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THE ERANOS CODE AND DATA SYSTEM FOR FAST REACTOR NEUTRONIC ANALYSES

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ABSTRACT

The main modelling options of ERANOS 2.0, the latest version of the ERANOS fast reactor analysis code and data system, are described. These include the ECCO cell and lattice code (Collision Probability Method in many groups using the sub-group method), the BISTRO 2-D S_n transport code, the TGV/VARIANT 3-D Nodal Variational Transport code, and a special procedure for creating equivalent homogeneous cross sections for control rods. The recommended "reference" core calculation route is presented.

A summary of the ERANOS extensive validation is provided. It is concluded that ERANOS 2.0 can predict the main characteristics of conventional as well as advanced liquid-metal-cooled fast reactors with an excellent accuracy, and that it can also be used for modelling advanced fast reactor cores, source-driven sub-critical media and gas-cooled fast reactors.

1. INTRODUCTION

Fast reactors have a potentially important role to play in the future as they can either overcome the

shortage of uranium ore by transmuting uranium into plutonium or burn effectively plutonium and minor actinides. The core characteristics of advanced fast reactors require reliable methods and data in order to address the challenges of their new features.

The European Reactor ANalysis Optimized calculation System, ERANOS, has been developed and validated with the aim of providing a suitable basis for reliable neutronic calculations of current, as well as advanced fast reactor cores.

This paper describes the main features of ERANOS 2.0, the latest version of the ERANOS software. A summary of the code extensive validation is also provided.

2. GENERAL OVERVIEW OF THE ERANOS 2.0 CODE AND DATA SYSTEM

The deterministic ERANOS neutronic system consists of data libraries, codes and calculation procedures which have been developed within the European Collaboration on Fast Reactors over the past 15 years or so [1].

The latest version of the ERANOS code and data system, ERANOS 2.0, contains all of the functions required for reference and design calculations of Liquid Metal Fast Reactor (LMFR) cores (as well as blankets, reflectors and shields), with extended capabilities for treating advanced reactor fuel subassemblies and cores, Accelerator Driven Systems (ADS) and Gas Cooled Fast Reactors (GCFR).

The ERANOS code system was developed to answer the needs of both industrial and R&D organisations. ERANOS is written with the ALOS software which requires only standard FORTRAN compilers and includes advanced programming features. A modular structure was adopted to allow the incorporation of the most recent research and development innovations. Blocks of data (EDL's) can be created or used by the modules themselves or by the user *via* the LU control language. Dynamic memory allocation is performed by the ESOPE language. External temporary storage and permanent storage capabilities are provided by the GEMAT and ARCHIVE functions, respectively. ESOPE, LU, GEMAT and ARCHIVE are all part of the ALOS software.

This modular structure allows different modules to be linked together in procedures corresponding to recommended calculation routes ranging from fast-running and moderately-accurate "routine" procedures to slow-running but highly-accurate "reference" procedures.

The ERANOS 2.0 reference calculation scheme is based on the ECCO cell and lattice code [2] (Collision Probability Method in many groups using the sub-group method), the TGV/VARIANT code (3-D Nodal Variational Transport Code) [3,4] and a procedure for creating equivalent homogeneous cross sections for control rods, based on the S_n transport code BISTRO and its associated perturbation modules. These main characteristics of ERANOS 2.0 are described below.

Many other modules and procedures are available but are not described in this paper. For example,

it is possible to model reactor actual operating conditions, determine detailed (with separate gamma contribution) or average (for burn up calculations) energy releases, calculate damage rates, perform fuel depletion calculations and carry out perturbation analyses (using either direct, general or harmonic perturbation theory).

3. MAIN FEATURES AND MODULES OF ERANOS 2.0

3.1. NUCLEAR DATA LIBRARIES

The ECCO/ERANOS 2.0 code package contains several neutron cross section libraries, all derived from the JEF-2.2 nuclear data evaluated files [5]. These include:

- a 1968-group library for the 37 main (resonant) nuclides,
- a 33-group library for fast-spectrum applications,
- a 175-group library for shielding calculations,
- a 172-group library for thermal-spectrum applications.

These libraries were obtained by processing the JEF-2.2 files with the NJOY and CALENDF codes [6]. Probability tables are included for the main 37 resonant nuclides.

Other nuclear data (fission yields and energies, decay constants, gamma production and interaction libraries, etc.) are provided in separate files.

The ERALIB1 neutron cross section libraries [7] are improved versions of the above libraries, obtained by applying a statistical adjustment procedure. The experimental basis for the adjustment is provided by a large number of integral values (more than 350) measured on clean critical cores. The calculation-versus-measurement discrepancies on the parameters used in the adjustment process form the starting point of the ERANOS validation.

3.2. THE ECCO CELL AND LATTICE CODE

The ECCO cell/lattice code [8] uses the subgroup method to treat resonance self-shielding effects. This method is particularly suitable for calculations involving complex heterogeneous structures.

ECCO prepares self-shielded cross sections and matrices by combining a slowing-down treatment in many groups (1968 groups) with the subgroup method within each fine group. In the reference calculation scheme, ECCO treats the heterogeneous geometry in fine groups (1968) for the 37 most important nuclides while broad group libraries (33 or 172 groups) are used for the less important nuclides. The sub-group method takes into account the resonance structure of heavy nuclides by means of probability tables and by assuming that the neutron source is uniform in lethargy within a given fine group. These calculations are very accurate as the fine group plus sub-group scheme have been set up to represent accurately the reaction thresholds and the resonances in any situation, narrow or wide.

If one were to adopt a uniform lethargy grid, at least 80000 points in energy would be required to

describe U238 in the resonance energy range, compared with only about 32000 points with the subgroup technique. More generally, 200000 points would be required to represent all the elements present in fast neutron reactors.

The self shielding formula for a standard effective cross section σ_x , where *x* can be the total (Legendre order 0), capture, fission, elastic or inelastic reaction for each energy group g, is the following:

$$\widetilde{\sigma}_{xi}^{g} = \frac{\sum_j S_j^g \sum_k \alpha_k^g \, \sigma_{x_k}^g \, p_{ij}\left(\Sigma_{t_k}^g\right)}{\sum_j S_j^g \sum_k \alpha_k^g \, p_{ij}\left(\Sigma_{t_k}^g\right)} \qquad [1]$$

where S_j^g is the neutron source in energy group *g* and spatial region *j*,

α_k^g is the probability in the group *g* to find the partial cross section $\sigma_{x_k}^g$ to which corresponds the total cross section $\sigma_{t_k}^g$ (used to calculate the macroscopic cross section $\Sigma_{t_k}^g$ in each region),

$p_{ij}\left(\Sigma_{t_k}^g\right)$ is the reduced collision probability for subgroup *k* within group *g*.

The self shielding of the Legendre order-one total cross section (as well as order-one elastic cross section) has a different formulation coming from the fact that this type of cross section is current-weighted, rather than flux-weighted:

$$\widetilde{\sigma}_{tr_i} = \frac{\sum_j S_j \sum_k \alpha_k \, \sigma_{tr_k} \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)}{\sum_j S_j \sum_k \alpha_k \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)} \qquad [2]$$

The flux and current are calculated with the self-shielded cross sections and matrices in a P1 consistent approximation:

$$\phi_i^g = \sum_j \left(-B^g \, J_j^g + S_{jj}^g + \sum_{g'} \Sigma_{s_{o,j}}^{g' \to g} \, \phi_j^{g'} \right) p_{ji}\left(\Sigma_t^g\right)$$

$$J_i^g = \sum_j \left((B^g/3)\, \phi_j^g + \sum_{g'} \Sigma_{s_{1,j}}^{g' \to g} \, J_j^{g'} \right) p_{ji}\left(\Sigma_t^g\right) \qquad [3a,b]$$

Self-shielded cross sections and matrices are condensed and smeared to provide effective cross sections and matrices in the user required broad group scheme.

One usually distinguishes wide and narrow resonances depending on their width compared to the neutron energy loss by scattering collision, which is smallest for scattering by heavy nuclides. Translated into lethargy gain, the value for U238 is almost constant and is equal to 0.008. This

compares well with the fine group width of 1/120 = 0.0083 and explains the fact that 3/4 of the neutrons having a collision in a given group escape from that group. Wide resonances are treated explicitly, the resonances in that case having a width larger than the fine group width. On the other hand, narrow resonances are represented by probability tables, and hence use of the subgroup method can be applied in a very accurate way.

The same calculation scheme can be used for thermal reactor problems as well as radiation shielding applications. This is an important point as new aspects in advanced reactors include optimisation of shields (internal storage, steel reflectors, boron carbide assemblies) as well as special subassemblies containing moderating materials for efficient transmutation of minor actinides or fission products.

Finally, the fact that the neutron balance is preserved in ECCO after condensation and smearing provides a final internal validation of the ECCO calculations.

The effective cross-sections and matrices produced by ECCO are subsequently used in full-core ERANOS calculations, for example with the S_n transport module BISTRO.

Many types of geometries are available within the ECCO code, but the most important ones are (i) a 2-D rectangular lattice of cylindrical and/or square pins within a square tube, (ii) a 3-D slab with the sides of the boxes and the tube described explicitly, and (iii) a 2-D hexagonal lattice of cylindrical pins within an hexagonal wrapper. In particular, a description of CAPRA subassemblies with a mixture of diluent pins and fuel pins is possible, such as for modelling the ECRIN incineration sub-assembly concept [2].

3.3. THE BISTRO S_N TRANSPORT CODE

The BISTRO code [9] is a finite difference code with a highly efficient convergence algorithm. S_n transport and diffusion options are both available. The diffusion option is also used in the transport module for convergence acceleration.

The standard S_n method is used to discretize the Boltzmann equation in two-dimensional geometries (X-Y, R-Z). Different algorithms (step, diamond and "θ-weighted") and a negative flux fix-up capability exist. The inner iterations are accelerated by the DSA method using the source correction scheme.

An efficient solution of the diffusion equation is obtained by using either the successive line over-relaxation method (SLOR), the alternating direction implicit method (ADI) or the strongly implicit method (SI). All three options are available within BISTRO. In addition, it is possible to determine a solution correctly and efficiently for cases with voided regions, external sources, up-scattering, and anisotropic scattering.

For the calculation of the sensitivities required in the cross-section adjustment studies, perturbation theory calculations are performed within ERANOS using either the transport theory module (for

the critical masses and reactivity coefficients) or the diffusion theory module (for parameters described with a fundamental mode distribution).

3.4. THE REACTIVITY EQUIVALENCE METHOD

The preparation of cross sections for regions containing control rods requires a special treatment due to the very high coupling of the heterogeneous control rod structure to the surrounding core cells. The method used is the reactivity equivalence method [10] which has been validated on the BALZAC 1H experiments [11]. This method uses the S_n transport option of the BISTRO code and its associated perturbation modules.

The calculation is set up as follows:

- the heterogeneous control rod is described in X-Y geometry with a representative surrounding core zone,
- ECCO cell calculations are performed to prepare cross sections for the different zones of the control rod and the core,
- homogenised cross sections are prepared for BISTRO S_4 P_0 transport calculations (the P_1 effect is sufficiently small to be neglected).

The equivalence method is carried out by applying the following procedure:

- angular direct flux calculation of the heterogeneous control rod,
- angular adjoint flux calculation of the homogenised control rod (starting with the volume weighted cross sections in the initial step),
- reactivity variation calculation using the perturbation method,
- determination of group- and reaction-dependent correction factors, f_i, to be applied to the homogeneous cross sections in order to obtain a zero reactivity variation between the heterogeneous and homogeneous representations of the control rod (equivalence),
- iterations on the homogeneous adjoint flux calculation until convergence of the f_i's.

Figure 2 summarises the above iterative procedure.

The validity of such an approach for control rod calculations has been evaluated not only in terms of reactivity effect, but also in terms of absorption rates in the control rod and surrounding core regions. Table 1 compares the rod worths of a typical large fast reactor computed by several different methods.

Table 1 shows the validity of the reactivity equivalence method adopted in ERANOS (errors in the last column), but also the inadequacy of simpler methods (homogenisation by volume or by flux) for the determination of the control rod worths.

Figure 2 Homogenisation of control rods

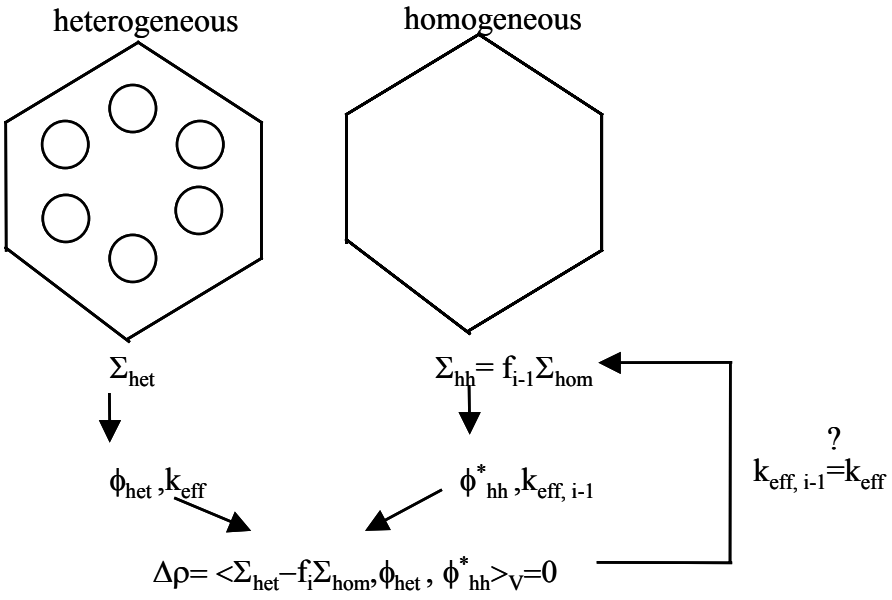


Table 1. Control and Safety Rod Worth Calculations by Various Procedures

Main Control Rod Bank (SCP)	Heterogeneous (reference)	Homogenisation by volume (error %)	Homogenisation by flux (error %)	Homogenisation by equivalence (error %)
Anti-reactivity (pcm)	8846	23.8	6.8	- 0.1
Absorption rate	0.345	24.1	7.0	- 2.0

Safety Rods (SAC)	Heterogeneous (reference)	Homogenisation by volume (error %)	Homogenisation by flux (error %)	Homogenisation by equivalence (error %)
Anti-reactivity (pcm)	6401	23.0	4.2	0.0
Absorption rate	0.258	23.0	4.2	- 1.0

3.5. THE TGV/VARIANT NODAL VARIATIONAL TRANSPORT CODE

The Variational Nodal Method developed for the VARIANT code [3,4] has been implemented in ERANOS 2.0 as the TGV/VARIANT module. This method is based on the second-order form of the even-parity transport equation. The problem is cast in the form of a linear functional minimization problem for the following (group-dependent) unknowns:

- the even-parity flux $\psi \equiv \frac{1}{2}\left[\Psi(\underline{\Omega}) + \Psi(-\underline{\Omega})\right]$ within the nodes,
- the odd-parity flux $\chi \equiv \frac{1}{2}\left[\Psi(\underline{\Omega}) - \Psi(-\underline{\Omega})\right]$ at the node interfaces.

A solution is searched in the form of expansions for the even- and odd-parity fluxes in pre-computed angular and spatial basis functions with unknown coefficients.

The basis functions used are:

- orthogonal polynomials for the spatial variables,
- spherical harmonics for the angular variables.

Scattering anisotropy can be taken into account as P_n moments up to the order N of the Legendre expansion of the flux.

Both Cartesian (X-Y, X-Y-Z) and hexagonal (Hex or Hex-Z) geometries are available within TGV/VARIANT. In addition, users may select different options depending on the order of the expansions chosen (See Table 2).

Table 2. Maximum Order of the TGV/VARIANT Expansions in ERANOS 2.0

Angular Expansion	within a node	on the boundary of a node
Diffusion	P1	P1
Simplified Transport	SP3	SP3
Transport	P3	P3

Spatial Expansion	Source within a node	Flux within a node	Flux at the boundary of a node
Maximum order of the polynomials	6 (in the plane) 4 (in the z-direction)	6	2

In the simplified transport option, the angular developments both within the nodes and at the node boundaries are truncated by neglecting high-order cross terms.

As running time and available memory are the main limitations to the use of such a code, the simplified transport option has been selected for the recommended reference route, all the more as this option was shown to be quite accurate in practice. Recommended values for the orders of the spatial expansion of the sources, the flux within a node and the flux at the interfaces are 3, 6, and 1, respectively. With this simplified transport option, the control-rod reactivity worths and the power map distribution are accurately predicted, as mesh effects are negligible and control-rod interaction effects are correctly treated.

A kinetics driver named KIN3D [12] was developed around the TGV/VARIANT module and integrated into ERANOS. Various types of fast reactor transients can be investigated with this 3-D time-dependent transport calculation option.

3.6 THE ERANOS REFERENCE CALCULATION ROUTE

With the algorithms available in the ERANOS 2.0 code system, it was possible to define a much improved reference calculation route with respect to previous versions of the software. The recommendations forming this reference route are:

- use of the ECCO cell code with a fully explicit description of the subassembly, including the wrapper tube and the array of pins, and with a fine (1968) group calculation including a sub-group treatment for the self shielding calculation. Results are given in 33 groups for the equivalent homogenised cell,

- use of the reactivity equivalence method for the preparation of the cross-sections for control rods,

- use of the nodal variational code TGV/VARIANT for the determination of the critical mass, the control-rod reactivity worth, the power map distribution and also for the burn-up reactivity swing,

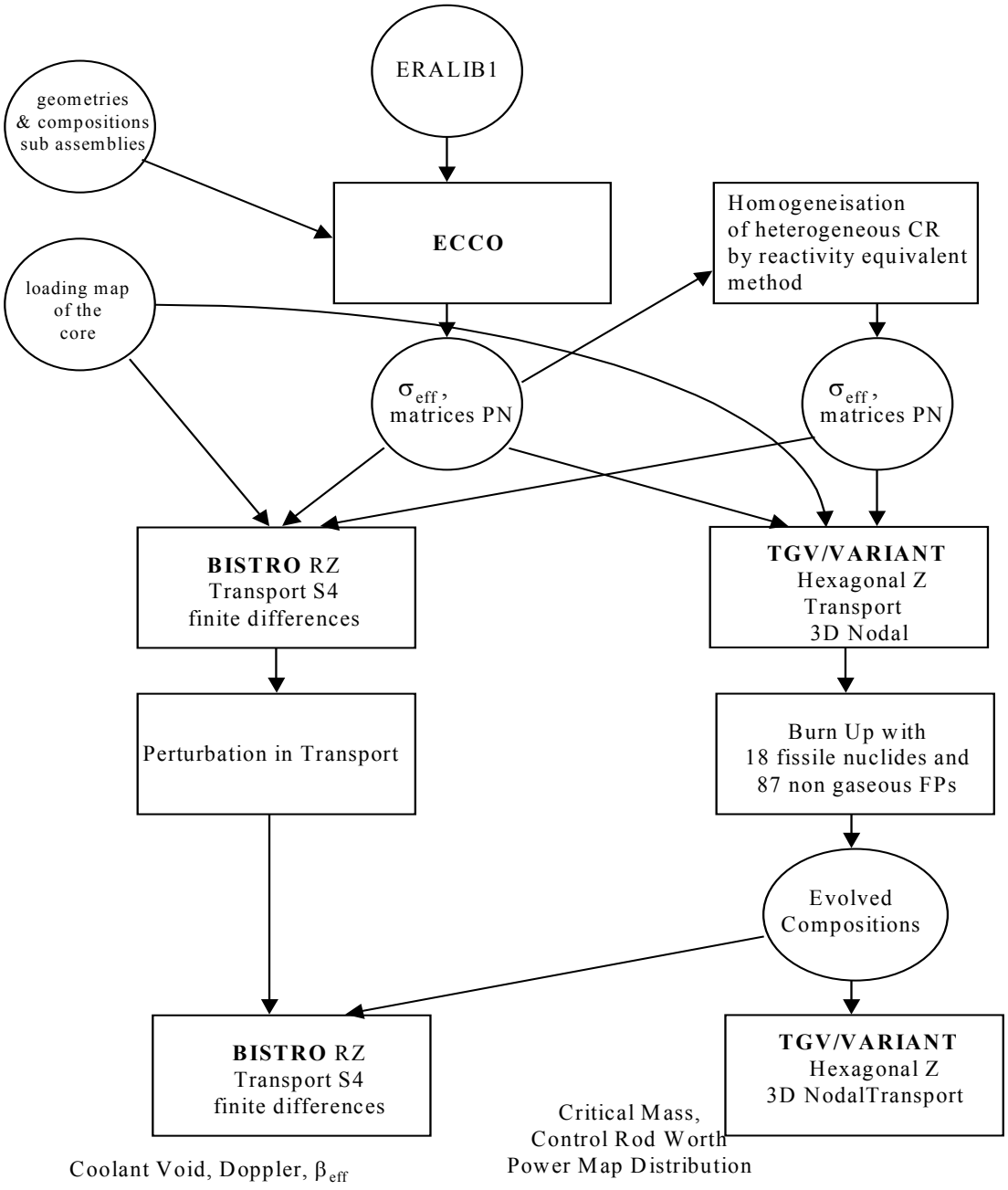
- use of decay chains made of 18 heavy nuclides and 87 fission products for fuel burn-up calculations,

- use of the S_n transport module BISTRO in R-Z geometry for the determination of certain parameters which are not very sensitive to the geometrical representation of the core; including β_{eff}, the sodium-void reactivity worth and the Doppler coefficient,

- use of perturbation modules associated with the BISTRO code for the characterisation of kinetics parameters.

A schematic view of this ERANOS 2.0 reference calculation scheme is provided in Fig 1. Additional schemes are available for core design studies, experiment analyses, shielding calculations including γ-heating [13], etc.

Fig 1: Reference Calculation Scheme ERANOS (Core)



4. VALIDATION OF ERANOS 2.0 FOR FAST REACTOR NEUTRONIC ANALYSES

The validation of the ERANOS data and code system for LMFR applications is based on a large experimental data base (over 500 measurements) accumulated by CEA over the years from the MASURCA zero-power critical assembly, as well as from other facilities or reactors. This data base includes in particular physics measurements performed in the PHENIX and SUPER-PHENIX plants, most notably the PROFIL irradiations [14] in PHENIX and the start-up core critical mass, control-rod reactivity worths, power map distribution and burn-up reactivity swing in SUPER-PHENIX [15]. As shown in Table 3, calculation-versus-experiment (C/E) comparisons are very satisfactory and demonstrate a significant improvement over the past calculation schemes.

Table 3. Summary of ERANOS LMFR Validation Results

Physical Quantity of Interest	C/E Discrepancy with ERANOS	C/E Discrepancy with Old Methodology (after application of correction factors)	Observations Regarding the ERANOS Calculation
Reactivity	≤ 100 pcm	≤ 300 pcm	No need of method corrections.
Rod Worth	≤ 5%	≈ 20%	New procedure eliminates the need for method correction.
Flux and Power Profiles	Residual radial power tilt of 5%	Unexplained radial power tilt of 17%	Long-standing problem in SUPER-PHENIX. Tilt partly explained with ERANOS.
Burn-up Swing	Under-estimation of about 6%	Under-estimation of about 17%	Improvement with respect to old methodology. Additional improvements could come from better MA and FP data.
β_{eff}	Measurement N/A in power reactors	Measurement N/A in power reactors	Very good results for zero-power criticals.
Doppler Effect	C/E = 1.00	C/E = 0.90	Old methodology did not take into account Doppler effect in iron and the effective temperature
Sodium void worth	Measurement N/A in power reactors. Spectral component OK	Measurement N/A in power reactors. OK with correction factors	Experiments in zero-power criticals show that the leakage component is still underestimated by ~20%. Improvements are expected from new algorithm + new Na data.

For each calculated LMFR neutronic quantity, ERANOS biases and uncertainties were assessed, together with the corresponding parametric domain of validity. From these validation studies, it was concluded that ERANOS 2.0 can predict LMFR core characteristics in a satisfactory manner, with negligible biases and reduced uncertainties.

The analysis of recent experiments (the CIRANO [16, 17], COSMO [18] and MUSE experimental programmes in MASURCA) has made it possible to extend the ERANOS domain of validity to plutonium-burning cores, i.e. cores with a higher plutonium content (equivalent plutonium enrichment of up to 53%), degraded plutonium quality (Pu240 fraction of up to 35%), large fuel dilutions, steel reflectors, moderated subassemblies, and also to source-driven sub-critical systems. In particular, the analysis of experiments such as MUSE-3 [19] has provided valuable insight into the physics of sub-critical multiplying media and has contributed to the ERANOS validation for MOX-fueled ADS applications.

Finally, recent studies performed with ERANOS [20] have shown that a satisfactory treatment of heterogeneity and streaming effects in a GCFR can be achieved by using a 2-D exact representation of fuel subassemblies, combined with the directional Benoist formulation in the ECCO cell code, to produce equivalent homogeneous cross sections for use in whole core BISTRO or TGV/VARIANT transport theory calculations. This result is obtained without a significant increase in running time; its accuracy has been proven by comparison with Monte Carlo calculations.

5. CONCLUSIONS

ERANOS 2.0, the latest version of the ERANOS fast reactor neutronic data and code system, is a comprehensive set of nuclear data libraries, multi-dimensional neutron transport modules and recommended calculation procedures which have been developed to cover a wide range of applications ranging from conventional LMFR's to advanced plutonium-burning fast reactors. The excellent performance of this system has been demonstrated by years of numerical and experimental validation. The ERANOS 2.0 experimental data base includes hundreds of measurements performed in MASURCA and in other critical facilities, as well as in power reactors. Recent work has demonstrated that ERANOS can also be successfully applied to the analysis of source-driven MOX-fuelled fast sub-critical media, as well as to the modelling of heterogeneity and streaming effects in GCFR's.

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