Status of Nuclear Data Uncertainty Reduction Activities at INL

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NPWG Meeting

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Introduction

- At INL several activities are being carried out for reducing uncertainties related to nuclear data on neutronic reactor design parameters. These activities have different source of funding: AFCI, Office of Science, ATR NUF, LDRD. Activities include:
  - Analysis of experiments in order to perform data adjustment and provide feedbacks to evaluators and experimenters. (AFCI)
  - Uncertainty analysis, target accuracy assessment, and impact of fuel composition on reactivity coefficients. (LDRD)
  - Coordination of the OECD/NEA subgroup 33 on “Methods and issues for the combined use of integral experiments and covariance data”. (LDRD)
  - Consistent data assimilation for improvement of basic nuclear parameters. (Office of Science FOA)
  - MANTRA (Measurement of Actinide Neutron Transmutation Rate by Accelerator mass spectrometry). Separate presentation by G. Youinou. (Office of Science FOA, ATR NUF)

Progress on INL's Integral Experiment Analyses

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AFCI Physics Working Group Meeting

Brookhaven National Laboratory

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Introduction

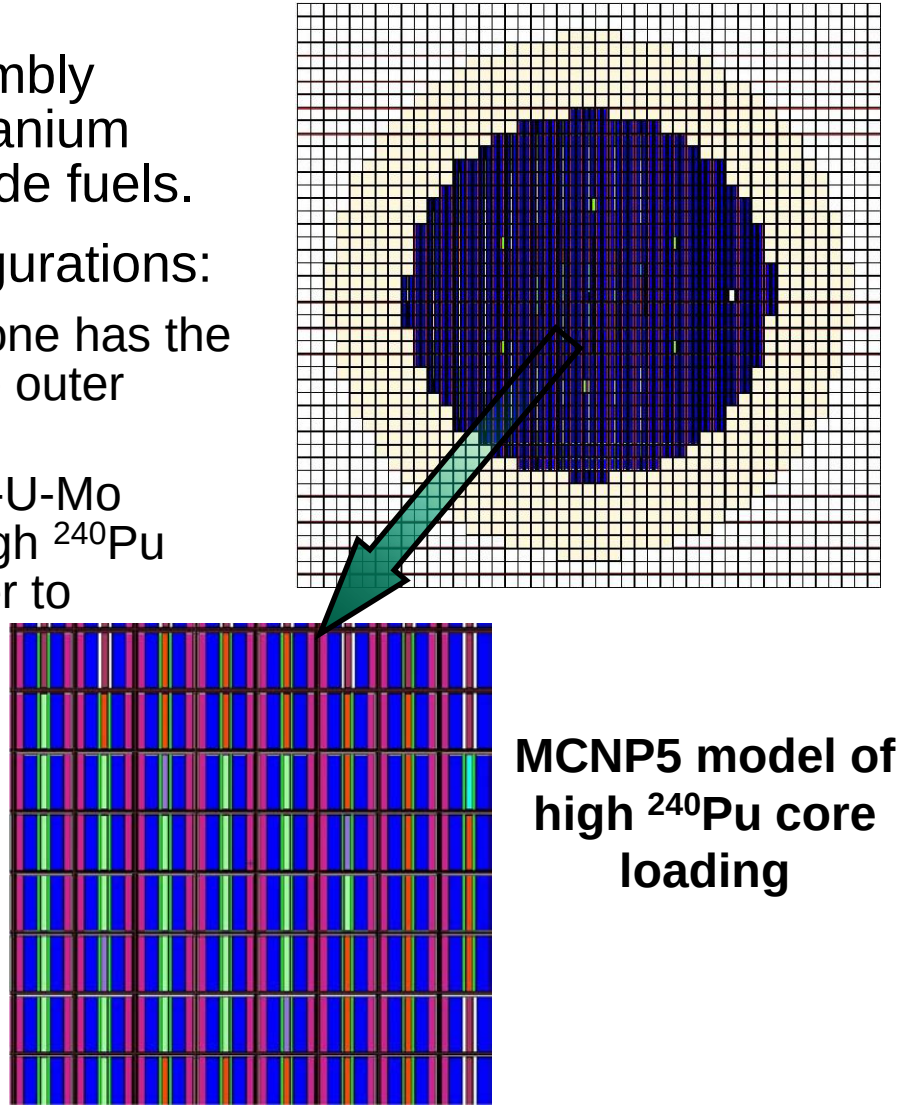
- We present progress on some of integral experiment analyses performed in FY210 that can be potentially used for the nuclear data adjustment, in order to provide feedbacks to evaluators and experimentators.

- The analysis used ENDF/B-VII data and the Monte Carlo neutron transport code MCNP5 in order to obtain the best estimates of discrepancies between calculated and measured values.

- In this presentation:
  - Analyses of ZPR6-7 Assemblies
  - Status of PROFIL Experiment Analyses
  - ZPPR-10

Analyses of ZPR6-7 Assemblies

- ZPR6-7 is a large cylindrical assembly surrounded by a thick depleted-uranium reflector based on mixed Pu-U oxide fuels.
- There are two principal core configurations:
  - Uniform core loading: A central zone has the same average composition as the outer region.
  - High ^{240}Pu-zone core loading: Pu-U-Mo plates in the central zone have high ^{240}Pu (27%) content. Composition closer to LMFBR core with high burnup.
- Analyses were performed using both detailed and simplified (cylindrical) geometry models.



MCNP5 model of high ^{240}Pu core loading

Analysis of ZPR6-7 Assemblies

- Our detailed MCNP models significantly underestimated k_{eff}.
- There was no significant dimensional mismatch. However, there are some possible differences in material compositions.
- Thus, we decided to use available models from the recent IRPhEP document.

- Comparison of k_{eff} calculated for detailed geometry models:

Assembly	Reference	MCNP5 (old models)	MCNP5 (new models from DVD)
Uniform core loading	1.00051±0.00087	0.99796±0.00007	1.00094±0.00007
High ^{240}Pu core loading	1.0008±0.0009	0.99240±0.00007	1.00017±0.00011

ZPR6-7 Spectral Indices

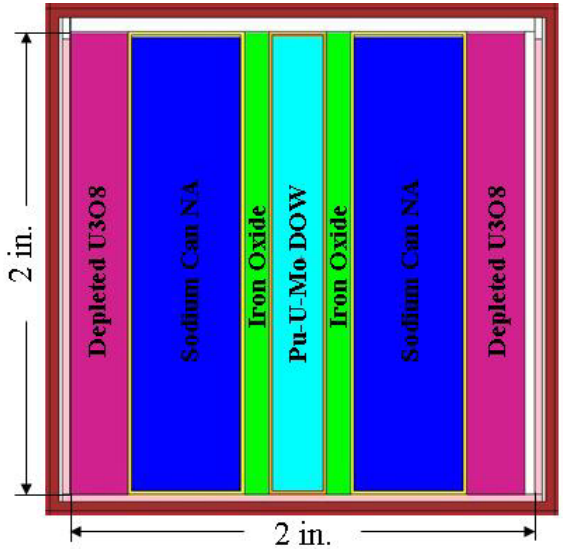
- Spectral indices has been re-evaluated by averaging over 2-2-2 inch box at the central drawer.

$$\text{Reaction rate of Isotope } n = \frac{\sum_i R_i^n A_i^n}{\sum_i A_i^n}$$

$R_i^n \equiv$ Reaction rate of Isotope n at Fuel plate i;

$A_i^n \equiv$ Atomic density of Isotope n at Fuel plate i.

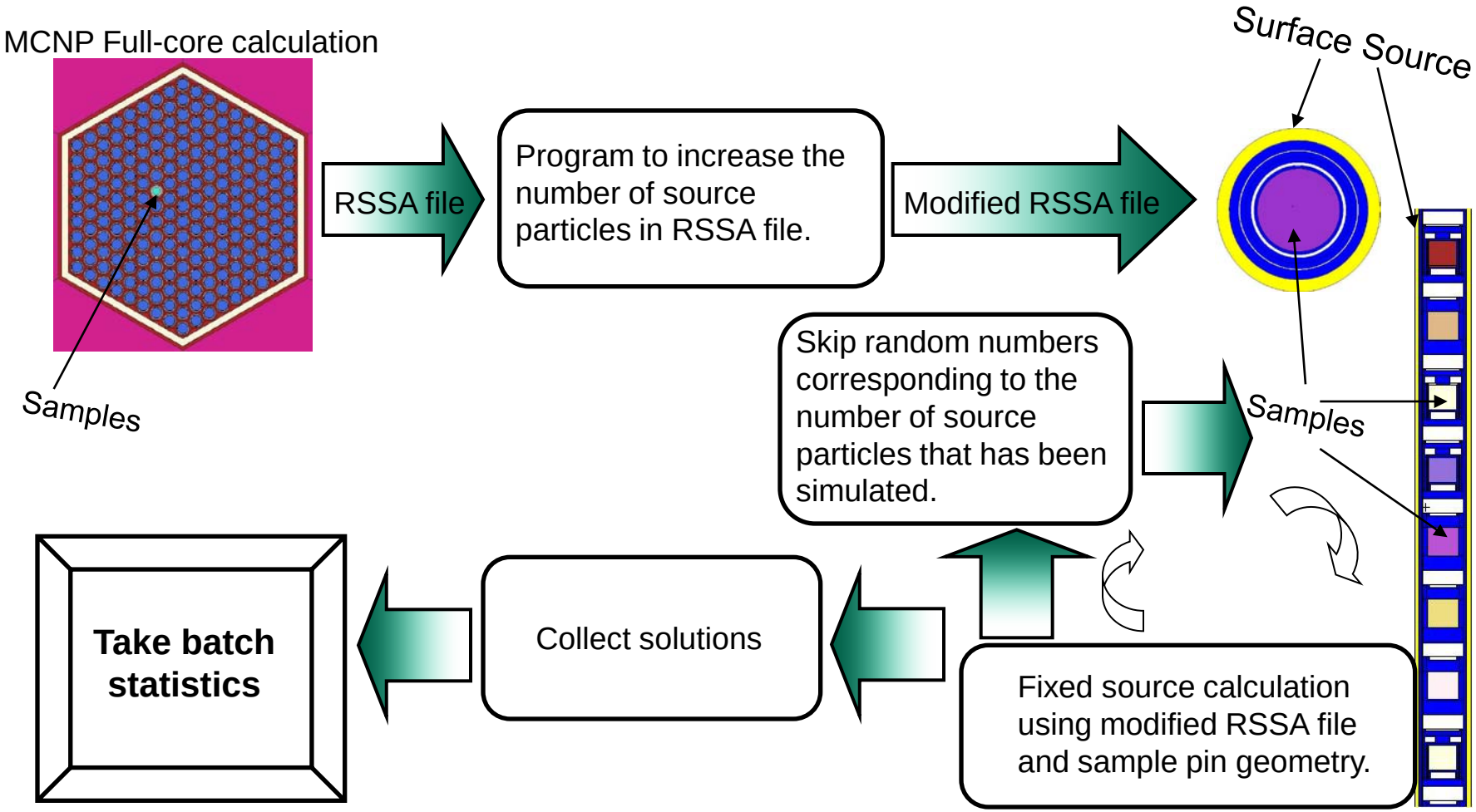
Spectral Index	Experiment	C/E
$\sigma_f(^{235}U)/\sigma_f(^{239}Pu)$	1.0599 ± 0.0223	1.0354 ± 0.0226
$\sigma_f(^{238}U)/\sigma_f(^{235}U)$	0.0223 ± 0.0007	1.0045 ± 0.0328
$\sigma_f(^{238}U)/\sigma_f(^{239}Pu)$	0.0234 ± 0.0007	1.0556 ± 0.0341
$\sigma_{n,\gamma}(^{238}U)/\sigma_f(^{235}U)$	0.1323 ± 0.0032	1.0098 ± 0.0252
$\sigma_{n,\gamma}(^{238}U)/\sigma_f(^{239}Pu)$	0.1402 ± 0.0032	1.0478 ± 0.0250
$\sigma_{n,\gamma}(^{238}U)/\sigma_f(^{238}U)$	5.8740 ± 0.1891	1.0139 ± 0.0342



PROFIL Analysis

- We found out that the original PROFIL-1 document states a factor of 10 less amount of U-238 in the radial blanket.
- k_{eff} changed from 1.00006 (±8 pcm) to 1.00758 (±3 pcm).
- Discrepancies in some of one-group cross sections were due to incorrectly taking into account for power scaling factors.
- Now we are good to proceed burnup calculations.

Proposed procedure to calculate one-group cross sections over each sample



Calculated Cross Sections on U235 Sample 1

Detector 10											
MT	**Isotope**	**XS [barn]**	**Relative Error [%]**	**MT**	**Isotope**	**XS [barn]**	**Relative Error [%]**	**MT**	**Isotope**	**XS [barn]**	**Relative Error [%]**
102	U234	4.463E-01	0.506	**102**	Pu239	4.609E-01	0.420	**102**	Nd148	1.138E-01	1.369
16	U234	2.667E-04	5.222	**16**	Pu239	4.671E-04	3.068	**16**	Nd148	7.989E-04	5.578
17	U234	2.710E-08	35.621	**17**	Pu239	1.293E-07	34.354	**107**	Nd148	1.021E-07	7.427
18	U234	3.499E-01	0.320	**18**	Pu239	1.784E+00	0.227	**103**	Nd148	2.051E-08	25.088
102	U235	5.249E-01	0.272	**102**	Nd143	2.479E-01	1.264	**102**	Nd150	1.337E-01	2.093
16	U235	1.558E-03	2.745	**16**	Nd143	9.324E-04	4.338	**16**	Nd150	7.239E-04	5.750
17	U235	3.399E-07	33.861	**107**	Nd143	1.361E-04	0.466	**107**	Nd150	1.715E-08	17.383
18	U235	1.847E+00	0.218	**103**	Nd143	1.138E-06	5.513	**103**	Nd150	7.149E-09	28.748
102	U236	4.163E-01	0.498	**102**	Nd144	6.880E-02	1.115				
16	U236	8.193E-04	4.342	**16**	Nd144	4.741E-04	6.759				
17	U236	1.580E-06	33.793	**107**	Nd144	5.016E-06	1.034				
18	U236	1.143E-01	0.427	**103**	Nd144	3.117E-07	12.227				
102	U238	2.778E-01	0.495	**102**	Nd145	4.118E-01	0.891				
16	U238	1.966E-03	3.615	**16**	Nd145	1.602E-03	3.828				
17	U238	4.883E-06	32.160	**107**	Nd145	2.542E-05	0.257				
18	U238	4.937E-02	0.538	**103**	Nd145	2.784E-07	9.972				
102	Np237	1.521E+00	0.256	**102**	Nd146	8.267E-02	1.063				
16	Np237	4.017E-04	4.041	**16**	Nd146	6.310E-04	6.243				
17	Np237	1.216E-07	33.798	**107**	Nd146	7.467E-07	2.540				
18	Np237	3.738E-01	0.330	**103**	Nd146	6.058E-08	20.489				

ZPPR-10A Benchmark for Reactivity Effects

- Control rod worth and sodium void reactivity are calculated by MCNP using total of 8 cases selected for IRPhEP benchmark.

- Based on MCNP solutions, the control rod worth is obtained by:

$$\Delta\rho_{CR} = \frac{k_{ref} - k_{rod}}{k_{ref} k_{rod} \beta_{eff}} \qquad \text{where} \quad \beta_{eff} \cong \frac{k_{ref} - k_{prompt}}{k_{ref}}$$

- The standard deviation is calculated by:

$$\sigma_{\Delta\rho_{CR}} = \sqrt{\left(\frac{1}{k_{ref}^2 \beta_{eff}}\right)^2 \sigma_{k_{ref}}^2 + \left(\frac{1}{k_{rod}^2 \beta_{eff}}\right)^2 \sigma_{k_{rod}}^2 + \left(\frac{1}{k_{ref} \beta_{eff}^2} - \frac{1}{k_{rod} \beta_{eff}^2}\right)^2 \sigma_{\beta_{eff}}^2}$$

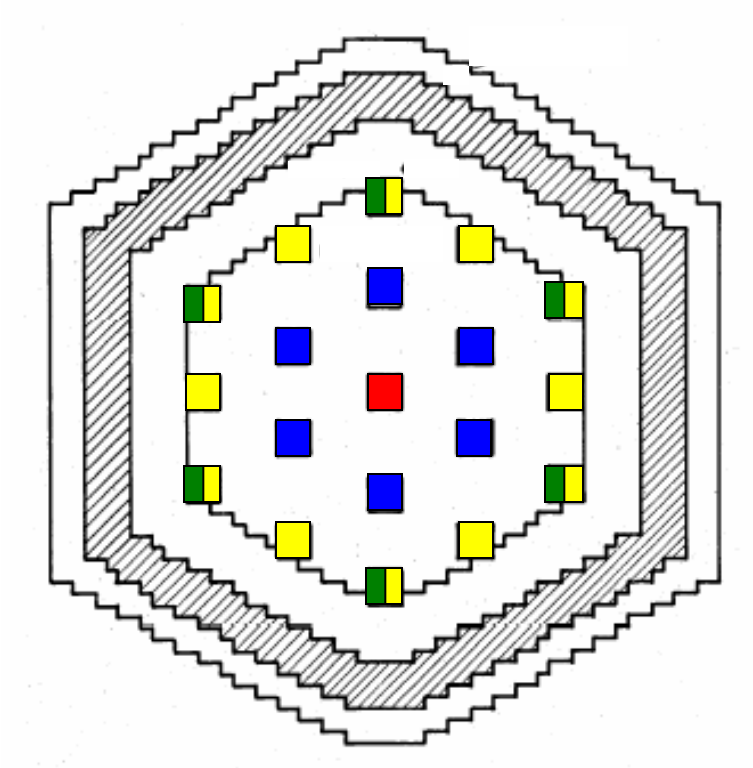
$$\text{where} \quad \sigma_{\beta_{eff}} = \frac{k_{prompt}}{k_{ref}} \sqrt{\left(\frac{\sigma_{k_{prompt}}}{k_{prompt}}\right)^2 + \left(\frac{\sigma_{k_{ref}}}{k_{ref}}\right)^2}$$

- Similar formulations for sodium void reactivity calculations.

ZPPR-10A Control Rod Worth

CR Positions	Experiment [$] (Measured Value)	C/E
Center	2.61 ± 0.03	1.0496 ± 0.0385
Ring 4	13.25 ± 0.14	1.0608 ± 0.0368
Ring 7	21.09 ± 0.31	1.0440 ± 0.0377
Ring 7	9.54 ± 0.11	1.0501 ± 0.0368

(β_{eff} = 0.00343323±0.00011305)



ZPPR-10A CR locations

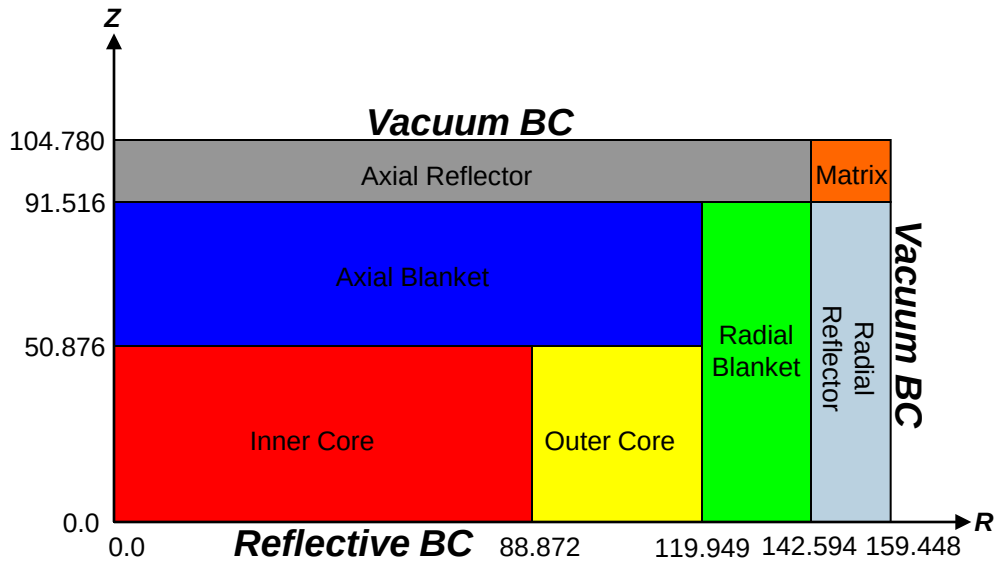
ZPPR-10A Sodium Void Reactivity

Voiding Zones	Experiment [cents] (Measured Value)	C/E
88 drawers per half, ± 8 in.	22.26 ± 0.26	1.2252 ± 0.0569
172 drawers per half, ± 8 in.	42.64 ± 0.46	1.0035 ± 0.0335
172 drawers per half, ± 16 in.	55.15 ± 0.61	1.0411 ± 0.0317
172 drawers per half, ± 20 in.	46.73 ± 0.52	0.9921 ± 0.0313

(β_{eff} = 0.00343315±0.00004252)

ZPPR-9 Benchmark

- Calculations of k_{eff} for ZPPR-9 were performed in RZ model using MCNP5 and ERANOS (BISTRO).
- 33-group, S4P1 and S4P3 for ERANOS calculations.
- *The reference value was obtained by multiplying the geometric correction factor, provided by JAEA, to the experimental value.



RZ Model of ZPPR-9 Core

Comparison of k_{eff} for ZPPR-9 models

	Reference*	MCNP5	ERANOS (33-group, S4P1)	ERANOS (33-group, S4P3)
k_{eff}	0.99215 (±153pcm)	0.98656 (±14pcm)	0.98830	0.98840

Future Work

- Work on experiment analysis will continue by finalizing the PROFIL 2 and TRAPU irradiation experiments

- The final adjustment is postponed waiting for availability of the AFCI 2.0 covariance matrix, ZPPR-15 benchmark (important for metal fuelled systems) and possibly ZPPR-9 and ZPPR-19 detailed models.

NUCLEAR DATA TARGET ACCURACIES FOR GENERATION-IV SYSTEMS BASED ON THE USE OF NEW COVARIANCE DATA

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Introduction

- As new high fidelity covariance data become available they can be used to assess nuclear data target accuracies for future innovative nuclear systems. The new covariance data produced at BNL (with the support of LANL and ORNL) and called AFCI 1.2, have been used to update the findings of the NEA/WPEC Subgroup 26.
- The difference with the respect to the previous study of the Subgroup 26 (where the BOLNA covariance matrix was used) has been found in some cases be significant.
- However, this work is devoted to target accuracy studies. In particular, one major (theoretical) issue has been investigated. This issue is related to the fact that in previous studies correlation terms have been neglected in target accuracy assessments.
- We will first illustrate the theory behind the target accuracy assessment, then provide results for applications to the advanced fast reactor systems considered in the NEA/WPEC Subgroup 26 study, and finally provide some indications on how to proceed for future studies.

THEORY

- When covariance data matrix (i. e. standard deviations on diagonal, and correlations on off-diagonal term) ***D*** and sensitivity coefficient arrays $\boldsymbol{S_R}$ for an integral parameter ***R***, one can calculate the uncertainty $\boldsymbol{\Delta R^2}$ on the integral parameter using the sandwich formula:

$$\Delta R^2 = S_R^+ D S_R$$

- A successive step is the assessment of target accuracy requirements Target accuracy assessments are the inverse problem of the uncertainty evaluation. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data.
- In fact, the unknown uncertainty data requirements can be obtained by solving a minimization problem where the sensitivity coefficients in conjunction with the existing constraints provide the needed quantities to find the solutions

THEORY

- The unknown uncertainty data requirements $\boldsymbol{d_i}$ can be obtained (e.g., for variables $\boldsymbol{i}$ not correlated among themselves), by solving the following minimization problem for the functional $\boldsymbol{Q}$:

$$\boldsymbol{Q} = \sum_{\boldsymbol{i}} \lambda_{\boldsymbol{i}} / \boldsymbol{d}_{\boldsymbol{i}}^2 = min \qquad \boldsymbol{i} = 1 \ldots \boldsymbol{I}$$

with the following constraints:

$$\sum_{\boldsymbol{i}} \boldsymbol{S}_{\boldsymbol{ni}}^2 \boldsymbol{d}_{\boldsymbol{i}}^2 \leq \left(\boldsymbol{R}_{\boldsymbol{n}}^{\boldsymbol{T}}\right)^2 \qquad \boldsymbol{n} = 1 \ldots \boldsymbol{N}$$

where $\boldsymbol{N}$ is the total number of integral design parameters, $\boldsymbol{S}_{\boldsymbol{ni}}$ are the sensitivity coefficients for the integral parameter $\boldsymbol{R}_{\boldsymbol{n}}$ and $\boldsymbol{R}_{\boldsymbol{n}}^{\boldsymbol{T}}$ are the target accuracies on the $\boldsymbol{N}$ integral parameters; $\lambda_{\boldsymbol{i}}$ are “cost” parameters related to each $\boldsymbol{\sigma}_{\boldsymbol{i}}$ and should give a relative figure of merit of the difficulty of improving that parameter (e.g., reducing uncertainties with an appropriate experiment).

THEORY

- In practical cases, in order to limit the number of variables (we remind that the unknown d_i variables are the standard deviations of the cross-sections for which target accuracies are required) and make the problem feasible, the number I is obtained by selecting the variables based on their contribution to the uncertainties; for instance, by selecting only those which globally account at least for a fixed quantity (e. g. 98%).
- When taking into account correlations the constraints become:

$$\sum_i G_i^n + \sum_{ii'} C_{ii'}^n + \sum_i F_i^n + P_n \leq \left(R_n^T\right)^2 \qquad n = 1 \ldots N$$

$$G_i^n = S_{ni}^2 d_i^2 \qquad C_{ii'}^n = S_{ni} d_i Corr_{ii'} d_{i'} S_{ni'}^+$$

$$F_i^n = S_{ni} d_i Corr_{ij} d_j S_{nj} \qquad j = 1 \ldots K$$

P_n represent the constant residual uncertainty for integral parameter R_n due to the unselected variables

THEORY

- In order to solve the nonlinear minimization problem with nonlinear constraints we have used the SNOPT code. SNOPT uses a sequential quadratic programming (SQP) algorithm that obtains search directions from a sequence of quadratic programming subproblems. Each QP subproblem minimizes a quadratic model of a certain Lagrangian function subject to a linearization of the constraints. An augmented Lagrangian merit function is reduced along each search direction to ensure convergence from any starting point.
- As many other optimization codes SNOPT needs the problem Jacobian. The code can calculate derivatives in a numerical manner, but our experience is that it better performs both in execution time and accuracy when derivatives are directly provided by the user. Derivatives with respect to variable $\boldsymbol{d_i}$ can be analytically calculated so their corresponding analytical formulation was implemented in the user function subroutines that were provided to SNOPT.

TARGET ACCURACY ASSESSMENT FOR ADVANCED FAST REACTOR SYSTEM

- For the practical application we have chosen as reactor design those of fast reactor system that were used in the Subgroup 26 study: EFR (Na-cooled European Fast Reactor), GCFR (Gas Cooled Fast Reactor), SFR (Sodium Fast Reactor), LFR (Lead Fast Reactor), ADMAB (Accelerator Driven Minor Actinide Burner).
- We have used the new available AFCI 1.2 covariance data. One major difference of this matrix with respect to the BOLNA one used in the the NEA/WPEC Subgroup 26 study, is the energy group structure adopted that consists in 33 energy groups mostly intended for fast reactor applications.
- For integral parameter we have used only the multiplication factor K_{eff} in order to simplify calculations and better understand the obtained results.
- For the target value on the integral parameter the value of 300 pcm has been adopted for all fast systems.

EFR

Target accuracy assessment for EFR (pcm). 146 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**631**	**-**	**-**	**631**	**-**	**631**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**631**	**1044**	**164**	**1231**	**248**	**1256**
	Final	**93**	**122**	**71**	**169**	**248**	**300**

EFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
U8 σ^{inel} Gr. 5	**20.6**	**3.8**	**0.5**
U8 σ^{inel} Gr. 4	**19.4**	**3.2**	**0.5**
U8 σ^{inel} Gr. 6	**16.9**	**4.4**	**0.6**
U8 σ^{inel} Gr. 3	**20.1**	**5.5**	**0.7**
Pu1 σ^{fis} Gr. 10	**20.0**	**6.4**	**0.9**

GCFR

Target accuracy assessment for GCFR (pcm). 173 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**982**	**-**	**-**	**982**	**-**	**982**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**982**	**1640**	**174**	**1919**	**278**	**1939**
	Final	**52**	**81**	**59**	**113**	**278**	**300**

GCFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
U8 σ^{inel} Gr. 5	**20.6**	**2.1**	**0.3**
U8 σ^{inel} Gr. 4	**19.4**	**2.3**	**0.3**
U8 σ^{inel} Gr. 3	**20.1**	**3.1**	**0.4**
U8 σ^{inel} Gr. 6	**16.9**	**3.1**	**0.4**
Pu1 σ^{fis} Gr. 10	**20.0**	**4.2**	**0.5**

SFR

Target accuracy assessment for SFR (pcm). 201 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**903**	**-**	**-**	**903**	**-**	**903**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**903**	**1858**	**186**	**2074**	**251**	**2090**
	Final	**80**	**121**	**76**	**164**	**251**	**300**

SFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
Pu8 σ^{fis} Gr. 7	**50.0**	**4.7**	**0.9**
Pu8 σ^{fis} Gr. 8	**50.0**	**4.8**	**0.9**
Pu8 σ^{fis} Gr. 6	**50.0**	**5.1**	**1.0**
Pu1 σ^{fis} Gr. 10	**20.0**	**3.6**	**0.7**
Pu8 σ^{fis} Gr. 9	**50.0**	**6.2**	**1.1**

ADMAB

Target accuracy assessment for ADMAB (pcm). 270 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**1124**	**-**	**-**	**1124**	**-**	**1124**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**1124**	**2125**	**194**	**2411**	**257**	**2425**
	Final	**72**	**119**	**68**	**155**	**257**	**300**

ADMAB target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
Am1 σ^{fis} Gr. 6	**10.0**	**1.6**	**0.4**
Am1 σ^{fis} Gr. 5	**10.0**	**1.7**	**0.4**
Pu1 σ^{fis} Gr. 10	**20.0**	**2.8**	**0.5**
Pu1 σ^{fis} Gr. 9	**18.9**	**2.8**	**0.5**
Cm5 σ^{fis} Gr. 10	**50.0**	**4.8**	**0.9**

Conclusions

- We have performed a target accuracy assessment using new available covariance data, the AFCI 1.2 covariance data matrix, and looking at the issue of taking into account correlation terms. The major conclusions and recommendations obtained by this study are:
  - The impact of correlation terms is very significant in target accuracy assessment evaluation and produces very stringent requirements on nuclear data
  - For this type of study a broader energy group structure should be used, in order to smooth out requirements and provide better information to evaluators and cross section measurement experts
  - The main difference in results between using BOLNA or AFCI 1.2 covariance data are related to minor actinides, minor Pu isotopes, structural materials (in particular Fe56), and coolant isotopes (Na23)

Conclusions

- For future target accuracy requirements study a possible broader energy structure that we propose contains 6 energy groups. This structure covers the entire spectrum and could be used for studies of fast, epithermal, and thermal reactors.

Proposed 6 energy groups structure (eV).

Group	Up Energy	Group	Up Energy
1	**$1.96403\ 10^{7}$**	**4**	**$2.03468\ 10^{3}$**
2	**$4.97871\ 10^{5}$**	**5**	**$2.26033\ 10^{1}$**
3	**$6.73795\ 10^{4}$**	**6**	**$5.40000\ 10^{-1}$**

- The energy limits are based on physical consideration with bands that cover the region above the threshold of fertile isotope fission cross-sections, and of many inelastic cross-sections, the region of the continuum down to the upper unresolved resonance energy limit, the unresolved resonance energy region, the resolved resonance region, the epithermal range, and thermal range.

Report on Status of SG33

WPEC/SG33

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Idaho National Laboratory

- Title: “Methods and issues for the combined use of integral experiments and covariance data”
- Cordinators: M. Salvatores, G. Palmiotti

- Goals, Mandate, Working Method:
  - *Review current methods and practices, including feedback from past work*
  - *Define test cases and input data to be used in the evaluation of the pre-selected methods.*
  - *On the basis of the test results and analysis, recommend a general methodology for data assimilation and for assessing the needs for additional experiments*

- Participants: ANL, BNL, CEA, CIAE, INL, IPPE, JAEA, JSI, NRG, ORNL

- Third meeting held on June 2nd

- First phase is very well advanced:
  - 6 organizations have sent documentation on their adjustment methodology (ANL, CEA, INL, IPPE, JAEA, JSI). ORNL should send their relatively soon.
  - Agreement has been reached on content of first deliverable: Identification of merit and drawbacks of existing methodologies (C. De Saint-Jean), comparison of mathematical formulations and specific features (M. Ishikawa), criteria for assessing methodology (G. Palmiotti)
  - First deliverable should be issued in a few months

- Second phase is under way:
  - Exercise has been defined and details have been agreed
  - First preliminary results on adjustment provided by JAEA (some issues with treatment of calculational uncertainties/errors)
  - First uncertainty evaluation on FBR (JAEA using JENDL 4 covariance matrix) and ABR (INL using AFCI 1.3 covariance matrix)

Goals of exercise

- Assess if in a multigroup nuclear data adjustment we end up with the same (similar) set of isotope cross sections when a common shared set of integral experiments is used and different data adjustment methodologies are used.
- Assess the impact of using different starting cross section libraries and/or different covariance matrices.
- Assess if the attained reduced uncertainties on a target design for a set of integral parameters of interest is consistent among the different solutions.

Benchmark exercise

Every participant to the benchmark exercise will use the same integral experiment values (E) and uncertainties, but their own calculated value (C), sensitivity coefficients, and adjustment/assimilation method.

The benchmark will consist of a three-step exercise using:

1. **own initial cross sections, own nuclear data covariances, w/wo integral correlation**
2. **own initial cross sections, same nuclear data covariances, w/wo integral correlation**
3. **same initial cross sections, same nuclear data covariances, w/wo integral correlation**

Benchmark output

The main benchmark results relevant for comparison are,

- Adjusted nuclear data,
- Final nuclear data covariances,
- Initial and final integral C/E values and associated uncertainties,
- Initial and final results of reactor project calculations including uncertainties.

The initial/final nuclear data and covariance matrices will be tested on the ABR (start up) configuration. In order to test the ability to extrapolate the results, it has been suggested to consider also a different target design. As possible candidates: ABR at equilibrium, JAEA FBR

- ***Integral data*** *: A total of 20 integral experiments are considered in 7 different assemblies*

  - **Jezebel 239-Pu configuration: 1 critical mass, 3 spectral indices: F28/F25, F49/F25, F37/F25,**
  - **Jezebel (240-Pu configuration: 1 critical mass),**
  - **Flattop Pu configuration: 1 critical mass, 2 spectral indice: F28/F25, F37/F25,**
  - **ZPR6-7 Standard configuration: 1 critical mass, 3 spectral indices: F28/F25, F49/F25, C28/F25,**
  - **ZPR6-7 (High 240Pu content: 1 critical mass),**
  - **ZPPR-9 1 critical mass, 3 spectral indices: F28/F25, F49/F25, C28/F25, 2 Na voids: central void and leakage-dominated configurations,**
  - **Joyo 1 critical mass.**

ABR Uncertainty on K_{eff} (pcm)

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	Total
U238	294	31	118	29	559	644
PU239	332	238	201	9	77	462
FE56	161	0	0	243	146	325
PU240	53	20	86	1	14	104
NA23	27	0	0	16	82	88
O16	6	0	0	42	2	42
CR50	16	0	0	3	2	16
PU241	11	9	4	0	2	15
Total	476	241	248	249	589	869

U238 Uncertainty on K_{eff}

Uncertainty (pcm)

Ener. ev	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}
1.96E+07	-0.4	2.1	5.7	0.1	2.4
1.00E+07	-1.1	7.6	25.1	1.3	59.5
6.07E+06	-2.3	12.1	41.3	5.0	193.3
3.68E+06	6.6	17.8	72.5	9.2	333.0
2.23E+06	21.3	19.4	76.7	12.3	345.9
1.35E+06	23.5	5.9	17.4	11.2	190.7
8.21E+05	29.4	2.2	1.3	8.3	40.2
4.98E+05	33.1	0.8	0.5	4.6	20.9
3.02E+05	43.8	0.5	0.3	6.7	17.6
1.83E+05	53.9	0.7	0.4	8.0	22.9
1.11E+05	58.3	0.4	0.2	7.9	41.6
6.74E+04	61.9	0.5	0.3	8.1	12.3
4.09E+04	61.4	0.3	0.2	6.3	0.0
2.48E+04	115.6	0.6	0.2	8.0	0.0
1.50E+04	120.4	0.6	0.2	1.1	0.0
9.12E+03	91.0	0.6	0.2	0.5	0.0
5.53E+03	77.4	0.0	0.0	0.3	0.0
3.35E+03	55.6	0.0	0.0	0.3	0.0
2.03E+03	89.6	0.0	0.0	0.3	0.0
1.23E+03	82.6	0.2	0.4	0.5	0.0

AFCI 1.3 Standard Deviat. %

Group	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}
1	22.3	0.6	1.4	7.4	31.6
2	21.2	0.7	1.4	12.3	30.3
3	19.9	0.6	1.3	13.1	20.1
4	5.9	0.6	1.3	15.1	19.4
5	6.1	0.6	1.3	18.8	20.6
6	3.1	1.8	1.1	9.5	16.9
7	1.7	4.9	2.0	2.6	5.6
8	1.5	5.1	2.0	2.2	4.3
9	1.5	6.8	2.0	1.8	4.1
10	1.7	5.2	2.0	1.9	6.0
11	1.7	5.1	2.0	2.8	19.2
12	1.7	5.1	2.0	3.4	17.9
13	1.6	5.2	2.0	4.3	0.0
14	3.2	100.0	2.0	2.3	0.0
15	3.9	98.8	2.0	0.9	0.0
16	3.3	100.0	2.0	0.8	0.0
17	2.8	14.5	2.0	0.7	0.0
18	2.9	66.8	2.0	0.8	0.0
19	2.9	68.0	2.0	0.8	0.0
20	2.8	6.9	2.0	1.0	0.0

ABR Uncertainty on Sodium Void (%)

Isotope	σ_{cap}	σ_{fiss}	ν	σ_{el}	σ_{inel}	Total
U238	3.9	0.1	0.5	0.6	4.1	5.8
NA23	1.5	0.0	0.0	1.5	4.9	5.3
PU239	1.4	3.2	2.9	0.2	0.8	4.6
FE56	1.2	0.0	0.0	3.7	0.9	3.9
PU240	0.6	0.1	0.6	0.0	0.1	0.8
O16	0.0	0.0	0.0	0.5	0.0	0.5
PU241	0.1	0.2	0.0	0.0	0.0	0.2
CR50	0.0	0.0	0.0	0.0	0.0	0.1
Total	4.6	3.2	3.0	4.0	6.5	10.0

USE OF COVARIANCE MATRICES IN A CONSISTENT (MULTISCALE) DATA ASSIMILATION FOR IMPROVEMENT OF BASIC NUCLEAR PARAMETERS IN NUCLEAR REACTOR APPLICATIONS: FROM METERS TO FEMTOMETERS

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Consistent Data Assimilation

- The major drawbacks of the classical adjustment method are related to the multigroup cross section approach. This implies several constraints:
  - potential limitation of the domain of application of the adjusted data
  - fixed multigroup structure
  - dependence on the neutron spectrum used as weighting function and the code used to process the basic data file
- A new approach has been developed in order to adjust physical parameters and not multigroup nuclear data, the objective being now to correlate the uncertainties of some basic parameters that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, high accuracy integral experiments.
- This new approach is the first attempt to build up a link between the wealth of precise integral experiments and basic theory of nuclear reactions. By using integral reactor physics experiments (meter scale), information is propagated back to the nuclear physics level (femtometers). In this way, the worlds of reactor nuclear physicists and that of nuclear physicists are bridged together.

Consistent Data Assimilation

- The classical statistical adjustment method can be improved by “adjusting” reaction model parameters rather than multigroup nuclear data.
- The objective is to associate uncertainties of certain model parameters (such as those determining neutron resonances, optical model potentials, level densities, strength functions, etc.) and the uncertainties of theoretical nuclear reaction models themselves (such as optical model, compound nucleus, pre-equilibrium and fission models) with observed discrepancies between calculations and experimental values for a large number of integral experiments.
- The experiments should be clean (i.e., well documented with high QA standards) and high accuracy (i.e., with as low as possible experimental uncertainties and systematic errors), and carefully selected to provide complementary information on different features and phenomena, e.g., different average neutron spectrum energy, different adjoint flux shapes, different leakage components in the neutron balance, different isotopic mixtures and structural materials etc.

Consistent Data Assimilation Approach

- The Consistent Data Assimilation methodology involves the following steps:
  - Selection of the appropriate reaction mechanisms along with the respective model parameters to reproduce adopted microscopic cross section measurements with the EMPIRE code calculations.
  - Determination of covariances matrices for the set of nuclear reaction model parameters obtained in the previous step.
  - Sensitivity of cross sections to the perturbation of the above mentioned reaction model parameters are calculated with the EMPIRE code.
  - Use of the adjoint technique to evaluate sensitivity coefficients of integral reactor parameters to the cross section variations.
  - Performing analysis of selected experiments using the best calculation tools available.
  - Performing consistent data assimilation on basic nuclear parameters using integral experiment C/E, covariance data, and sensitivity coefficients.
  - Constructing new ENDF/B type data files based on modified reaction theory parameters for use by neutronic designers.

Nuclear Parameter Sensitivity

- The sensitivities of integral experiments to fundamental parameters p_k are defined as:

$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta \sigma_j} \times \frac{\Delta \sigma_j}{\Delta p_k}$$

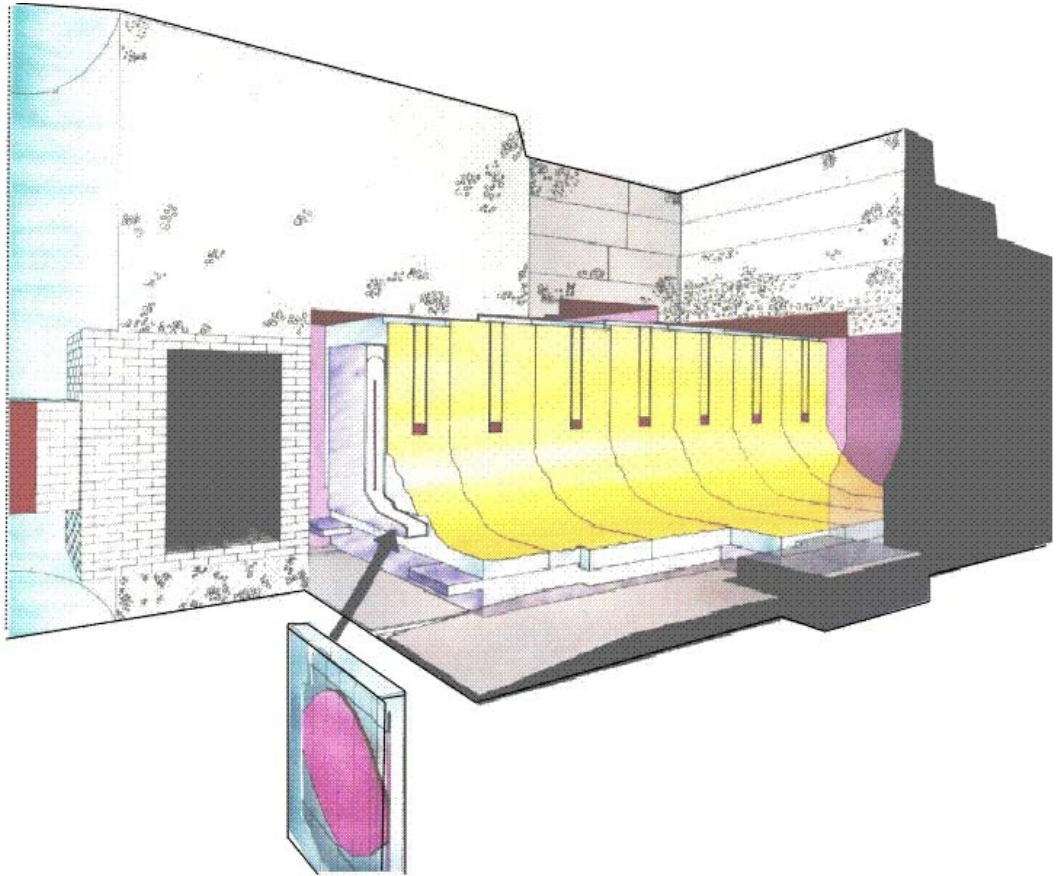
- R is an integral reactor physics parameter (e. g. K_{eff}, reaction rates, reactivity coefficient, etc.), and σ_j a multigroup cross section.
- In order to compute σ_j one use EMPIRE with an appropriate set of parameters p_k to generate an ENDF/B file for that specific isotope, and NJOY for producing multi-group cross sections.
- Covariance of the nuclear parameters p_k in conjunction with NJOY are used to generate the $\Delta\sigma_j / \Delta p_k$.
- The multigroup sensitivity coefficients $\Delta R / \Delta \sigma_j$, are provided by reactor physics calculations, using the Generalized Perturbation Theory and the ERANOS code system.

INTEGRAL EXPERIMENT ANALYSIS

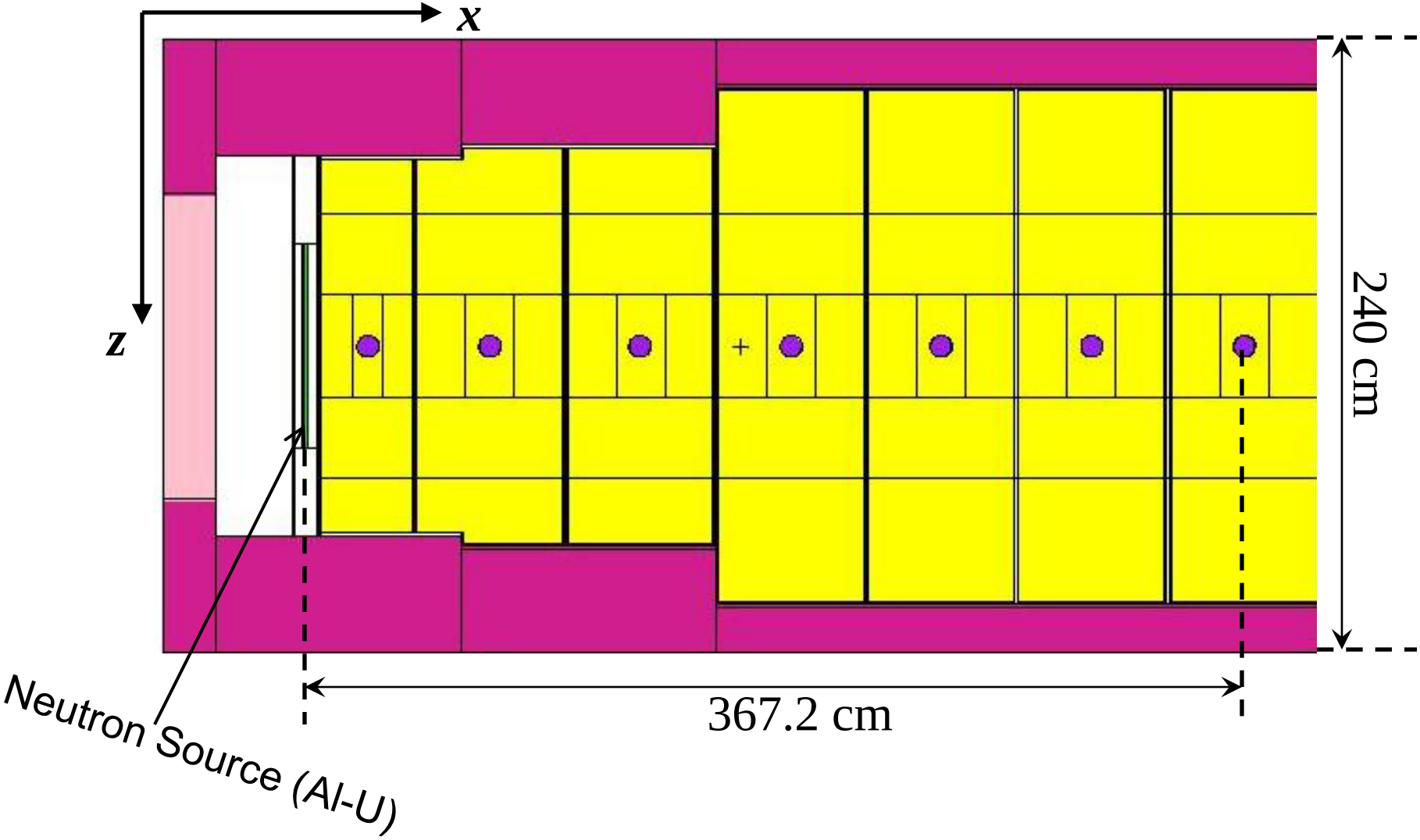
- As a practical example we have considered the case of the ^{23}Na isotope.
- For this case we have used propagation experiments of neutrons in a medium dominated by this specific isotope.
- These kinds of experiments were specifically intended for improving the data used in the shielding design of fast reactors.
- Two experimental campaigns taken from the SINBAD database have been used in this practical application:
  - the EURACOS campaign
  - the JANUS-8 campaign

EURACOS

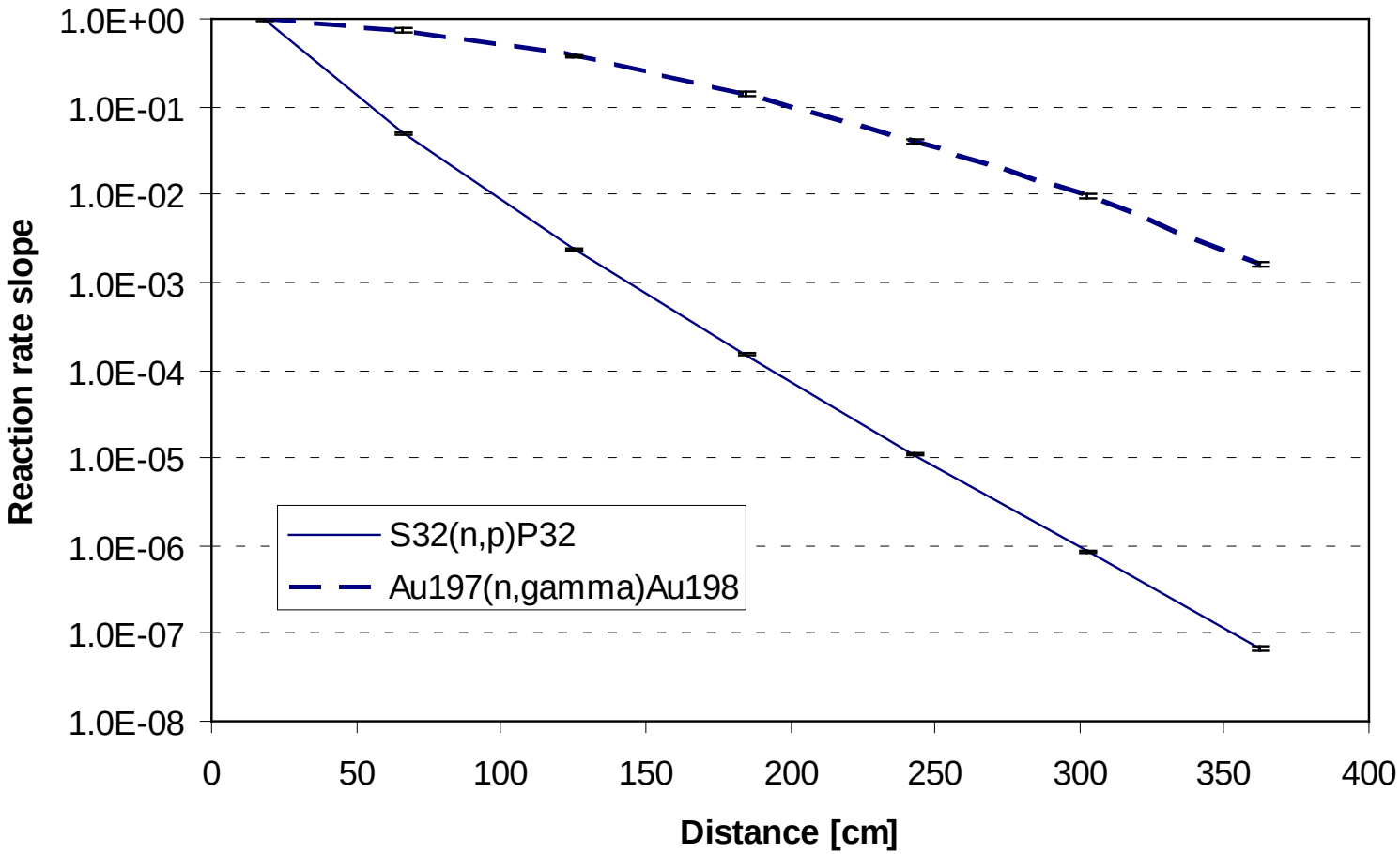
- The Ispra sodium benchmark project was performed under the EURACOS (Enriched URAnium COnverter Source) irradiation facility.
- Measurements with activation detectors were carried out at distances from the source for $^{32}S(n,p)$ and ^{197}Au (n,γ) in order to analyze fast and epithermal neutron attenuations.



EURACOS Na-Experimental Facility

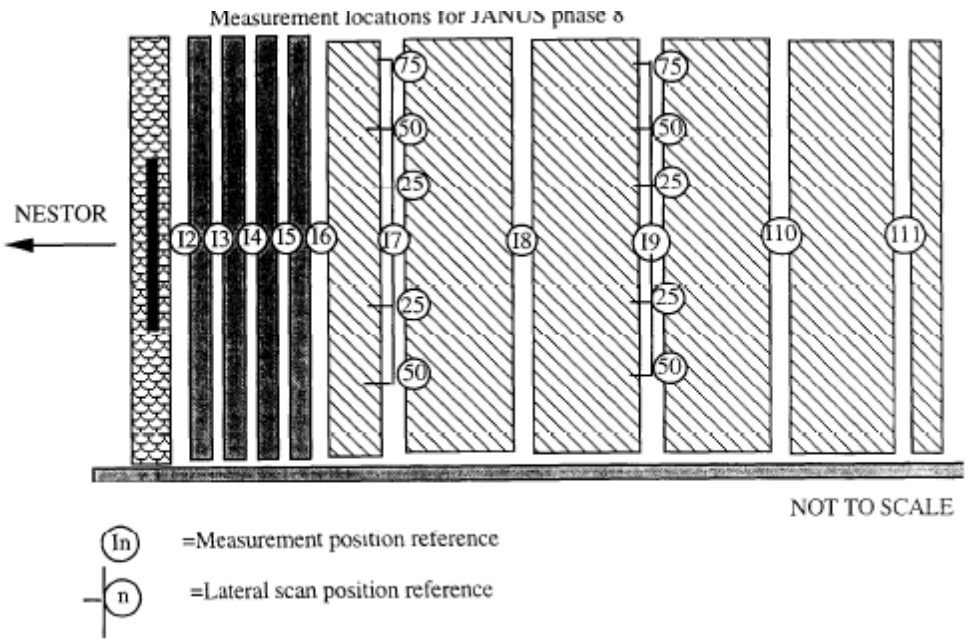


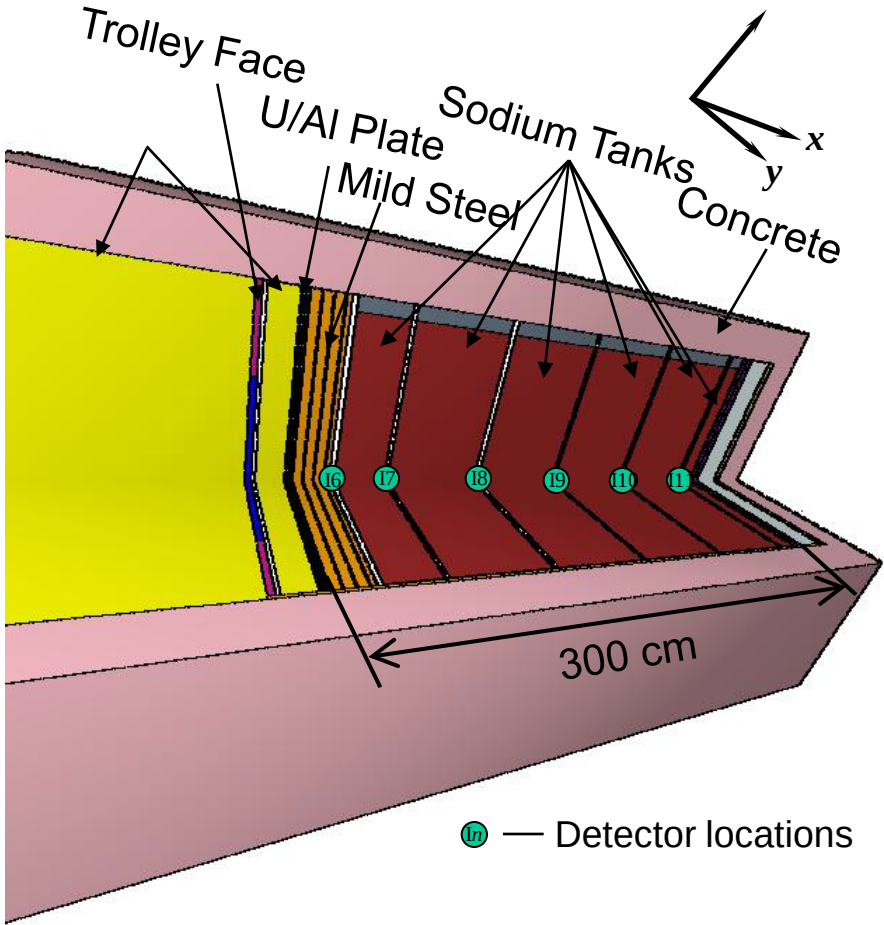
EURACOS Calculated (MCNP5 and EMPIRE σ) Attenuations



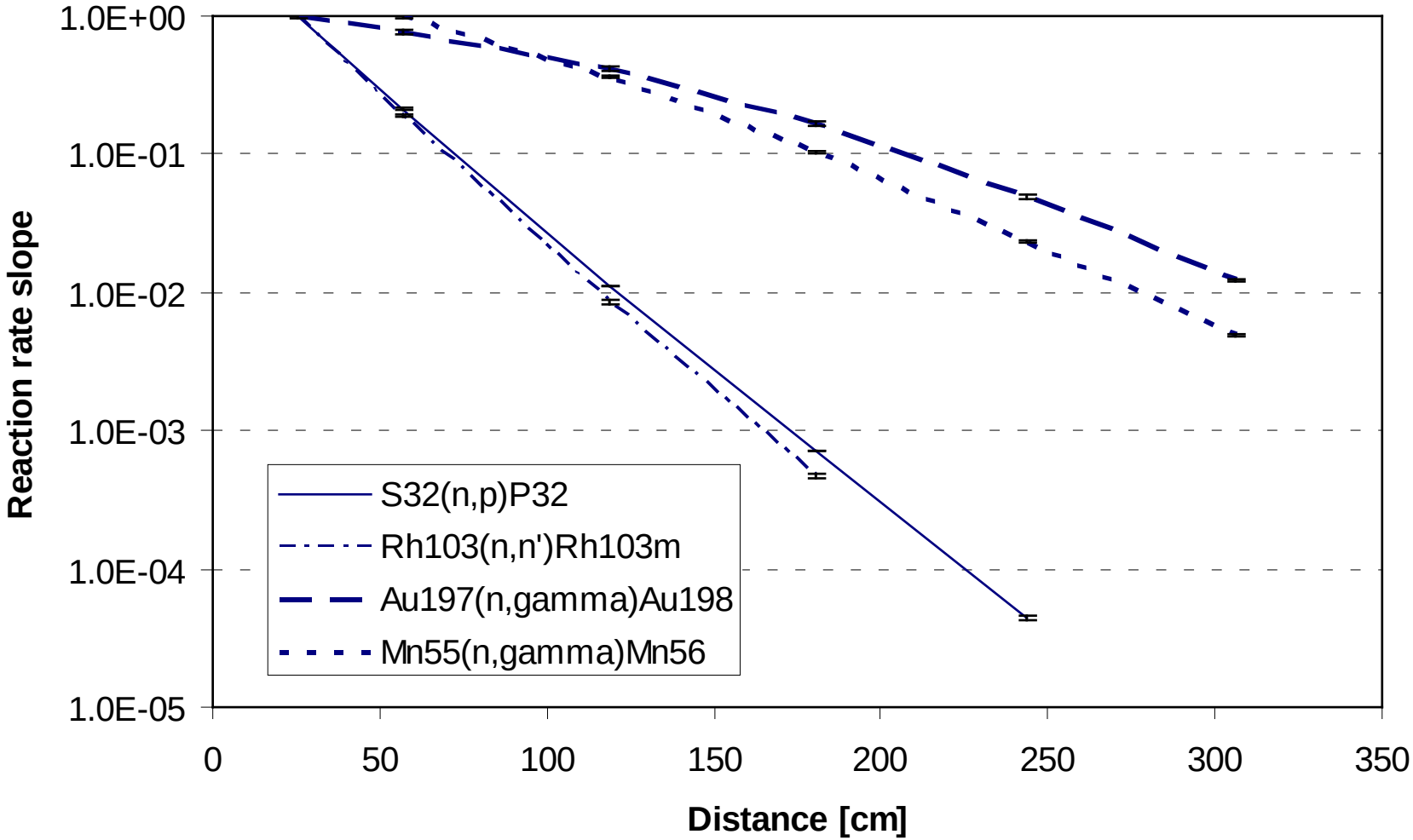
JANUS-8 Sodium Propagation Experiment

- The JANUS Phase 8 experiments were performed at the ASPIS facility.
- The neutron attenuations of several different detectors were analyzed and in particular for the following reaction rates: $^{32}S(n,p)^{32}P$, $^{103}Rh(n,n')^{103m}Rh$, $^{197}Au(n,\gamma)^{198}Au$, and $^{55}Mn(n,\gamma)^{56}Mn$.





JANUS-8 Calculated (MCNP5 and EMPIRE σ) Attenuations



^{23}Na CONSISTENT DATA ASSIMILATION

- In order to perform the consistent data assimilation on the ^{23}Na a set of 136 nuclear parameters were selected and sensitivities to them in terms of multigroup cross section were calculated. The selected parameters include:
  - nuclear scattering radius
  - bound level and 33 resonances (for each one: E_n resonance peak energy, Γ_n neutron width, Γ_g radiative width, for a total of 102 parameters).
  - 21 Optical model parameters
  - 7 Statistical Hauser-Feshbach model parameters
  - 5 Preequilibrium Exciton model parameters

Selection of Reaction Rate Slopes

- A set of reaction rate slopes (one for each detector in the two experiment campaigns) was selected.
- The selection was based, on:
  - low experimental and calculation uncertainty,
  - good depiction of the neutron attenuation for the energy range to be characterized by the corresponding detector,
  - complement of information (obtained by correlation calculations using the sensitivity coefficients)
  - good consistency among the C/E on the selected slopes
- The selected slopes were the ratios of the fourth position to the first one for both detectors in the EURACOS experiment, while for the JANUS-8 experiment we selected the fourth to first position ratio for the ^{32}S and ^{197}Au detectors, fourth to second position for the ^{55}Mn (there was no measurement in the first position), and third to first for the ^{103}Rh (the fourth position has a very large experimental uncertainty)

Selection of Reaction Rate Slopes

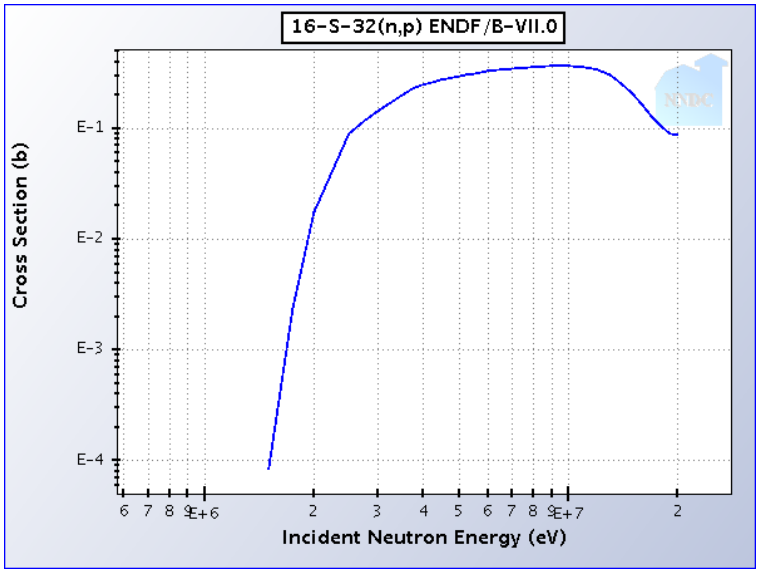
C/E of the selected slopes

Detector	C/E
EURACOS ^{32}S	**0.770 ± 0.085**
EURACOS ^{197}Au	**0.954 ± 0.102**
JANUS-8 ^{32}S	**0.538 ± 0.022**
JANUS-8 ^{197}Au	**1.010 ± 0.033**
JANUS-8 ^{55}Mn	**1.158 ± 0.025**
JANUS-8 ^{103}Rh	**0.960 ± 0.106**

Selection of Reaction Rate Slopes

^{32}S sensitivity coefficients.

Upper Energy (Mev)	Sensit. $\sigma^{elastic}$ EUR.	Sensit. $\sigma^{elastic}$ JANUS	Sensit. $\sigma^{inel.}$ EUR.	Sensit. $\sigma^{inel.}$ JANUS
19.64	**$-7.3\ 10^{-3}$**	**$-4.5\ 10^{-2}$**	**$-4.8\ 10^{-2}$**	**$-1.6\ 10^{-1}$**
10.00	**$-1.3\ 10^{-1}$**	**$-2.1\ 10^{-1}$**	**$-6.6\ 10^{-1}$**	**$-9.9\ 10^{-1}$**
6.065	**$-8.4\ 10^{-1}$**	**-1.4**	**-1.9**	**-2.9**
3.678	**$-9.0\ 10^{-1}$**	**-4.0**	**-1.1**	**-2.8**
2.231	**$-2.9\ 10^{-1}$**	**-2.4**	**$-1.8\ 10^{-1}$**	**$-8.6\ 10^{-1}$**



Selection of Reaction Rate Slopes

Correlations among experiments.

	^{32}S EUR.	^{197}Au EUR.	^{32}S JAN.	^{197}Au JAN.	^{55}Mn JAN.	^{103}Rh JAN.
^{32}S EUR.	**1.00**	**-0.13**	**0.08**	**0.00**	**0.00**	**0.02**
^{197}Au EUR.	**-0.13**	**1.00**	**0.04**	**-0.02**	**0.46**	**-0.29**
^{32}S JAN.	**0.08**	**0.04**	**1.00**	**0.00**	**0.00**	**0.04**
^{197}Au JAN.	**0.00**	**-0.02**	**0.00**	**1.00**	**0.31**	**-0.16**
^{55}Mn JAN.	**0.00**	**0.46**	**0.00**	**0.31**	**1.00**	**0.28**
^{103}Rh JAN.	**0.02**	**-0.29**	**0.04**	**-0.16**	**0.28**	**1.00**

$$Corr_{12} = \frac{S_1 DS_2^+}{[(S_1 DS_1^+)(S_2 DS_2^+)]^{1/2}}$$

Data Assimilation

C/E after statistical adjustment

Detector	C/E after adj.
EURACOS ^{32}S	**0.997 ± 0.057**
EURACOS ^{197}Au	**0.946 ± 0.010**
JANUS-8 ^{32}S	**1.000 ± 0.022**
JANUS-8 ^{197}Au	**0.959± 0.028**
JANUS-8 ^{55}Mn	**1.028 ± 0.023**
JANUS-8 ^{103}Rh	**0.976 ± 0.047**

Data Assimilation

Parameter variations and standard deviations obtained by data assimilation

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
Scat. Rad.[a)]	**1.9**	**4.1**	**1.7**
Γ_n Bou. Lev.[b)]	**-6.4**	**8.0**	**6.4**
Γ_n 2.8 Kev[c)]	**0.6**	**1.9**	**1.9**
Γ_γ 2.8 Kev[c)]	**10.5**	**11.8**	**10.5**
Γ_n 538 Kev[c)]	**-57.2**	**65.9**	**58.4**
R. Vol. Rad.[d)]	**-1.8**	**2.8**	**1.6**
R. Surf. Dif.[e)]	**-0.8**	**5.0**	**4.7**
R. Vol. Dif.[f)]	**-0.4**	**2.1**	**2.1**
TOTRED[g)]	**-1.1**	**3.5**	**3.2**
FUSRED[h)]	**-0.8**	**5.0**	**4.0**

a) Nuclear Scattering Radius b) Bound Level resonance c) Resonance Peak Energy d) Optical model real volume radius for target nucleus e) Optical model real surface diffuseness for target nucleus f) Optical model real volume diffuseness for target nucleus g) Optical model scaling of total cross sections due to intrinsic model uncertainty h) Optical model scaling of absorption cross sections due to intrinsic model uncertainty

Data Assimilation

Contribution of the parameter variation to the relative change of the C/E

^{32}S

Parameter	EURACOS Contrib. (%)	JANUS-8 Contrib. (%)
R. Vol. Rad.	**20.2**	**61.6**
TOTRED	**3.9**	**13.4**
FUSRED	**2.0**	**2.9**
R. Surf. Dif	**1.7**	**5.2**
R. Vol. Dif.	**1.9**	**3.3**
Total	**29.5**	**85.8**

^{55}Mn

Parameter	Contribution (%)
Scat. Rad.	**-12.4**
Γ_n Bou. Lev.	**8.0**
Γ_γ 2.8 Kev	**4.4**
Γ_n 538 Kev	**-2.6**
R. Vol. Rad.	**1.0**
Γ_γ 2.8 Kev	**-1.3**
Total	**-11.2**

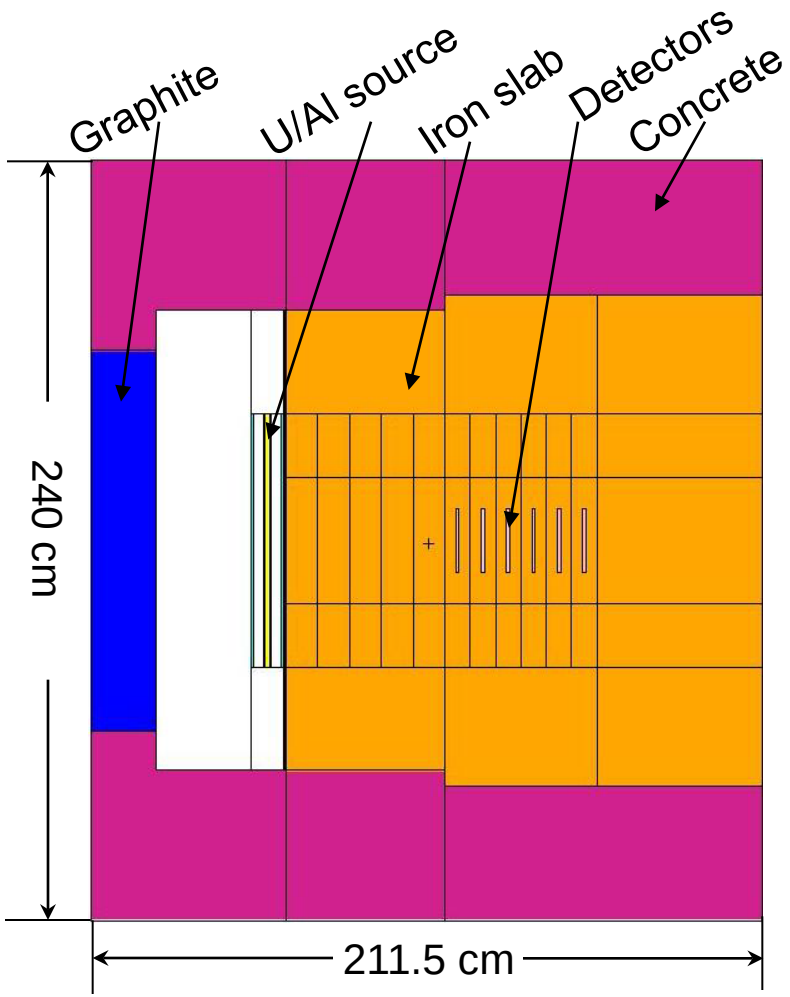
$$\chi^2=5.95$$

Conclusion and Future Work

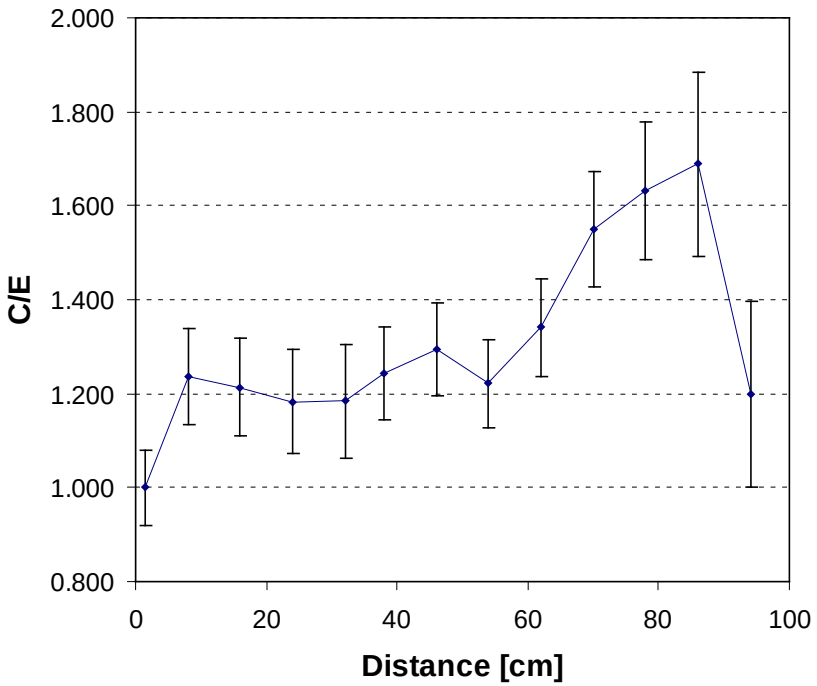
- We have proposed and implemented a new approach to link integral experiment results to basic nuclear parameters used by evaluators for generating point cross section data files. In this way the improvement in cross sections obtained by data assimilation can be general and not linked to a specific energy group structure as done in the past.
- A practical application employing experimental results of neutron propagation in sodium has shown that “adjustments” in a few nuclear parameters of ^{23}Na can produce remarkable improvements in the agreement between calculation and experiments.
- Next steps will involve the use of the modified “adjusted” parameters in EMPIRE to generate ENDF/B type of files that will be used to generate (via NJOY) multigroup data. These multigroup cross sections will be checked against those obtained by a multigroup adjustment where the same experiments used in the consistent data assimilation will be applied.
- In the next future, the consistent data assimilation will be extended to other isotopes: ^{56}Fe, Fission products, actinides.

EURACOS Iron Experiment for Consistent Method

- EURACOS II Iron experiment from SINBAD database.
- Analyze neutron attenuations in various energy range through the iron slab (~140cm).
- Preliminary analysis has been performed for S32(n,p)P32 reaction rate slope.
- The sulfur detectors within the first 50cm of the slab were simulated by point detectors. Other detectors beyond 50cm were modeled explicitly.



EURACOS II Iron Experiment Model

S32(n,p)P32 Reaction Rate Slope

	MCNP (C)		Experiment (E)		C/E	
Distance [cm]	Slope	Stdv [%]	Slope	Stdv [%]	C/E	Stdv [%]
1.5	1.00E+00	0.86	1.00E+00	7.92	1.000	7.97
8	2.59E-01	0.89	2.10E-01	8.28	1.237	8.33
16	5.36E-02	0.86	4.42E-02	8.50	1.214	8.55
24	1.16E-02	0.88	9.81E-03	9.28	1.183	9.32
32	2.57E-03	0.91	2.17E-03	10.10	1.184	10.14
38	8.27E-04	0.97	6.65E-04	7.92	1.244	7.98
46	1.84E-04	0.94	1.42E-04	7.57	1.295	7.63
54	4.09E-05	0.78	3.35E-05	7.64	1.222	7.68
62	1.00E-05	0.80	7.46E-06	7.71	1.341	7.75
70	2.42E-06	0.81	1.56E-06	7.92	1.551	7.96
78	5.80E-07	0.83	3.55E-07	8.89	1.632	8.93
86	1.38E-07	0.87	8.19E-08	11.55	1.689	11.58
94	3.32E-08	0.92	2.77E-08	16.48	1.199	16.51