems become more difficult to solve. The resolution method is based on a scheme with an implicit time step ( $\vartheta$  method). The delayed neutron equations are integrated exactly. The spatial resolution technique used for the MINOS solver has been adapted to kinetics to improve calculation time. Recently, the method was extended to SPN transport equations, taking into account the time dependence of the current.

The Improved Quasi-Static method (IQS) is also available in CRONOS2 [20]. The possibility to take large time steps for shape flux calculation allowed by the IQS method, allow us to reduce considerably the computing time of the calculations.

### 3.2.4 Source calculations

The importance of source calculations can be illustrated by the study of the repositioning of fuel assemblies, which are very small sources in relation to the size of the reactor. Since the equations to be solved are of the same nature as the kinetic equations after time discretization, this new possibility has been introduced into CRONOS2, taking advantage of the most sophisticated resolution techniques. The method was extended to SPN transport equations to take into account anisotropic sources. This new feature allowed considerable progress to be made, particularly when it came to determining equivalent reflector constants [19].

### 3.2.5 General perturbation calculations

Perturbation calculations are used to obtain estimates of the variations in physical quantities said to be “observable” (reaction rates, reactivity, local power, axial power imbalance or axial offset etc.) in relation to parameters such as the position of a control rod or the soluble boron concentration. The estimates are obtained extremely quickly without any need for the flux variation to be known. This means that the method can be used for reactor control, where rapid responses are required. The strong point of the method used in CRONOS2 [21] is that it has been generalized to cover any order so that better estimates can be obtained and its variational approach makes it possible to obtain a consistent approximation for associated calculations, which is not always the case with nodal methods.

### 3.2.6 Feedback effect, neutronic/thermal hydraulics coupling

If neutron distribution and power density inside the core are to be computed accurately, the thermal hydraulics of the coolant and the heat released by the fuel rods have to be taken into account. These phenomena are computed using special codes associated with each field and coupled by exchanging boundary conditions. The thermal hydraulics of the core can be dealt with by the FLICA4 code coupled with CRONOS2 via the ISAS application. This coupling has a part to play in the study of accident situations such as steam line break or control rod ejection.

For very simple situations, CRONOS2 has its own simplified thermal-hydraulics model.

### 3.2.7 Isotopic depletion

CRONOS2 includes a special method for processing isotopic depletion. Depending on the shape of the modification sequence, analytical resolution is used for triangular systems and in appropriate steps and degrees in general cases.

For the most common types of studies, it is possible to replace detailed evolution of isotopes by parametric evolution. With this approach, the assumption is that the depletion of the concentrations, when the fuel assembly is in an infinite environment, is sufficiently close to their evolution in the core as a whole. Once the state parameters have been re-assessed, the new isotope concentrations are calculated by interpolation of the concentrations in the APOLLO2 library.

## 4 NUMERICAL EXAMPLES

### 4.1 LARGE CLUSTER CALCULATIONS

The APOLLO2 code, dedicated to the assembly calculations, has the capability to treat large clusters of assembly. In [22], a review of different deterministic methods integrated in the APOLLO2 code has been presented and has been applied to the calculation of those geometries. They used, for solving the neutron transport equation, the collision probability ( $P_{ij}$ ) method, the recently implemented Characteristic method as well as the so-called two-level scheme (TLS). Those methods and schemes have been run for calculating a large and heterogeneous cluster representing a usual French PWR lattice configuration. The various results are in good agreement with those obtained with a precise Monte Carlo simulation.

### 4.2 PWR REFERENCE CALCULATIONS

The study focused on axial activity (fission rate) calculations for the core of St Laurent B1 French nuclear power plant. The 900 MWe core was wired with 50 fission chamber detectors placed in the central water duct of the 17x17 array. The measurements were taken in 56 planes distributed over the entire height of the core and the values were then integrated axially. The results of the non-adjusted calculations carried out with the SAPHYR system were compared to the measurements made by EDF over three cycles (105, 106 and 107). The CRONOS2 calculation (2-group diffusion) was carried out in two stages corresponding to superimposition of a homogeneous 3D calculation and an average pin-by-pin 2D calculation. Thus the local flux value at the center of the wired fuel assemblies can be obtained. To eliminate the radial drift that occurs at the start of the cycle, the results are centered on an average plane. Figure 6 shows the statistics for the deviations between the non-adjusted activity values obtained using CRONOS2 and those obtained from measurements. The result is a well-centered Gaussian curve and a small standard deviation for the UOX assemblies, proving the good quality of the results.

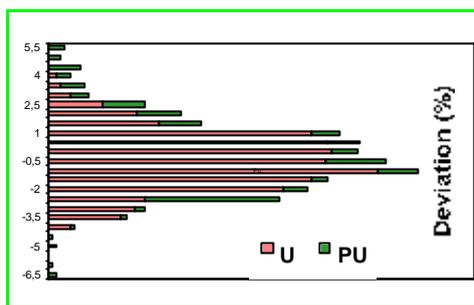


Figure 6 - Statistics showing deviations between measurement and calculation results for the core at St Laurent nuclear power plant

### 4.3 HTGR REACTORS

The SAPHYR system, initially dedicated to PWR calculations, has been transposed to HTGR calculations [23]. The benchmark problems of the HTTR's start-up core physics experiments initially proposed by JAERI through the IAEA in a Coordinated Research Program, has been performed in order to validate and qualify the SAPHYR codes that will serve to evaluate the future HTGR generation. For the analysis, a calculation scheme based on a deterministic approach is used.

The double heterogeneity calculations of the coated fuel particles and the self-shielding in the resonance region are taken into account in a fuel cell calculation performed with APOLLO2.

The core diffusion calculations are performed with CRONOS2, using a homogenized fuel element and without taking into account the streaming effect. The new finite elements have been used in the code CRONOS2 in order to improve the description of the fuel element radial heterogeneity in the core calculations [14]. Some limitations appear in the APOLLO2/CRONOS2 calculation scheme for thin annular core configuration where fundamental mode approximation seems to be hardly applicable. After all, it can be stressed that all calculation results obtained for the fully loaded core configuration fit well each other and with the experiment, considering the experimental uncertainties.

### 4.4 BWR CALCULATIONS

BWR fuel assembly heterogeneity causes steep thermal flux gradients. The 2D collision probability method with exact boundary conditions, associated with a two-level flux calculation, makes possible to compute accurately the flux in BWR fuel assemblies with APOLLO2 [24]. Void fraction variations in assemblies involve big spectrum changes that it is necessary to consider in core calculation. So, a void history parameter is used to generate cross-sections libraries for the core calculation with CRONOS2. Core calculations associating neutronic and thermal hydraulic effects have been performed [25]. APOLLO2 calculations using the Characteristic method are in progress.

### 4.5 RESEARCH REACTORS

The research reactors are usually characterized by a small core, a very complex heterogeneous geometry and a large leakage. For this type of cores, the classical 2 stages "2D transport - 3D diffusion" treatment results in unacceptable errors in the prediction of the flux map and the power

distribution, and one has to resort to the full transport scheme. For the Orphée research reactor, a multigroup albedo model has been implemented in the APOLLO2 code [26], and few-group 3D  $S_N$  transport calculations have been done with the CRONOS2 code. Comparisons between 2D whole core transport calculations with external vacuum boundary condition and 2D multigroup albedo calculations have proved the precision and the efficiency of the method.

#### 4.6 NUCLEAR SAFETY REVIEWS: THE RBMK SERIES

The effective cross-section libraries were to be created using the WIMS code. CRONOS2 was therefore adapted so that it could read these libraries. 3D kinetics calculations have been carried out and compared to those obtained using various codes. CRONOS2 has also been used to model the control system and its logic during a control rod withdrawal transient. The CEA was the only organization able to present this type of model [27].

#### 4.7 NUCLEAR SAFETY: A CONTROL ROD EJECTION BENCHMARK

The Institute for Nuclear Safety and Protection (IRSN) is working on a 3D kinetics benchmark for control rod ejection, which was instigated by the Nuclear Regulatory Commission (the American safety authority), using the SAPHYR system [28]. The calculations are currently based on a cell-by-cell diffusion approximation and are coupled with FLICA4. It is planned to continue these studies with kinetic transport calculations. This new function will be a welcome addition to CRONOS2 since it is essential to be able to check whether the power reconstitution methods of industry tools, which have been validated in normal operating conditions, continue to be valid in accidental situations where there is a strong power level variation with high power peaks. None of the existing software can be used as a reference in this area.

### CONCLUSIONS

Thanks to a continuous developmental effort, the SAPHYR system has become an outstanding tool for diversified applications covering a large domain of applications, from sophisticated R&D studies that need state-of-the-art methodology to routine industrial calculations for reactor and criticality analysis. It is powerful enough to carry out calculations for all types of reactors and is invaluable for understanding complex phenomena. SAPHYR will be in use in most of the French nuclear companies such as Electricité de France, Framatome, Cogema, SGN, Transnucléaire and Technicatome.

Even though it is being widely used already and has numerous functions, SAPHYR continues to be developed to improve current performance levels and acquire the new functions constantly required by users concerned with modeling and numerical methods.

It also acts as a reference for validating the R&D ideas that are set to lead to certain specifications for the new generation of DESCARTES tools, due to replace the existing ones in 2010.

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their criticism and support to make SAPHYR a better system. Thanks are due, in particular, to the entire SAPHYR project team. Last but not least, we want to thank our friends from Framatome and Electricité de France that financially and through constant cooperation have backed CEA's effort to elaborate the successive versions of SAPHYR codes.

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