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Validation of Simulation Codes for Future Systems: Motivations, Approach and the Role of Nuclear Data

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Abstract: The validation of advanced simulation tools will still play a very significant role in several areas of reactor system analysis. This is the case of reactor physics and neutronics, where nuclear data uncertainties still play a crucial role for many core and fuel cycle parameters. The present paper gives a summary of validation motivations, objectives and approach. A validation effort is in particular necessary in the frame of advanced (e.g. Generation-IV or GNEP) reactors and associated fuel cycles assessment and design.

Validation and verification

Validation of simulation codes is complementary to the “verification” process. In fact, “verification” addresses the question “are we solving the equations correctly” while validation addresses the question “are we solving the correct equations with the correct parameters”.
Verification implies comparisons with “reference” equation solutions or with analytical solutions, when they exist. Most of what is called “numerical validation” falls in this category.
Validation strategies differ according to the relative weight of the methods and of the parameters that enter into the simulation tools. Most validation is based on experiments, and the field of neutronics where a “robust” physics description model exists and which is function of “input” parameters not fully known, will be the focus of this paper. In fact, in the case of reactor core, shielding and fuel cycle physics the model (theory) is well established (the Boltzmann and Bateman equations) and the parameters are the nuclear cross-sections, decay data etc.
Two types of validation approaches can and have been used:

a) Mock-up experiments (“global” validation): need for a very close experimental simulation of a reference configuration. Bias factors cannot be extrapolated beyond reference configuration;
b) Use of “clean”, “representative” integral experiments (“bias factor and adjustment” method). Allows to define bias factors, uncertainties and can be used for a wide range of applications. It also allows to define “adjusted” application libraries or even “adjusted” data files.

The use of this last approach has been particularly successful in the design of SUPERPHENIX. In fact the prediction of the critical mass has been remarkably close to the experimental value observed at reactor start up (discrepancy of ~3 out of ~400 core sub-assemblies).

Validation: motivation and objectives

The recent extensive sensitivity/uncertainty studies, have allowed to preliminary quantify the impact of current nuclear data uncertainties on design parameters of the major Gen-IV and transmutation systems, and in particular on fast reactors with different coolants, with different fuels (oxide, metal, carbide, nitride), fuel composition (e.g. different Pu/TRU ratios), MA content and different conversion ratios. In general, innovative characteristics of future reactor cores will in fact imply new core architectures (e.g. without fertile blankets), reduced void reactivity coefficients, wide range of possible Pu vectors, significant presence of minor actinides in innovative fuels (metal, oxide, carbide, nitride) in burner or breeder core configurations.
These studies [1 to 4] have pointed out that 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 be able to meet design target accuracies.
This point can be illustrated by the inspection of the review of current and targeted uncertainties for some SFR design parameters, as indicated in Tables 1-3 (consistent with the requirements of [5]):

Table 1. Neutronics: Core

Parameter	Current uncertainty (SFR) Input Data Origin (A Priori)	Current uncertainty (SFR) Modeling Origin	Targeted Uncertainty
Multiplication Factor, k_{eff} ($\Delta k/k$)	1%	0.5%	0.3%
Power Peak	1%	3%	2%
Power Distribution	1%	6%	3%
Conversion Ratio (Absolute Value)	5%	2%	2%
Control Rod Worth: Element	5%	6%	5%
Control Rod Worth: Total	5%	4%	2%
Burnup Reactivity Swing ($\Delta k/k$)	0.7%	0.5%	0.3%

Parameter	Current uncertainty (SFR) Input Data Origin (A Priori)	Current uncertainty (SFR) Modeling Origin	Targeted Uncertainty
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%

Table 2. Neutronics: Shielding

Parameter	Current uncertainty (SFR) Input Data Origin (A Priori)	Current uncertainty (SFR) Modeling Origin	Targeted Uncertainty
Out of Core Coolant Activation	70%	70%	50%
Shield Dimensioning (Total Flux)	70%	30%	20%
Structural Damage Out of Core (Total Flux)	40%	30%	20%

Table 3. Neutronics: Fuel Cycle

Parameter	Current uncertainty (SFR) Input Data Origin (A Priori)	Current uncertainty (SFR) Modeling Origin	Targeted Uncertainty
Neutron Dose at Fuel Fabrication	15%	15%	10%
Decay Heat of Spent Fuel at Repository	50%	15%	20%
Radiotoxicity at Repository	50%	15%	20%

These tight design target accuracies, which justified in a consolidated phase of design, in order to comply with safety and optimization requirements and objectives, can only be met if very accurate nuclear data are used for a large number of isotopes, reaction types and energy ranges.
The required accuracies on the nuclear data are such that it is difficult to meet them 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. In some cases, these integral experiments have been documented in an effective manner and associated uncertainties are well understood.
A combined use of scientifically based covariance data and of integral experiments can be made using advanced statistical adjustment techniques (see, e.g., [6]). These techniques can provide in a first step adjusted nuclear data for a wide range of applications, together with new, improved covariance data and bias factors (with reduced uncertainties) for the required design parameters, in order to meet design target accuracies.
The method can be further improved to “adjust” physical parameters and to obtain in a second phase, a fully “adjusted” data file.

Uncertainty reduction needed to meet integral parameter target accuracies for all systems

As an example of the accuracy requirements to meet design target accuracies for innovative fast reactors, in [7] a study has been performed in order to quantify the requirements to meet simultaneously target accuracies such those indicated in Table 1 for a wide range of fast reactors with different coolants, fuel type, MA content in the fuel, being iso-generators or burners and critical or sub-critical. In practice the following systems have been considered:

ABTR: Na-cooled Pu burner, with Conversion Ratio CR~0.5;
SFR: Na-cooled TRU burner with CR~0.25;
EFR: Na-cooled FR for homogeneous TRU recycle and CR~1;
GFR: Gas-cooled FR for homogeneous TRU recycle and CR~1;
LFR: Lead-cooled FR for homogeneous TRU recycle and CR~0.8;

ADMAB: Lead-cooled ADS with U-free fuel and Pu/MA~1/2.
A summary of the results is given in the following table:

Table 4. *ABTR, SFR, EFR, GFR, LFR, ADMAB: Uncertainty Reduction Requirements to Meet Integral Parameter Target Accuracies*

Isotope Cross-Section	Energy Range	Uncertainty (%) Initial	Uncertainty (%) Target
U238 σ_{inel}	19.6 - 6.07 MeV	29.3	9.0
	6.07 - 2.23 MeV	19.8	2.0
	2.23 - 1.35 MeV	20.6	2.1
	1.35 - 0.498 MeV	11.6	2.3
	498 - 183 keV	4.2	3.8
	183 - 67.4 keV	11.0	4.2
Pu241 σ_{fiss}	6.07 - 2.23 MeV	14.2	5.0
	2.23 - 1.35 MeV	21.3	3.9
	1.35 - 0.498 MeV	16.6	2.1
	498 - 183 keV	13.5	1.7
	183 - 67.4 keV	19.9	1.7
	67.4 - 24.8 keV	8.7	1.9
	24.8 - 9.12 keV	11.3	2.0
	9.12 - 2.03 keV	10.4	2.1
	2.03 - 0.454 keV	12.7	2.7
	454 - 22.6 eV	19.4	5.4
Cm244 σ_{fiss}	6.07 - 2.23 MeV	31.3	3.0
	2.23 - 1.35 MeV	43.8	2.6
	1.35 - 0.498 MeV	50.0	1.5
	498 - 183 keV	36.5	4.0
	183 - 67.4 keV	47.6	7.3
U238 σ_{capt}	24.8 - 9.12 keV	9.4	1.8
	9.12 - 2.03 keV	3.1	1.8
Fe56 σ_{inel}	6.07 - 2.23 MeV	7.2	2.6
	2.23 - 1.35 MeV	25.4	1.7
	1.35 - 0.498 MeV	16.1	1.5

Isotope Cross-Section	Energy Range	Uncertainty (%) Initial	Uncertainty (%) Target
B10 σ_{capt}	498 - 183 keV	15.0	2.9
	183 - 67.4 keV	10.0	2.7
	67.4 - 24.8 keV	10.0	3.3
	24.8 - 9.12 keV	8.0	3.9
	9.12 - 2.03 keV	8.0	6.0
Pu239 σ_{capt}	1.35 - 0.498 MeV	18.2	6.6
	498 - 183 keV	11.6	4.4
	183 - 67.4 keV	9.0	4.0
	67.4 - 24.8 keV	10.1	4.2
	24.8 - 9.12 keV	7.4	3.8
	9.12 - 2.03 keV	15.5	3.2
O16 σ_{capt}	19.6 - 6.07 MeV	100.0	37.9
	6.07 - 2.23 MeV	100.0	37.9
Am243 σ_{inel}	6.07 - 2.23 MeV	17.9	4.9
	2.23 - 1.35 MeV	35.3	3.9
	1.35 - 0.498 MeV	42.2	2.3
	498 - 183 keV	41.0	3.7
	183 - 67.4 keV	79.5	3.7
	67.4 - 24.8 keV	80.8	12.4
Am242m σ_{fiss}	1.35 - 0.498 MeV	23.4	21.4
	498 - 183 keV	16.5	6.3
	183 - 67.4 keV	16.6	4.7
	67.4 - 24.8 keV	16.6	4.8
	24.8 - 9.12 keV	14.4	5.6
	2.04 - 0.454 keV	11.8	5.9
Na23 σ_{inel}	1.35 - 0.498 MeV	28.0	10.5

Isotope Cross-Section	Energy Range	Uncertainty (%) Initial	Uncertainty (%) Target
Pu240 σ_{fiss}	6.07” - 2.23 MeV	4.8	2.9
	2.23 - 1.35 MeV	5.7	2.6
	1.35 - 0.498 MeV	5.8	1.6
	498 - 183 keV	3.9	3.7
	2.03 - 0.454 keV	21.6	11.8
Si28 σ_{capt}	19.6 - 6.07 MeV	52.9	7.2
Si28 σ_{inel}	6.07 - 2.23 MeV	13.5	3.9
	2.23 - 1.35 MeV	50.0	7.4
Pb206 σ_{inel}	6.07 - 2.23 MeV	5.5	4.2
	2.23 - 1.35 MeV	14.2	4.0
	1.35 - 0.498 MeV	9.2	4.7
Pb207 σ_{inel}	6.07 - 2.23 MeV	5.0	4.9
	2.23 - 1.35 MeV	13.8	6.0
	1.35 - 0.498 MeV	11.3	3.6
Pb σ_{inel}	6.07 - 2.23 MeV	5.4	3.0
Am243 σ_{fiss}	6.07 - 2.23 MeV	11.0	2.3
	2.23 - 1.35 MeV	6.0	1.9
	1.35 - 0.498 MeV	9.2	1.7
Bi209 σ_{inel}	2.23 - 1.35 MeV	34.1	2.8
	1.35 - 0.498 MeV	41.8	4.3
N15 σ_{el}	2.23 - 1.35 MeV	5.0	3.1
	1.35 - 0.498 MeV	5.0	1.2
	498 - 183 keV	5.0	1.9
	183 - 67.4 keV	5.0	2.3
Zr90 σ_{inel}	6.07 - 2.23 MeV	18.0	3.3

These results confirm the very significant uncertainty reduction needed to meet target accuracies on important design parameters. In some cases (e.g. inelastic of U-238), the required reduction seems hard to be met with differential measurements only.

The data statistical adjustment and bias factor method

The adjustment and bias factor method [6] makes use of:
• “a priori” nuclear data covariance information,
• integral experiments analysis to define C/E values,
• integral experiment uncertainties,
in order to evaluate “a priori” uncertainties on reference design performance parameters, to reduce these uncertainties using integral experiments (“a posteriori” uncertainties on performance parameters) and to define “adjusted“ nuclear data and associated “a posteriori” covariance data.
A crucial step is the selection of a set of relevant experiments. This task can be performed using sensitivity analysis of selected configurations including reference design configurations for a wide range of integral parameters related to the core performances (critical mass, reactivity coefficients, control rod worth, power distributions etc), and fuel cycle parameters (reactivity loss/cycle, decay heat, transmutation rates, neutron sources and doses of spent fuel etc).
A second crucial step is the selection of science based covariance data for uncertainty evaluation and target accuracy assessment. Finally, the analysis of experiments should be performed using the best methods available, with some redundancy to avoid systematic errors. Finally the adjustment procedure allows to use calculation/experiment discrepancies (and associated uncertainties) in a statistical adjustment.
The “adjustment” procedure can be generalized and applied to the physical parameters that enter into the model description of a specific cross-section type. This generalized method is called “consistent method” [8], and is shortly described below.
If the cross-section is schematically described as:

$\sigma(E) = f(E, p_i)$

the sensitivity coefficients of the cross-section to the variations of the parameters p_i can be obtained from the model codes as:

$S_{pi} = (\delta f / \delta p_i)(p_i / f)$

These sensitivity coefficients can then be folded with standard sensitivity coefficients of integral parameters R to cross-section σ variations:

$(\delta R / \delta p_i)(p_i / R) = S_\sigma S_{pi}$

A correlation can now be established among integral parameters and basic physics parameters, and the adjustment procedure outlined previously, can be applied to the p_i parameters, if uncertainties (covariance data) are provided for the parameters.

Finally, if these parameters are part of the data file (e.g. the temperature values associated to the evaporation spectrum describing the secondary neutron distribution in inelastic scattering) the file itself can be in principle "adjusted".

Integral experiments

Integral experiments have been performed in large number in the past. Future experiments can be foreseen only on a few installations and at a later date (this is the case of the MASURCA critical facility at CEA-Cadarache).

Some of the most representative (and "clean") integral experiments are being collected within the NEA-NSC project IRPHEP [9]. In this respect, it should be stressed that documentation is essential: experimental conditions and environment, "credible" uncertainties, correlations among experiments.

Another very crucial point is the availability and share of power reactor experiments, e.g.

- Physics experiments at reactor start-up (e.g. SUPERPHENIX);
- Operation experiments (e.g. EBR-II, FFTF, PHENIX, JOYO);
- New experiments (e.g. at the future MONJU start-up);
- Irradiation experiments (e.g. PROFIL and TRAPU experiments in PHENIX).

Issues and perspectives

Innovative reactor system design and requirements for improved economy and safety, will require significant improvements beyond current simulation tools, associated to significant improvements in their validation, in particular in order to cope with very tight requirements on nuclear data uncertainties. In this respect, a robust validation approach can be used in the reactor core and fuel cycle physics field.

Powerful and flexible sensitivity analysis methods and tools are available (see [10]), and a large effort is underway to assess nuclear covariance data in very comprehensive way [11].

However, a choice of appropriate integral experiments has to be carefully made. There is the need for integral experiments with well documented uncertainty values and possible correlations among different experiment types. There is also the need for an increased role of power reactor integral experiments.

The experiment analysis should be performed with more than one reference methods, as far as possible independent from each other, in order to reduce or eliminate the risks of systematic method errors.

Since the result of the validation will provide bias factors and reduced uncertainties on most design parameters, together with statistically "adjusted" cross-sections with new associated covariance data, it will be needed to define the protocols for using them as application libraries. However, and more important, the "adjustments" will have to be interpreted as "trends" to be used by nuclear data evaluators, in order to improve current data files (such as ENDF/B-VII). We have also described in the present paper, how the statistical adjustment procedure can be generalized to provide "adjustments" of physics parameters that enter into the models which describe the different cross-sections.

Finally, it should be stressed that the present data bases of integral experiments are relatively wide, even if not always documented in a satisfactory way. Future design studies, new core and fuel types, new core configurations, could require selected, high accuracy integral experiments, to be performed in the few adapted critical facilities, still available world-wide.

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