Status of JEFF-3.1.1 and ERANOS-2 code system validation for fuel cycle calculation of Fast Reactors

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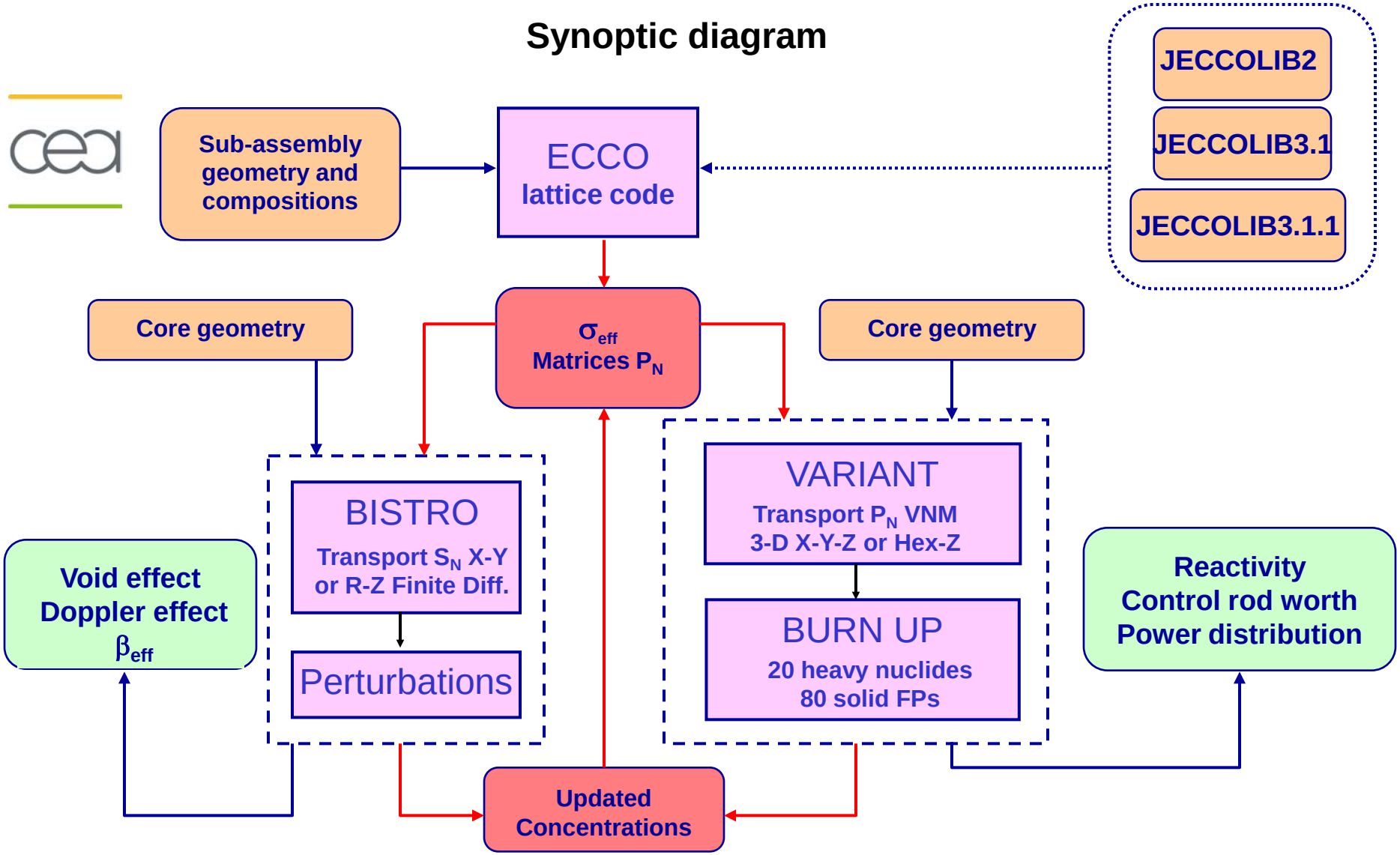
Existing Calculation Tools for fast reactor analysis

ERANOS

European Reactor ANalysis Optimised System

- A modular, integrated, neutron data and deterministic code system developed in the framework of a European R&D agreement
- A wide range of R&D and industrial applications
  - Investigation and design of critical and sub-critical liquid-metal-cooled (SFR,…) and gas-cooled cores (GFR)
  - Analysis of physics experiments in zero-power facilities
  - Analysis of irradiation experiments in power reactors
  - Neutron (and gamma) shielding calculations
  - Core-follow calculations in power reactors (PHENIX)
- ERANOS 2.0, released in 2002, is the outcome of a 12-year development and extensive validation effort
- Distributed by CEA to various international partners under bilateral collaboration agreements

Synoptic diagram

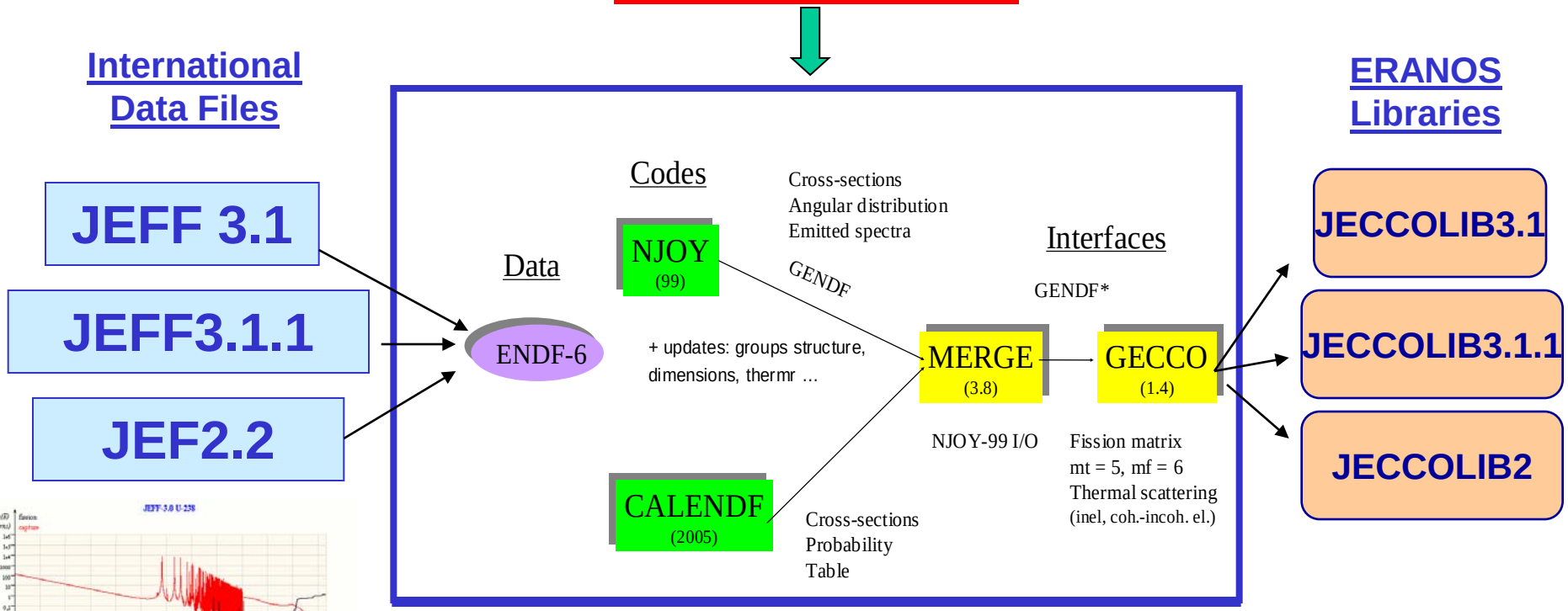


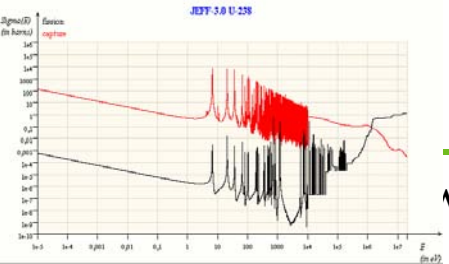
New Nuclear data libraries

Cross sections, activation, energy release, radioactive decay

1968 energy groups : Major nuclides, P1-5, 5 temperatures
+ **Probability tables**
172 energy groups : All nuclides, P1-3, 5 temperatures
33 energy groups : All nuclides from above
175 energy groups P5 for shielding calculations

Same Processing Tools





Nuclear data Libraries
33, 172, 175 and 1968 energy groups

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

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

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

$$\tilde{\sigma}_{tr_i} = \frac{\sum_j S_j \sum_k \alpha_k \sigma_{tr_k} \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)}{\sum_j S_j \sum_k \alpha_k \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)}$$

ECCO cell and lattice code

- **Fine-group calculations**
- **Resonant self-shielding by the sub-group method**
- **P_{ij} method for various geometries, including embedded bodies**
- **Energy collapsing and space homogenisation**
- **Macro-cell option**
- **Special model for anisotropic streaming effect**

Core calculation modules

- **Diffusion or transport, direct or adjoint, eigenvalue or with external source**
- **BISTRO 2-D transport, finite difference S_N**
- **VARIANT9 2-D or 3-D transport, Variational Nodal Method P_N et SP_N (ANL)**
- **H3D 3-D diffusion, finite volumes**
- **Geometries: 1-D, 2-D et 3-D Cartesian, cylindrical, 2-D et 3-D hexagonal**
- **Neutron/Gamma transport calculations**

Depletion

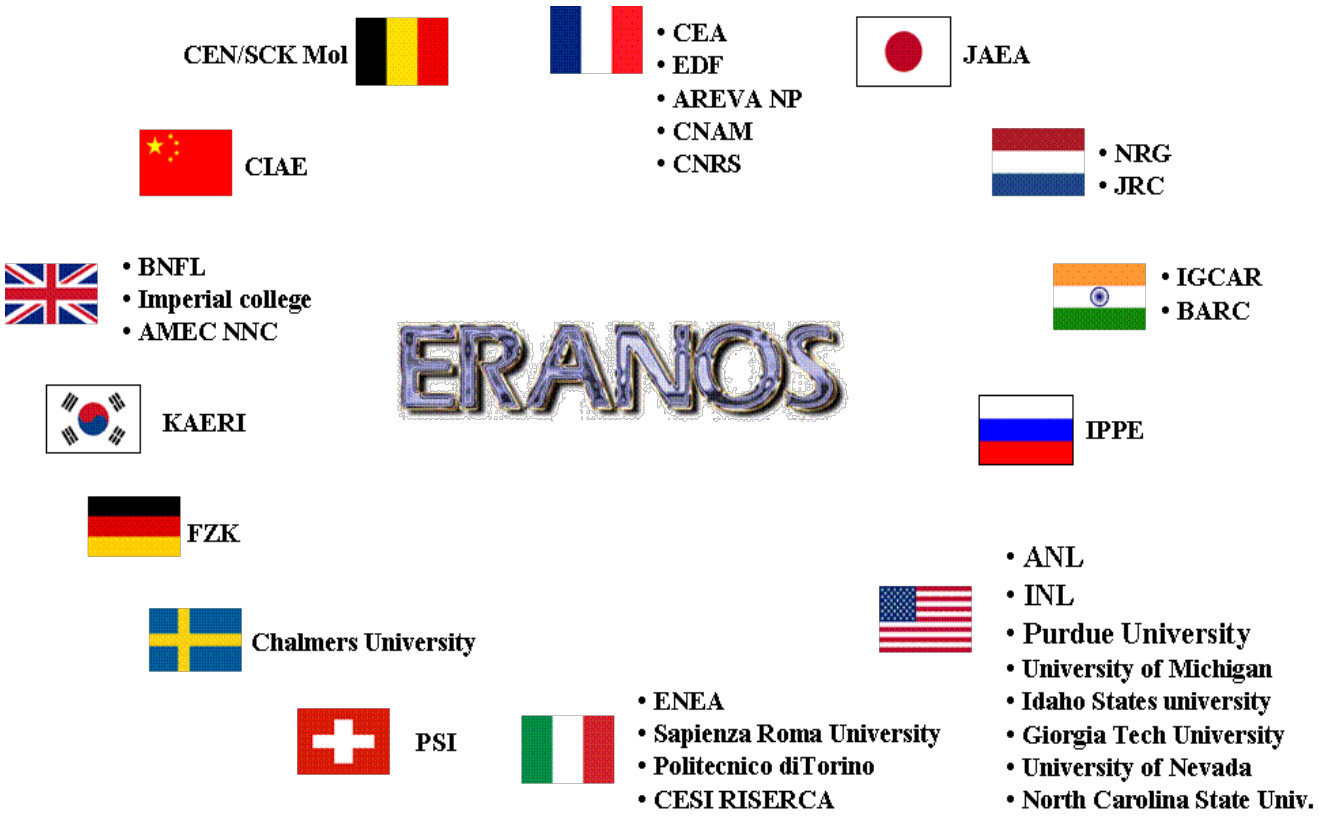
MECCYCO isotopic point depletion

- Direct and adjoint calculations
- Sensitivity calculations

KIN3D 3-D spatial **kinetics driver**

Various **interfaces**: CCCC format-compliant files, ANISN, SIMMER,…

Special **PROCEDURES** for control rod homogenisation, sensitivity and perturbation calculations, representativity analysis, intra-nodal homogeneous flux reconstruction, shielding calculations, etc.



Training

Training CEA/INSTN
User's workshop 2006 - 2009
User club for universities

Licensees

14 countries
~10 Universities
~15 National Laboratories
~4 Industrial companies

Criticality on cores with fertile blankets : summary

	ERANOS2.1 JEFF-3.1	fuel	r
MAS 1A'	+477	UPuFe + C, ≈25% Pu	0.30
MAS PRE-RACINE 1 het. POA	+423	$(U,Pu)O_2$ + Na ≈21% Pu	0.43
MAS PRE-RACINE 2 POA+P2A	+271		
MAS PRE-RACINE 2 PIT+P2A	+236		
MAS PRE-RACINE 4 het. PIT+P2A	+324		
MAS CIRANO ZONA2A	+442	$(U,Pu)O_2$ + Na, ≈27% Pu	0.54
Super-Phénix C1D	+444	$(U,Pu)O_2$ + Na ≈16% / 20% Pu	0.32 / 0.38
Super-Phénix lot 5	+462		
Super-Phénix CMP	+455		
Super-Phénix other crit. states	+425 to +545		

- Constant overshoot (≈400 pcm) with ERANOS2 + JEFF-3.1 on criticality calculation

  - would be increased by ≈100 pcm with JEFF-3.1.1 due to $^{16}O(n,\alpha)$

Doppler and β_{eff} validation : summary

- Doppler : performed in the **S**outhwest **E**xperimental **F**ast **O**xide **R**eactor (USA)
- General Electric & KfK (1969-72)
- Specific fuel design (segmented fuel ⇒ limited axial expansion)
- 2 neutron spectra, depending on the central rod : BeO (S1) or steel (S2)
- Static (heating) or dynamic (prompt jump) experiments : static ones analyzed

(C/E)	SEFOR-1	SEFOR-2
JEF-2.2	1.00 ± 0.07	1.00 ± 0.07
JEFF-3.1	**1.01 ± 0.07**	**1.00 ± 0.07**

- βeff : performed in MASURCA (BERENICE program, 1993-94) – R2 (U) & ZONA2 (Pu)
- Cf source method, pile noise method, Rossi-α method
- "experimental" value : a mix of direct measurement and computed coefficients
- JEFF-3.1 kinetic data : 8 time families, ν_d changes with respect to JEF-2.2

  (e.g. ^{235}U : -1.5% ; ^{238}U : +2.2% ; ^{239}Pu +1.2%, ^{241}Pu +2.2%)
- Pu core : **C/E = 1.028 ± 0.020**

The PROFIL and PROFIL-2 experiments in Phénix

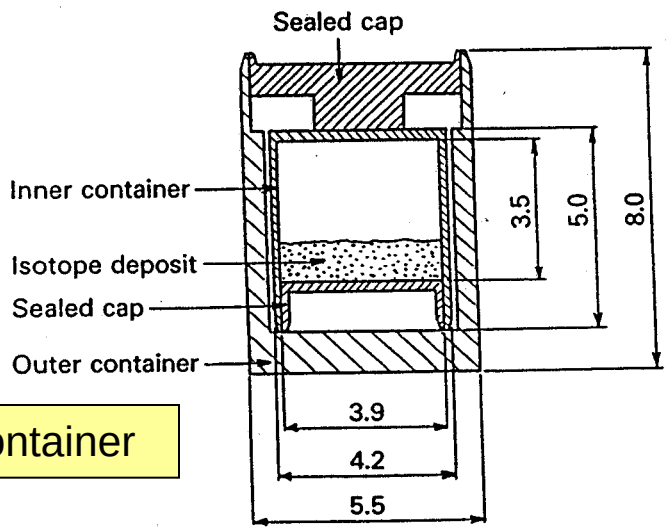
PROFIL :

- 1 exp. pin, within the central fuel S/A of Phénix
- Irradiation : 01/1974 → 01/1975 (179 equiv. full power days)
- 46 samples
- actinides : ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am
- FP : ^{95}Mo, ^{97}Mo, ^{101}Ru, ^{105}Pd, ^{133}Cs, ^{145}Nd, ^{149}Sm
- standards : B, Li

PROFIL-2 :

- 2 exp. pins in a fuel S/A of the first ring of Phénix
- Irradiation : 07/1979 → 09/1980 (316 efpd)
- 2 x 42 samples
- actinides : ^{232}Th, ^{233}U, ^{234}U, ^{235}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{244}Cm
- FP : ^{92}Zr, ^{106}Pd, ^{143}Nd, ^{144}Nd, ^{147}Sm, ^{151}Sm, ^{153}Eu
- standard : B

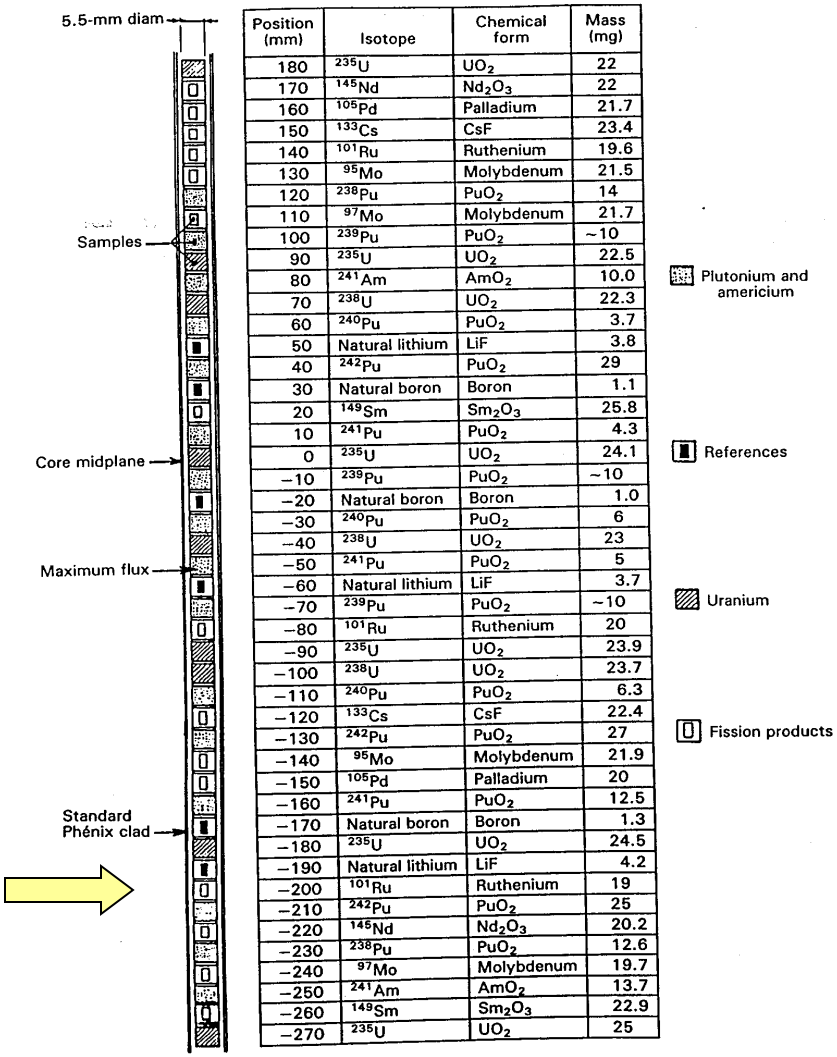
The PROFIL and PROFIL-2 experiments in Phénix



Double container

Axial sample pattern :

- Each sample is (at least) doubled
- ^{235}U distributed over the whole height



Position (mm)	Isotope	Chemical form	Mass (mg)
180	^{235}U	UO_2	22
170	^{145}Nd	Nd_2O_3	22
160	^{105}Pd	Palladium	21.7
150	^{133}Cs	CsF	23.4
140	^{101}Ru	Ruthenium	19.6
130	^{95}Mo	Molybdenum	21.5
120	^{238}Pu	PuO_2	14
110	^{97}Mo	Molybdenum	21.7
100	^{239}Pu	PuO_2	~10
90	^{235}U	UO_2	22.5
80	^{241}Am	AmO_2	10.0
70	^{238}U	UO_2	22.3
60	^{240}Pu	PuO_2	3.7
50	Natural lithium	LiF	3.8
40	^{242}Pu	PuO_2	29
30	Natural boron	Boron	1.1
20	^{149}Sm	Sm_2O_3	25.8
10	^{241}Pu	PuO_2	4.3
0	^{235}U	UO_2	24.1
−10	^{239}Pu	PuO_2	~10
−20	Natural boron	Boron	1.0
−30	^{240}Pu	PuO_2	6
−40	^{238}U	UO_2	23
−50	^{241}Pu	PuO_2	5
−60	Natural lithium	LiF	3.7
−70	^{239}Pu	PuO_2	~10
−80	^{101}Ru	Ruthenium	20
−90	^{235}U	UO_2	23.9
−100	^{238}U	UO_2	23.7
−110	^{240}Pu	PuO_2	6.3
−120	^{133}Cs	CsF	22.4
−130	^{242}Pu	PuO_2	27
−140	^{95}Mo	Molybdenum	21.9
−150	^{105}Pd	Palladium	20
−160	^{241}Pu	PuO_2	12.5
−170	Natural boron	Boron	1.3
−180	^{235}U	UO_2	24.5
−190	Natural lithium	LiF	4.2
−200	^{101}Ru	Ruthenium	19
−210	^{242}Pu	PuO_2	25
−220	^{145}Nd	Nd_2O_3	20.2
−230	^{238}Pu	PuO_2	12.6
−240	^{97}Mo	Molybdenum	19.7
−250	^{241}Am	AmO_2	13.7
−260	^{149}Sm	Sm_2O_3	22.9
−270	^{235}U	UO_2	25

The PROFIL and PROFIL-2 experiments in Phénix

C/E : standards

Ratio	PROFIL	PROFIL-2
$^{10}B/^{11}B$	0.956 ± 0.005	1.023 ± 0.004
$^{7}Li/^{6}Li$	1.004 ± 0.013	—

C/E : U and Pu

Nuclide	Reaction	Ratio	C/E
^{235}U	fission	$^{235}U/^{238}U$	1 : 1.007 ± 0.020 2A : **1.000 ± 0.001** 2B : 0.993 ± 0.003
	capture	$^{236}U/^{235}U$	1 : **1.000 ± 0.001** 2A : 1.000 ± 0.001 2B : **1.000 ± 0.001**
^{238}U	capture *(n,2n)*	$^{239}Pu/^{238}U$ *$^{237}Np/^{238}U$*	1.018 ± 0.002 *0.927 ± 0.028*
^{238}Pu	capture	$^{239}Pu/^{238}Pu$	1.024 ± 0.005
^{239}Pu	capture *(n,2n)*	$^{240}Pu/^{239}Pu$ *$^{238}Pu/^{239}Pu$*	0.981 ± 0.001 *0.793 ± 0.034*
^{240}Pu	capture *(n,2n)*	$^{241}Pu/^{240}Pu$ *$^{239}Pu/^{240}Pu$*	0.970 ± 0.004 *0.719 ± 0.044*
^{241}Pu	capture	$^{242}Pu/^{241}Pu$	**1.083 ± 0.001**
^{242}Pu	capture	$^{243}Am/^{242}Pu$	**1.175 ± 0.016**

ERANOS + JEFF-3.1

The PROFIL and PROFIL-2 experiments in Phénix

C/E : minor actinides

Nuclide	Reaction	Ratio	C/E
^{237}Np	capture	^{238}Pu/^{237}Np	0.915 ± 0.011
^{241}Am	capture	^{242m}Am/^{241}Am ^{242}Pu/^{241}Am ^{238}Pu/^{241}Am ^{242}Cm/^{241}Am	0.992 ± 0.005 (global average)
^{243}Am	capture	^{244}Cm/^{243}Am	0.933 ± 0.036
^{244}Cm	capture	^{245}Cm/^{244}Cm	**1.354 ± 0.003**
^{246}Cm	capture	^{247}Cm/^{246}Cm	**1.208 ± 0.035**

Corrected branching ratio : ^{241}Am(n,γ)^{242}Am : 80% → **85%**

C/E actinides of thorium cycle

Nuclide	Reaction	Ratio	C/E
^{232}Th	capture	^{233}U/^{232}Th	**0.898 ± 0.058**
^{233}U	capture	^{234}U/^{233}U	**0.915 ± 0.001**
^{234}U	capture	^{235}U/^{234}U	**0.889 ± 0.001**

ERANOS + JEFF-3.1

The PROFIL and PROFIL-2 experiments in Phénix

Fission products

ERANOS + JEFF-3.1

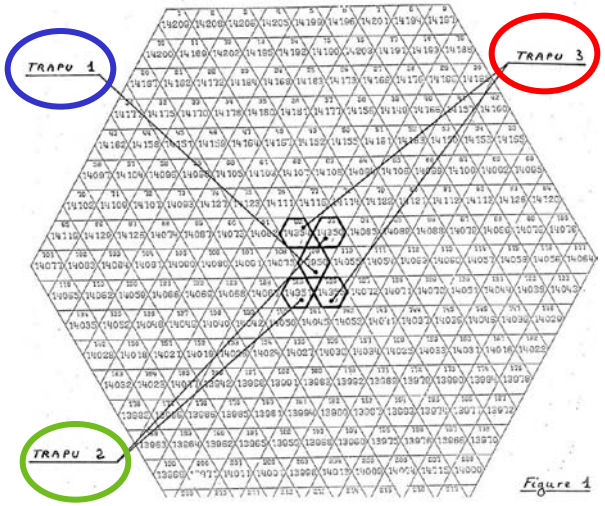
(C/E – 1) in %	Nuclide
-15 to -10%	^{105}Pd
-10 to -5%	^{106}Pd, ^{133}Cs, ^{134}Cs, ^{150}Sm, ^{154}Eu
-5 to 0%	^{144}Nd, ^{149}Sm, ^{153}Eu
0 to +5%	^{97}Mo
+5 to +10%	^{95}Mo, ^{101}Ru
+10 to +15%	^{143}Nd
+15 to +20%	^{145}Nd, ^{147}Sm
+20 to +30%	^{151}Sm
A factor 2	^{151}Eu

- These FP contribute to **≈38%** of the reactivity swing due to FP in a large SFR (EFR)
- Adjustment on capture (C/E=1 for each FP) reduces the reactivity swing due to FP by **3.7%** and the global (FP+HM) reactivity swing by 1.4%
- Additional use of the PF in PROFIL-R et PROFIL-M ⇒ cover **≈2/3** of the reactivity swing due to FP in a large SFR (EFR)
- GEN-IV (IBG ≈ 0) : strong compensation between $\Delta\rho$(HM)>0 et $\Delta\rho$(FP)<0 ⇒ increased relative uncertainties

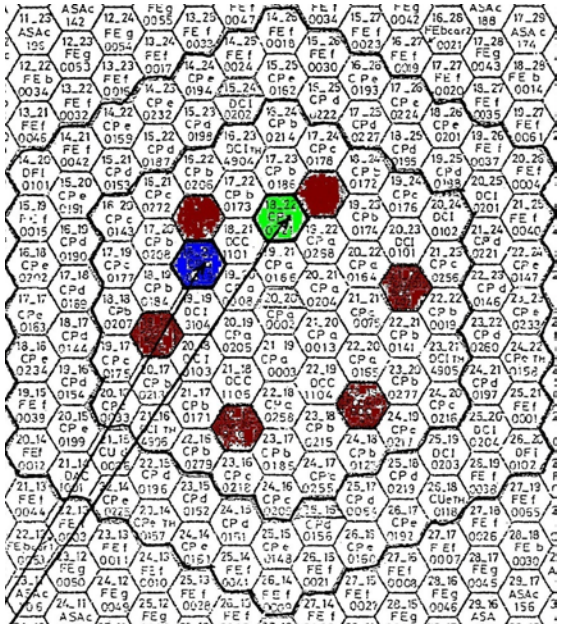
The TRAPU experiments in Phénix

Type fo pin		Pu^{238}	Pu^{239}	Pu^{240}	Pu^{241}	Pu^{242}	Initial Pu content
TRAPU-1	Pu UNGG	0.12	73.26	21.92	3.99	0.71	19,6 %
TRAPU-2	Pu « PWR»	0.77	71.37	18.54	7.42	1.90	19,25%
TRAPU-3	Pu with Pu^{240}	0.22	33.97	49.40	10.03	6.38	28,04%

Experimental sub assembly



PHENIX Core loading



The TRAPU experiments in Phénix

C/E

Ratio	TRAPU 2	TRAPU 3	Ratio	TRAPU 2	TRAPU 3
U234 / U238	1.01 ± 0.03	1.04 ± 0.03	Np237 / U238	0.86 ± 0.04	0.82 ± 0.04
U235 / U238	1.03 ± 0.02	1.02 ± 0.02	Am241 / Pu239	0.99 ± 0.03	0.99 ± 0.04
U236 / U238	0.98 ± 0.02	0.98 ± 0.02	Am242m / Am241	1.00 ± 0.03	0.98 ± 0.03
Pu239 / U238	1.00 ± 0.02	1.00 ± 0.02	Am243 / Am241	1.03 ± 0.03	1.06 ± 0.03
Pu238 / Pu239	0.97 ± 0.02	0.95 ± 0.02	Cm244 / Pu239	1.01 ± 0.05	1.03 ± 0.04
Pu240 / Pu239	0.98 ± 0.02	1.00 ± 0.02	Cm242 / Cm244	1.02 ± 0.04	0.99 ± 0.03
Pu241 / Pu239	0.97 ± 0.02	0.98 ± 0.02	Cm243 / Cm244	0.64 ± 0.05	0.62 ± 0.03
Pu242 / Pu239	1.01 ± 0.02	1.01 ± 0.02	Cm245 / Cm244	1.20 ± 0.03	1.50 ± 0.04

- Fluence adjustment performed to match Nd148 production ; slight discrepancy with U235 fission ⇒ additional 2% uncertainty in quadratic sum to experimental ones
- Good agreement on major actinides (but low sensitivity)
- Minor actinides : OK for Am, Cm242 and Cm244 ; large discrepancies for Np237 (n2n reaction), Cm243 (sensitivity to power history?) and Cm245 (consistent with PROFIL results)

Conclusion

- ERANOS-2 calculation package extensively used and validated for GEN-IV Fast Breeder Reactors
- JEFF3.1.1 Nuclear Data Library represents a strong improvement (compared to JEF2.2) and is generally satisfactory for FBR and fast spectra calculations.
- CEA has performed relevant critical experiments in MASURCA and MINERVE (critical masses, spectrum indices, reactivity worth), as well as irradiation experiments in PHENIX.
- The analysis of these experiments using ERANOS2/JEFF3.1 points out the ability of this calculation package to predict FBR core criticality and fuel assembly inventory.
- The OSMOSE experiment in Minerve will increase the qualification of Major and Minor Actinide nuclear data in intermediate spectra, thanks to the oscillation of separated isotope samples