Needs and issues of covariance data application

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- **Advanced simulation and nuclear data uncertainty impact: status of design target uncertainties**
- **Covariance data can have a significant impact on innovative design features: the physics issues.**
- **What has been learned with the pilot study of NEA-WPEC Subgroup26**
- **To go beyond: the adjustment project within GNEP. Covariance data needs and first results**
- **Areas for (not so far) future uncertainty data needs**
- **Conclusions**

Status of current design uncertainties and decomposition in « input data » and « modeling » contributions

Neutronics: Core

Parameter	Current Uncertainty (SFR)		Targeted Uncertainty
	Input data origin (a priori)	Modeling origin	
Multiplication factor, K_{eff} (Δk/k)	1.5%	0.5%	0.3%
Power peak	1%	3%	2%
Power distribution[d)]	1%	6%	3%
Conversion ratio (absolute value in %)	5%	2%	2%
Control rod worth: Element	5%	6%	5%
Control rod worth: Total	5%	4%	2%
Burnup reactivity swing (Δk/k)	0.7%	0.5%	0.3%

Neutronics: Core

Parameter	Current Uncertainty (SFR)		Targeted Uncertainty
	Input data origin (a priori)	Modeling origin	
Reactivity coefficients: total	7%	15%	7%
Reactivity coefficients: component	20%	20%	10%
Fast flux for damage	7%	3%	3%
Kinetics parameters	10%	5%	5%
Local nuclide densities: Major	5%	3%	2%
Local nuclide densities: Minor	30%	10%	10%
Fuel decay heat at shutdown	10%	3%	5%

Covariance data can have a significant impact on innovative design features: the physics issues

- A wide range of systems has been investigated, both within the AFCI and GNEP initiatives
- Some expected new significant features (core and fuel cycle) depend heavily on nuclear data knowledge and uncertainties.
- Typical examples of nuclear data dependent innovative design features are:
  - Cores with low reactivity loss during the cycle
  - Cores with increased inventory of Minor Actinides in the fuel
  - Cores with no uranium blankets
- Both core design and the associated fuel cycle features have to be considered

The case of the Na-void reactivity coefficient

At first order:

$$\Delta k / k = \frac{1}{F}\left\{ N_{Na}\sum_{j} \sigma^{c}_{Na,j}\Phi_{j}\Phi_{j}^{+} - N_{Na}\sum_{j,k}\sigma_{Na}(j \rightarrow k)\Phi_{j}(\Phi_{k}^{+} - \Phi_{j}^{+}) - \delta D_{j}\int grad\Phi_{j} grad\Phi_{j}^{+} dV - \right.$$

$$\left. - \sum_{i} N_{i} \sum_{j} \delta\sigma^{a}_{i,j}\Phi_{j}\Phi_{j} \right\} = A_{Na} - S_{Na} - L - A_{SelfSh}$$

Scattering component (→ S_{Na}) Leakage component (→ L)

$-S_{Na}>0$ or <0 according to the sign of $(\Phi_k^{+} - \Phi_j^{+})$, $-L<0$

The scattering component sign is determined by energy shape of the adjoint flux, which, at first approximation, is related to the energy dependence of eta:

$$\eta = \nu\sigma_{f} / \sigma_{a}$$

Fissile isotopes (Pu-239, U-235, U-233) and Minor Actinides have significantly different eta shapes. The result is very different adjoint flux shapes, in particular at high energy, and, as a consequence, different values of the Na void scattering component.

As consequence, significant potential impact of nuclear data uncertainties on core feasibility

a) Cores with internal breeding gain (IBG) close to zero

This type of cores is caracterized by a reactivity loss during the cycle, Δρ/cycle, close to zero (apart from the contribution of the fission products to the reactivity loss):

$$\Delta\rho/\text{cycle} \sim \text{const1} \times \left(\sum \Delta n_i \, \rho_i + n_{PF} \, \rho_{PF} \right) \sim \text{const2} \times \text{IBG} + \text{const1} \times \Delta\rho_{PF}$$

Data related uncertainties

i=1….HI heavy isotope index

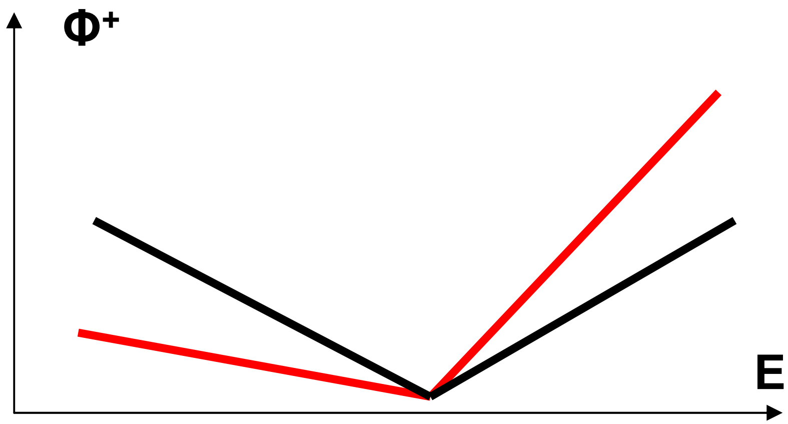
ρ_i reactivity/atom for isotope i with number density variation over the cycle Δn_i

ρ_{PF} reactivity/atom for pseudo-fission product PF with number density n_{PF}

IBG internal breeding gain

The competing effects of the build-up and of burn-up of the different fissile and fertile isotopes, require high accuracy fission, capture and inelastic data, as confirmed by the Subgroup 26 findings.

Moreover, the close-to-zero value of Δρ/cycle has potential safety implications and the trade-off between the Na void coefficient and the Δρ/cycle plays an important role in core design (e.g. number and position of control rods in the core)



Adjoint flux behavior as fonction of E:

$$\Phi^+ \sim \frac{\nu\Sigma_f}{\Sigma_a + DB^2}$$

High U-238/Pu-239 ratio (i.e. IBG ~0)

- **Positive Na void coefficient**
- **Low Δρ/cycle**

Low U-238/Pu-239 ratio (i.e. IBG<0)

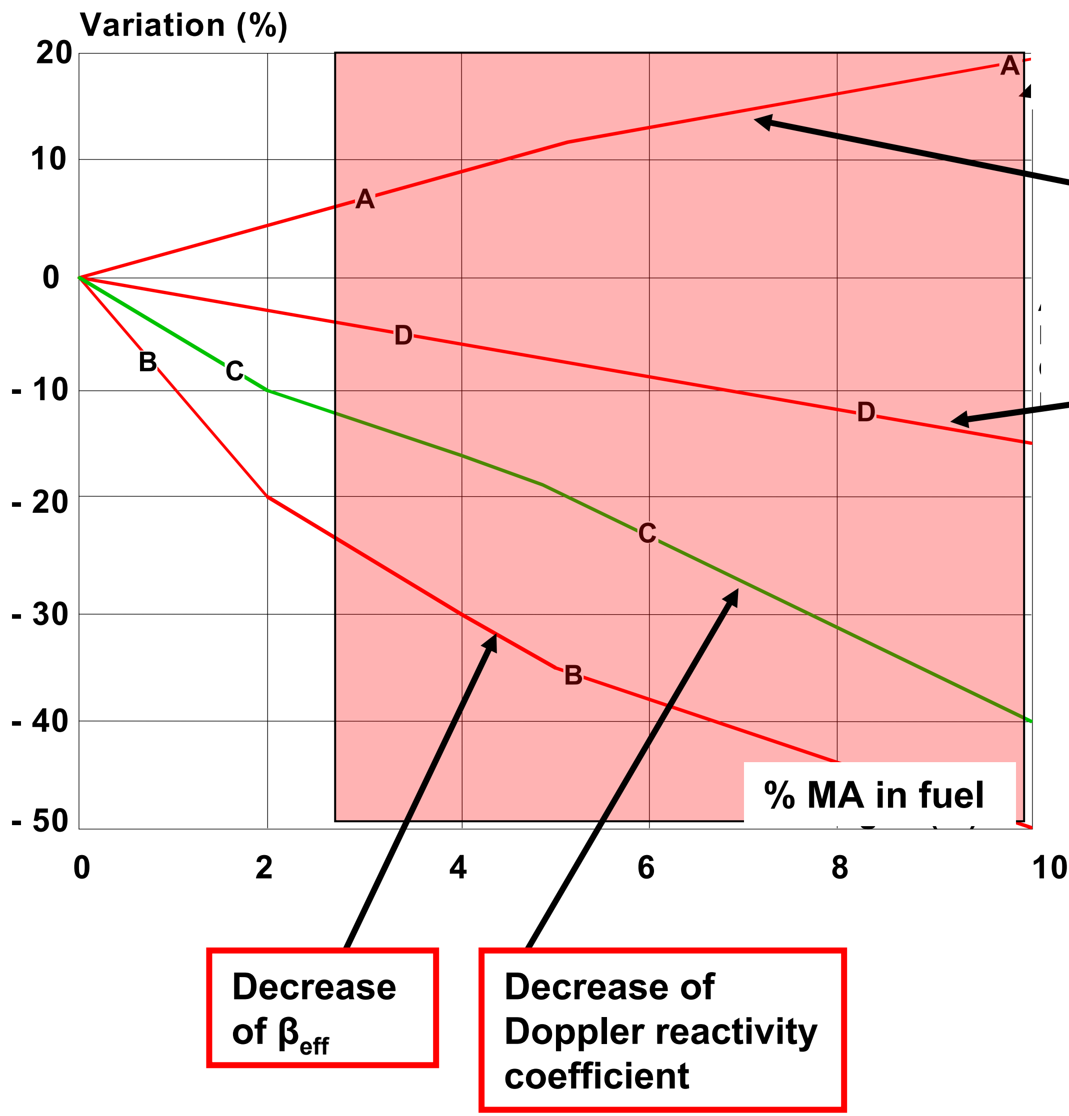
- **Negative Na void coefficient**
- **Δρ/cycle<<0**

- **As consequence, there can be a significant potential impact of nuclear data uncertainties on core feasibility and on its safety assessment.**

- **For example, the good compromise on IBG value and Na-void reactivity based on nominal values of both parameters could be revised to take into account uncertainties with practical consequences on, e.g., the core burn-up:**

an IBG more negative should be found in order to have a less positive Na-void coefficient, with a higher reactivity loss/cycle and consequently a potential reduction of the burn up.

b) Fast reactor cores with high content of Minor Actinides: Impact on reactivity coefficients (case of a SFR)



Max MA content ~ 2.5% for large size SFR (EFR) and 5-10 % for medium/small size (Phenix)

c) Blanket vs. Reflectors in FRs

- **Non proliferation issues suggest to avoid Uranium blankets in the next generation FRs, and replace them with reflectors.**

- **The presence of reflectors induces neutron spectrum transients at the core/reflector interface that need specific calculation methods.**

- **There are also significant data related effects. In the following table it is indicated the k_{eff} sensitivity to the different Fe-56 data, in configurations with blanket or with reflector.**

- **Very different sensitivities are shown, as expected.**

K_{eff} sensitivity (%) to Fe-56 data

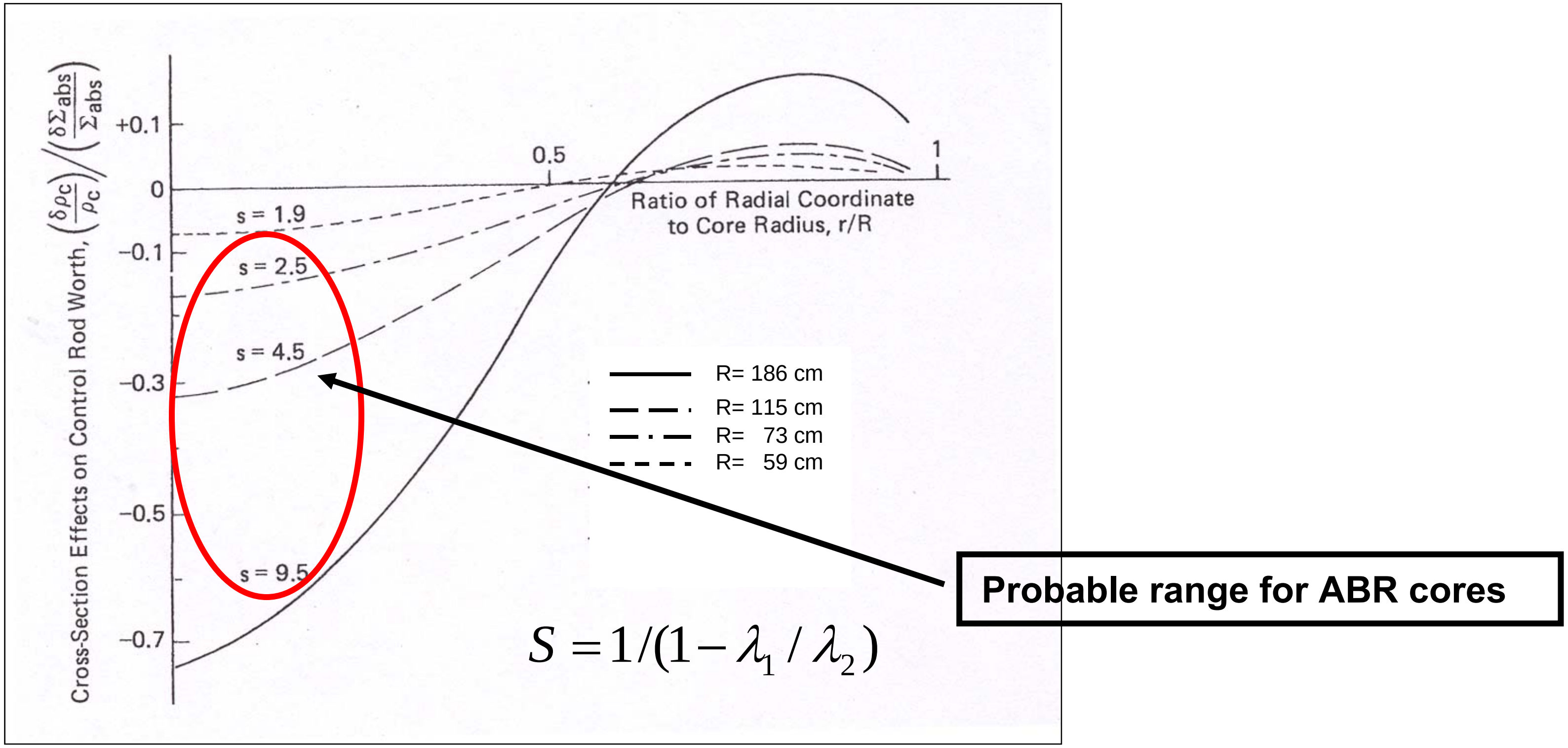
Experiment/ Configuration	Blanket (B) or Reflector (R)	Capt.	Elast.	Inel.	Total
ZPR3-53	B	-0.11	0.76	-0.02	0.63
ZPR3-54	R	-1.40	16.5	1.50	16.6
CIRANO	R	-1.50	6.28	-0.24	4.55
ZPPR-15	B	-1.54	1.67	-2.55	2.43
ABR-Metal	R	-1.49	3.05	-3.06	-1.51
ABR Oxide	R	-1.73	1.79	-3.29	-3.23

For example, 5% uncertainty on σ_{el} (or on σ_{in}) has a very different impact on the two ZPR3-53 and 54 experiments (up to 0.8% $\Delta k/k$) and up to 0.15% $\Delta k/k$ in the case of ABR-Metal.

d) Control rod spatial sensitivity to nuclear data uncertainties

A control rod worth is affected differently by cross section uncertainties according to the size of the core, its location and environment.

In the figure below, the spatial dependence of the sensitivity is shown as a function of space in cores of different sizes, each characterized by the related Boltzmann operator eigenvalue separation.



e) As for the Fuel Cycle, it is important to have a clear understanding (i.e. with low uncertainty) of isotope contributions to specific effects.

In the example below, it is shown that the decay heat at fuel unloading differs by a factor ~100 for FR cores with Conversion Ratio CR=0 or =1.

- **In the former case, Cm-244 is practically the only contributor, while in the latter several isotopes, with different decay constants, give comparable contributions.**

- **Their build-up during irradiation should be known rather accurately. This means the need of accurate capture and fission data in the related Bateman equations.**

	CR=0.0	CR=1.0
Total decay heat (MeV/s/g)	3.08 E+12	3.53 E+10
Pu-238 Contribution	3.00 E+11	6.50 E+09
Am-241 id	5.23 E+10	1.62 E+09
Cm-242 id	6.64 E+11	1.35 E+10
Cm-244 id	2.03 E+12	1.03E+10
% Cm-244 in the fuel	8.63 E-02	5.2E-04

Uncertainties and Target Accuracies: Lessons Learned with WPEC Subgroup 26

Recent work to assess uncertainties on a wide range of integral parameters and a wide range of systems, has been performed within an international initiative and a final report is being issued (Summer 2008):

"OECD/NEA WPEC Subgroup 26 Final Report: Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations"

This work has been made possible by the work on covariance data, led by BNL with LANL and ORNL participation (the so-called BOLNA covariance data set) , and by the availability of state-of-the-art sensitivity analysis tools

- **The Sub26 studies have pointed out that** ***the present uncertainties on the nuclear data should be significantly reduced, in order to get full benefit from the advanced modeling and simulation initiatives.***

- **Only a** ***parallel effort in advanced simulation and in nuclear data improvement*** **will enable to provide designers with more general and well validated calculation tools, that would allow to meet design target accuracies**

- **A further output: new entries in the OECD-NEA High Priority Request List can be proposed, based on uncertainty reduction requirements to meet design target accuracies. However, the requirements cannot be just the result of a mathematical procedure!**

The unknown uncertainty data requirements can be obtained by solving a minimization problem (the "inverse" problem) :

$$\sum_i \lambda_i / b_i'^2 = \min \qquad \text{i = 1 ... I}$$

$$\sum_i S_{Ri} b_i'^2 S_{Ri}^+ + \sum_{i,j} S_{Ri} b_i' b_j' c_{ij} S_{Rj}^+ < Q_R$$

The c_{ij} are the correlation coefficients of the original data covariance matrix, and the b_i' are the unknown variance values needed to meet the requirements .

The S_{Ri} are the sensitivity coefficients of integral parameter R to nuclear data i.

Q_R is the target accuracy on the integral parameter R, and λ_i are cost parameters.

To establish priorities in order to reduce uncertainties, the b_i' values should be compared to the variance data in the original covariance matrices. This helps to decide if an action should be undertaken to meet the requirement.

Apart for the approximation of the expression used to find the required variance reductions, three issues should be carefully assessed:

- **How realistic is the reference system**
- **The robustness of the initial covariance data**
- **The choice of λ_i**

Fast Reactor Uncertainty Reduction Requirements to Meet Design Target Accuracies, according to Subgroup 26 (no correlation effects accounted for)

		Energy Range	Current Accuracy (%)	Target Accuracy (%)
U238	σ_{inel}	6.07 ÷ 0.498 MeV	10 ÷ 20	2 ÷ 3
	σ_{capt}	24.8 ÷ 2.04 keV	3 ÷ 9	1.5 ÷ 2
Pu241	σ_{fiss}	1.35MeV ÷ 454 eV	8 ÷ 20	2 ÷ 8
Pu239	σ_{capt}	498 ÷ 2.04 keV	7 ÷ 15	4 ÷ 7
Pu240	σ_{fiss}	1.35 ÷ 0.498 MeV	6	1.5 ÷ 2
	ν	1.35 ÷ 0.498 MeV	4	1 ÷ 3
Pu242	σ_{fiss}	2.23 ÷ 0.498 MeV	19 ÷ 21	3 ÷ 5
Pu238	σ_{fiss}	1.35 ÷ 0.183 MeV	17	3 ÷ 5
Am242m	σ_{fiss}	1.35MeV ÷ 67.4keV	17	3 ÷ 4
Am241	σ_{fiss}	6.07 ÷ 2.23 MeV	12	3
Cm244	σ_{fiss}	1.35 ÷ 0.498 MeV	50	5
Cm245	σ_{fiss}	183 ÷ 67.4 keV	47	7
Fe56	σ_{inel}	2.23 ÷ 0.498 MeV	16 ÷ 25	3 ÷ 6
Na23	σ_{inel}	1.35 ÷ 0.498 MeV	28	4 ÷ 10
Pb206	σ_{inel}	2.23 ÷ 1.35 MeV	14	3
Pb207	σ_{inel}	1.35 ÷ 0.498 MeV	11	3
Si28	σ_{inel}	6.07 ÷ 1.35 MeV	14 ÷ 50	3 ÷ 6
	σ_{capt}	19.6 ÷ 6.07 MeV	53	6

How to meet requirements.

- Some of the most important requirements are difficult to be met using only differential experiments, even if innovative experimental techniques are used.

- The use of integral experiments has been essential in the past to insure enhanced predictions for power fast reactor cores.

- A combined use of scientifically based covariance data and of selected integral experiments can be made using classical statistical adjustment techniques

What is needed

- selection of a set of significant experiments,
- sensitivity analysis of selected configurations including reference design configurations for a wide range of integral parameters
- use of science based covariance data for uncertainty evaluation and target accuracy assessment,
- analysis of experiments using the best methods available, with some redundancy to avoid systematic errors,
- use of calculation/experiment discrepancies (and associated uncertainties) in a statistical adjustment

A warning: the credibility of an adjustment is dependent on the credibility of the covariance data and of the experimental uncertainties!

The outcome of the procedure should provide *reduced uncertainties for the full set of integral parameters* of the reference system:

$$\tilde{\mathbf{B}}_R = \mathbf{S}_R^T \tilde{\mathbf{B}}_p \mathbf{S}_R = \mathbf{B}_R \left\{ 1 - (\mathbf{S}_R^T \mathbf{B}_p \mathbf{S}_R)^{-1} (\mathbf{S}_A^T \mathbf{B}_p \mathbf{S}_A + \mathbf{B}_A)^{-1} \times \right.$$
$$\left. \times (\mathbf{S}_A^T \mathbf{B}_p \mathbf{S}_R)^2 \right\}$$

Experimental uncertainties should be as low as possible

where $\tilde{\mathrm{B}}_p$ is the new covariance matrix for the nuclear data.

S_R is the sensitivity *matrix* of the set of design parameters i=1….I in the reference system, to the nuclear data k=1….K.

S_A is the sensitivity *matrix* of the set of integral experiments j=1….J.

A new initiative: a GNEP/DOE sponsored 3-years Project with the participation of ANL, BNL, INL, LANL

The scope of the project is to produce a set of improved nuclear data using improved covariance data and a carefully selected set of integral experiments

- **As far as covariance data, such as inclusion of experimental data in the fast neutron region and inclusion of thermal and resonance integral data in the low energy region.**

- **Covariance data will be produced from the thermal energy to 20 MeV in a 33-energy group representation for 65 priority materials including actinides, structural materials and fission products.**

- **The covariance data are provided for elastic, inelastic, capture and n2n cross sections, while for actinides fission cross sections and nubar covariance data are also provided.**

- **The entire nuclear data covariance activities is coordinated by BNL with the support from LANL in the range of actinides and light nuclei.**

- **The resulting covariance data are utilized by ANL and INL for analysis.**

Some preliminary results, based on the selection of a limited number of existing, well documented integral experiments:

List of integral experiments used in the statistical adjustment

Experiment	Parameter analyzed			Fuel Type	Pu/(U+Pu)
	Critical mass	Reaction Rates	Irradiation Experiment		
GODIVA	Yes	Yes	-	U Metal	0.0
JEZEBEL[239]	Yes	Yes	-	Pu Metal	1.0
JEZEBEL[240]	Yes	-	-	Pu Metal	1.0
ZPR-3/53	Yes	Yes	-	PuC-UC	0.42
ZPR-3/54	Yes	Yes	-	PuC-UC	0.42
ZPPR-15	Yes	Yes		Pu-U Metal	0.13
COSMO[a]	-	Yes	-	PuO_2-UO_2	0.27
CIRANO[a]	Yes	Yes	-	PuO_2-UO_2	0.27
PROFIL[b]	-	-	Yes	PuO_2-UO_2	0.27
TRAPU[b]	-	-	Yes	PuO_2-UO_2	0.27

a) experiments performed in the MASURCA facility (NEA, 2005)
b) irradiation experiments performed in the PHENIX reactor (D'Angelo, 1990)

An example of the outcome

K_{eff} Uncertainties [pcm] Calculated with Original (BOLNA) and with Adjusted Covariance for the ABR (metal and oxide)

Reactor	BOLNA 4 groups	Adjusted Covariance
ABR Oxide	1439	639
ABR Metal	1460	639

Some examples of fission cross sections adjustments and uncertainty reduction

Parameter	Adjustment %	Standard Deviation %	
		Original	Adjusted
Pu238 σ^{fis} group 1	-11.6	18.3	7.7
Pu238 σ^{fis} group 2	-2.5	12.0	11.2
Pu238 σ^{fis} group 3	-1.0	11.6	11.4
Pu239 σ^{fis} group 1	0.2	0.5	0.3
Pu239 σ^{fis} group 2	0.1	0.6	0.5
Pu239 σ^{fis} group 3	-0.1	0.6	0.6
Pu240 σ^{fis} group 1	-2.6	3.7	1.7
Pu240 σ^{fis} group 2	-2.7	4.3	2.9
Pu241 σ^{fis} group 1	2.9	15.0	6.0
Pu241 σ^{fis} group 2	2.7	16.9	5.4
Pu241 σ^{fis} group 3	-0.6	9.1	7.4
Pu242 σ^{fis} group 1	-0.6	16.6	2.6

Group 1: 20 MeV-0.5 MeV
Group 2: 0.5 MeV- 67 KeV
Group 3: 67 KeV- 2 KeV
Group 4: 2 KeV- Thermal

Areas for future needs

- Neutron cross sections are not all the story!
- Fission spectrum uncertainty data needs have been pointed out by Subgroup 26, and several papers at this Workshop on that issue
- Photon production data (maybe, priority is data availability….)
- S(α,β) thermal scattering data. Need sensitivity first ?
- Mubar uncertainty needs: an example of sensitivity

Sensitivity of ABR (Oxide) k_{eff} to mubar of selected isotopes

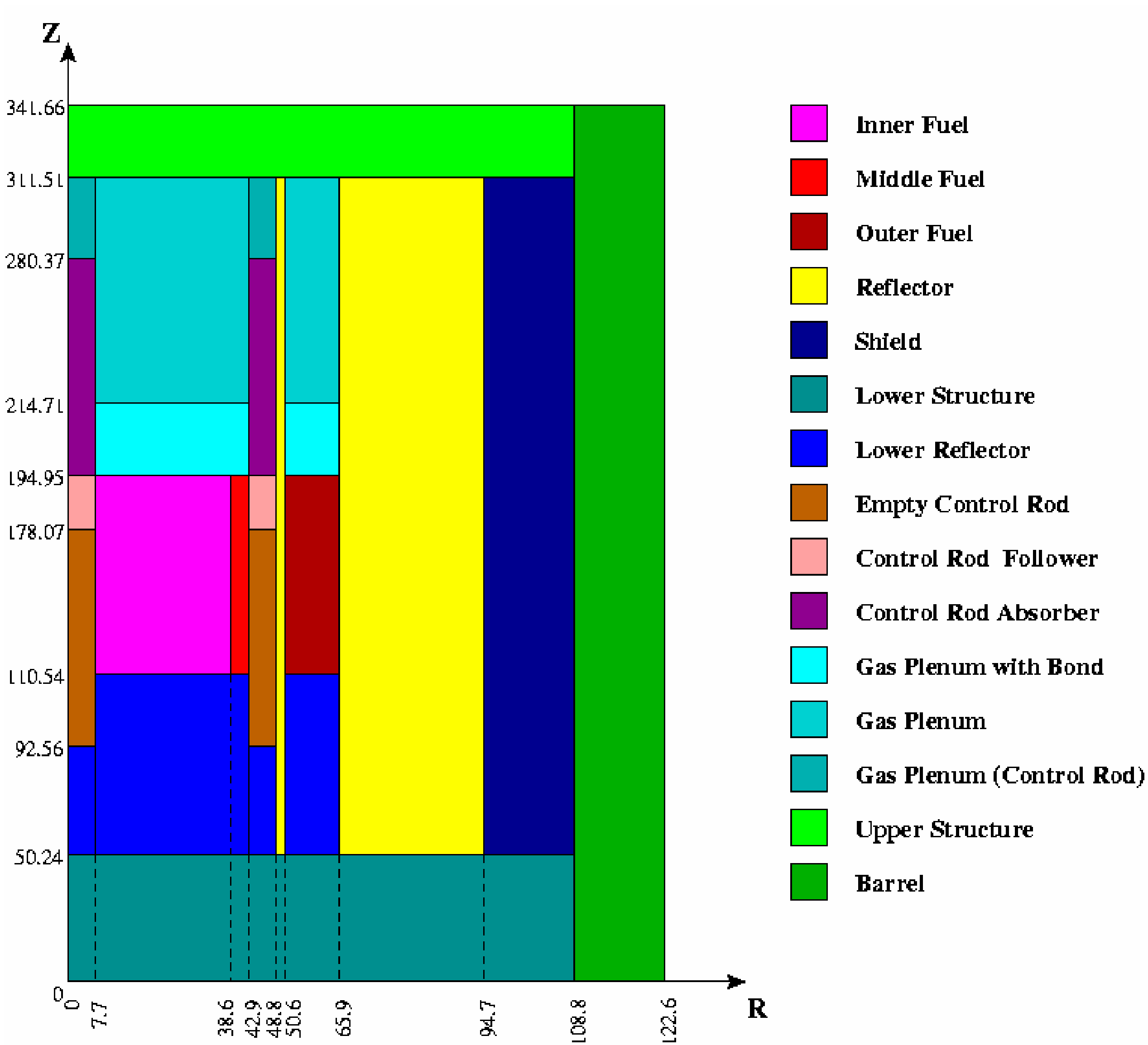
Isotope	System	Fission	Capture	Elastic	Inelastic	Mubar
O-16	ABR-Oxide	0	-0.002	-0.027	0	-0.004
	EFR	0	-0.003	-0.018	0	-0.008
	LFR	0	---	---	---	---
Na-23	ABR-Oxide	0	-0.002	-0.001	-0.009	-0.005
	EFR	0	-0.001	0.015	-0.005	-0.009
	LFR	0	---	---	---	---
Fe-56	ABR-Oxide	0	-0.023	-0.020	-0.036	-0.013
	EFR	0	-0.011	0.036	-0.018	-0.016
	LFR	0	-0.010	0.019	-0.017	-0.008
U-238	ABR-Oxide	0.065	-0.198	0.022	-0.042	-0.010
	EFR	0.074	-0.144	0.044	-0.032	-0.022
	LFR	0.060	-0.127	0.029	-0.038	-0.015
Pb	ABR-Oxide	---	---	---	---	---
	EFR	---	---	---	---	---
	LFR	0	-0.009	0.124	-0.029	-0.021

➔ **Sensitivity coefficients indicate potential not negligeable effects**

In conclusion:

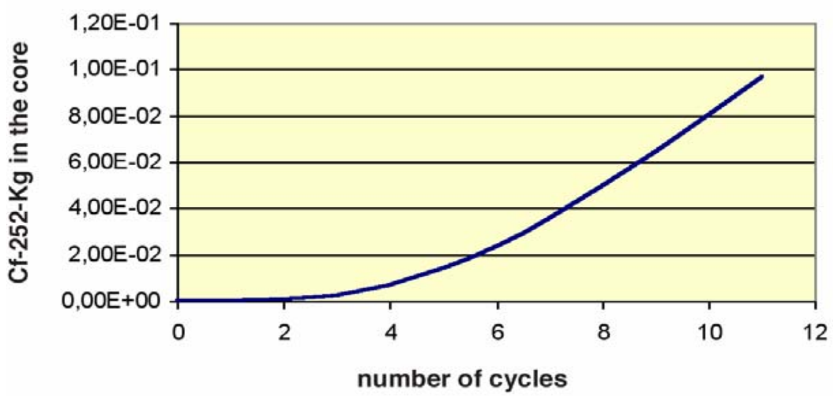
- **New innovative fast reactor systems (reactor and fuel cycle) will likely present specific features that are very sensitive to nuclear data uncertainties. This is probably also the case of innovative thermal reactors (e.g. VHTR)**
- **In preliminary phases of conceptual design scoping, larger uncertainties can probably be tolerated**
- **However, in further consolidated design phases, low uncertainties and sound correlation data are required for feasibility, safety and economic reasons**
- **There are challenging issues that can only be coped with the use of robust, science-based covariance data and high accuracy integral experiments**
- **Without that approach, advanced simulation objectives will be hard to meet.**

The reference system: ABR (Metallic Fuel: U,PU, Zr)

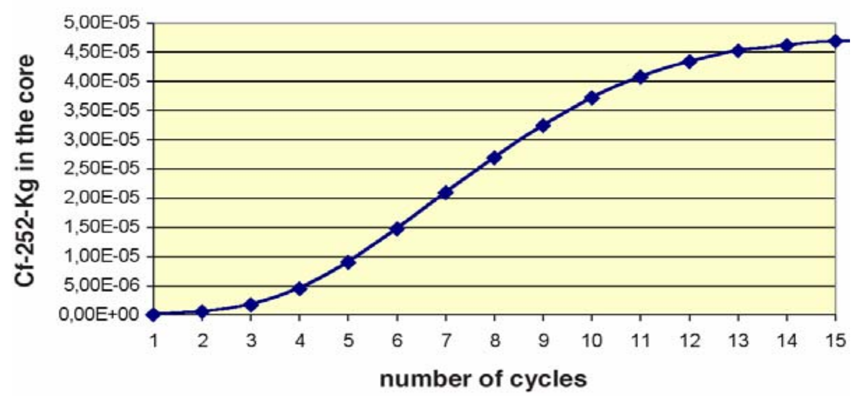


There is a negative impact on fuel cycle parameters of full TRU recycling in LWRs, e.g. at fuel fabrication due to the build-up of higher mass nuclei in a thermal reactor : unacceptable increase of neutron production due to high capture cross-sections in thermal spectra, which favour the production of Cf-252 (strong neutron emitter by spontaneous fission)

Cf-252 inventory in the core. Case of full TRU multirecycling in:



LWR



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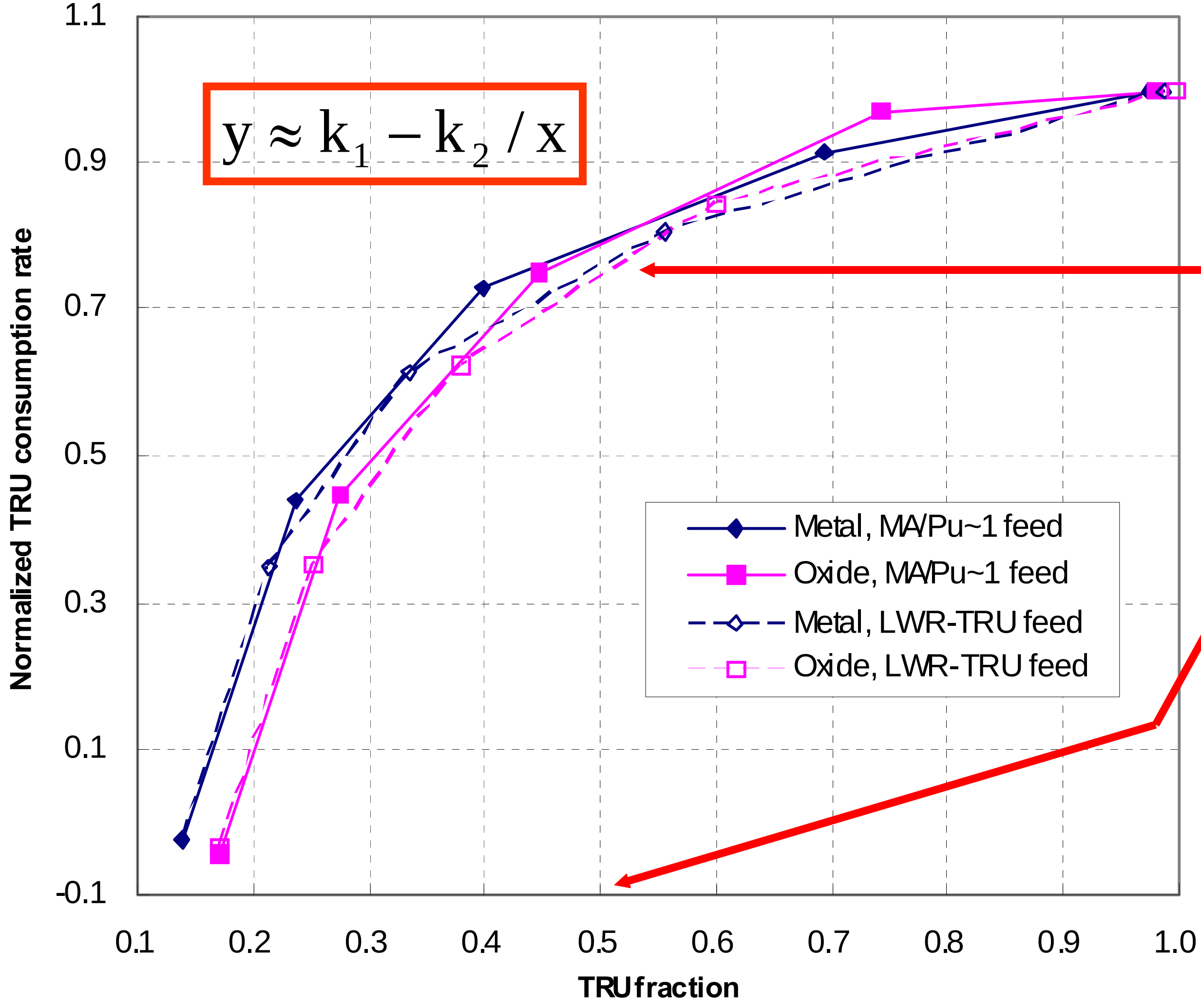
Nuclear data uncertainties can hardly change the picture…and the conclusions! However….

“Transmutation” fuels: is there any need for U-free fuels?

The cross section dependent relation between TRU consumption rate(=y) and TRU fraction (=x) (e.g. in critical Advanced Burner Reactors), gives the answer…



$$y \approx k_1 - k_2 / x$$

70-80% of max. theoretical consumption can be obtained with TRU/(U+TRU) ~0.4-0.6 both for metal or oxide fuelled cores and for a wide range of Pu/MA ratios

A quick « détour »: a « conservation » principle helps to define the appropriate covariance matrices D

The uncertainty on an integral parameter R_k is given by: $\Delta R_k^2 = S_{k,I} D_I S_{k,I}^+$

D_I is defined as: $D_I = \begin{pmatrix} d_{11} \ldots\ldots\ldots d_{I1} \\ \\ d_{I1} \ldots\ldots\ldots d_{II} \end{pmatrix}$ i=1……I (fine group grid)

and the sensitivity vectors $S_{k,I}$ have I components $s_{k,i}$ (i=1…..I)

One can define a broad group grid (j=1…..J, J<<I) such that **the fine group uncertainty is conserved:**

$$S_{k,J} D_J^k S_{k,J}^+ \equiv \Delta R_k^2 \quad \text{or} \quad S_{k,J} D_J^k S_{k,J}^+ = S_{k,I} D_I S_{k,I}^+$$

One can write for each element $d_{j,j'}^k$ of the matrix D_J^k

$$d_{j,j'}^k = \frac{\sum_{i \in j} s_{k,i} \sum_{i' \in j'} d_{i,i'}^k s_{k,i'}^+}{s_{k,j} s_{k,j'}^+} \quad \text{where} \quad s_{k,j} = \sum_{i \in j} s_{k,i} \quad \text{and} \quad s_{k,j}^+ = \sum_{i \in j} s_{k,i}^+$$

$D_J^k \longrightarrow$ is the appropriate broad group covariance matrix, since its use allows the conservation of the uncertainty on the parameter k calculated at the fine (reference grid) level.