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# Reference Values for Nuclear Criticality Safety

**Homogeneous and Uniform**
**$UO_2$, "UNH", $PuO_2$ and "PuNH",**
**Moderated and Reflected by $H_2O$**

**A demonstration study by an**
**Expert Group of the**
**Working Party on Nuclear Criticality Safety for the**
**OECD/NEA Nuclear Science Committee**

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NEA No. 5433

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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# FOREWORD

Since 1980 the OECD/NEA has supported international co-operation with studies on nuclear criticality safety issues, in particular the comparison of calculation methods and the associated validation. Past expert groups have studied typical transport packages for irradiated fuel, large arrays of units with fissile material, small fissile particles mixed with moderated fissile material and burn-up credit, which continues to be studied. To support validation, the OECD/NEA International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook has been updated with new and revised benchmarks and issued every year since 1995. Almost all of the benchmarks are based on critical experiments. The criticality safety expert groups, as well as the ICSBEP, work under the direction of the OECD/NEA Nuclear Science Committee (NSC), supported by its Working Party on Nuclear Criticality Safety (WPNCS).

In practice, criticality safety control, as well as emergency preparedness and response, often rely on simple systems and handbook data. These data include reference values, such as minimum critical mass, concentration and geometry as well as maximum critical moderation for well-defined systems. Since the systems are well-defined, the reference values are physical constants. The fissile materials in the study were eventually limited to uranium dioxide, uranium nitrate, plutonium dioxide and plutonium nitrate. They are each moderated and reflected by water. Several isotopic distributions of the uranium and plutonium elements were selected.

The accuracy of a reference value influences safety and economy of operations. In perceived and real emergency situations, large uncertainties in the data could result in inappropriate conclusions. Independent safety reviews, such as is required in international transport, could lead to conclusions based on less accurate data. This may be safe in the short term but discourages improvement of the data and methods, preserving large uncertainties in some areas.

The ICSBEP Handbook and other benchmark sources contain more or less complicated systems. They rarely can be used to directly determine the reference values of interest or their accuracies. Large deviations in reference values had been noticed between different criticality safety handbooks and guides. In 1998, some of the members of the WPNCS prepared a proposal for a study of reference values (minimum and maximum critical values). The proposal was accepted by the Working Party and the NSC and work began in 1999.

The present report contains a compilation and evaluation of reference values from various participants. Some of the values are from published handbooks, guides and other literature while other values were calculated mainly for the purpose of this study. As is apparent from the first OECD/NEA study in 1980 and onwards, validation is essential for the credibility of any evaluation or comparison. With proper validation, an accurate estimation of the reference value based on all contributions should be expected. The evaluation takes advantage of the ICSBEP Handbook as well as of recent developments in determination of similarities between benchmarks and applications (reference values). However, the validation process is not complete and does not sufficiently consider other error sources such as nuclide density determinations. A continuation of the study is thus recommended.

*Acknowledgements*

The collection of reference values was initially made on internet web pages supported primarily by NAIS Co. and for some time also by GRS. These were constructive efforts, showing the participants results continuously as they were being contributed. Dr. Susumu Mitake kindly organised an unofficial meeting by the Expert Group in Tokyo, October 2003. The new OECD/NEA scientific secretary to the Working Party, Dr. Yolanda Rugama, prepared JEFF 3.0 cross sections for use with MCNP to support the final evaluation leading to this report. Code developers and cross-section processing organisations have supported their products and this study by guidance and other services. Various organisations have supported the participants through sponsorship and other activities. The Swedish Nuclear Power Inspectorate (SKI), with short notice, sponsored some of the final evaluation and compilation of the report.

## TABLE OF CONTENTS

## ACRONYMS

| | |
|---|---|
| ANL | Argonne National Laboratory |
| ANS | American Nuclear Society |
| BfS | Bundesamt für Strahlenschutz |
| DfT | Department for Transport |
| DIN | Deutsches Institut für Normung |
| EALF | Energy corresponding to Average Lethargy of neutrons causing Fission |
| EMS | E Mennerdahl Systems |
| ENDF/B | Evaluated Nuclear Data File Version B |
| GRS | Gesellschaft für Anlagen- und Reactorsicherheit |
| HSE/NII | Health and Safety Executive/Nuclear Installations Inspectorate |
| IAEA | International Atomic Energy Agency |
| ICSBEP | International Criticality Safety Benchmark Evaluation Project |
| INL | Idaho National Laboratory |
| IPPE | Institute for Physics and Power Engineering |
| IRSN | Institute de Radioprotection et de Sûreté Nucléaire |
| ISO | International Standards Organisation |
| JAERI | Japan Atomic Energy Research Institiute |
| JEF | Joint European File |
| JEFF | Joint European Fission and Fusion library project |
| JENDL | Japanese Evaluated Nuclear Data File |
| LANL | Los Alamos National Laboratory |
| MCV | Minimum Critical Value |
| NAIS | Nippon Advanced Information Service |
| NEA | Nuclear Energy Agency |
| NSC | Nuclear Science Committee |
| NUPEC | Nuclear Power Engineering Corporation |
| OECD | Organisation for Economic Co-operation and Development |
| ORNL | Oak Ridge National Laboratory |
| PNL | Pacific Northwest Laboratory |
| PuNH | Plutonium Nitrate pentaHydrate |
| UNH | Uranyl Nitrate hexaHydrate |
| WPNCS | Working Party on Nuclear Criticality Safety |

# EXECUTIVE SUMMARY

## Introduction

A reference value for nuclear criticality safety is a physical constant that corresponds to a parameter value for a well-defined reference system of fissionable and other materials. A reference value should have no bias (estimated error) but will always have an uncertainty.

Improper bias corrections and large real or estimated uncertainties are problems. Inappropriate emergency preparedness and response may be a consequence. A safety margin may be unnecessarily large. Since a single reference value may be used in many operations, even a small extra margin could be costly. Underestimated errors may lead to safety hazards.

Information on calculation methods is important to safety evaluation reviewers. Simple reference systems are also useful in the validation of deterministic codes. They are also needed before studying other moderators, reflectors, absorbers, mixtures of fissionable materials, etc.

## Scope and objectives of the first study

The OECD/NEA expert group has selected a total of 132 reference systems from a wide scope of fissionable materials, moderators and reflectors. The fissionable materials are uranium and plutonium with valence numbers IV. They are not mixed. The uranium isotopes are $^{235}U$ and $^{238}U$ with the mass percentages of $^{235}U$ in the uranium 100, 20, 5, 4 and 3. The plutonium isotopes are $^{239}Pu$, $^{240}Pu$, $^{241}Pu$ and $^{242}U$ and the isotope distributions, with each isotope mass percentage of total plutonium given in that order, are 100/0/0/0, 95/5/0/0, 80/10/10/0, 90/10/0/0, 80/15/5/0 and 71/17/11/1. Chemical structures are uranium dioxide ($UO_2$), uranyl nitrate hexahydrate (UNH or $UO_2(NO_3)_2+6H_2O$), plutonium dioxide ($PuO_2$) and plutonium nitrate pentahydrate (PuNH or $Pu(NO_3)_4+5H_2O$).

All the selected fissionable materials are also fissile. Neutron moderation is thus an important issue. Water is the only additional moderating material. Mixing of the water with oxide, dissolution of hydrated nitrate in water and sometimes mixing of the saturated solution with hydrated nitrate are required to obtain optimum moderation. The moderated fissionable materials are uniform and homogeneous. The only external material is water sufficient for full (saturated) reflection.

The reference parameters are mass, volume, cylinder diameter, slab thickness, fissionable element concentration and moderation atomic ratios H/U and H/Pu. The expected but not postulated (concave surfaces represent heterogeneity and are excluded) geometries are spheres (mass, volume), infinitely long cylinders, infinite slabs in the transverse dimensions and “infinite seas” for concentrations and moderation ratios. Environmental conditions include room temperature, normal atmospheric pressure and gravity (unspecified). The reference values correspond to optimum moderation under the given system conditions for mass, volume, cylinder diameter and slab thickness. The minimum fissionable element concentration value makes an infinite system critical. The same system gives the maximum moderation atomic ratio value H/U or H/Pu. The moderation ratio is more appropriate for criticality safety control since it contains sufficient information in itself.

## Results

The scope and objectives were developed after the initialisation of the study. The selection of reference systems was modified during the study. Web sites were developed for collection of reference values and this worked quite well. Major problems and delays in the progress of the study included a lack of reported validation for contributed values, to different qualities of the values, to different interests and changed priorities expressed by participants or their sponsors and finally to differences between participant opinions and the defined scope and objectives. A more formal structure for the Expert Group study compared with previous OECD/NEA criticality safety studies was set up by the newly created Working Party on request from OECD/NEA. The short study time (three years) together with the lack of formal management and review procedures contributed to delays and discussions. The Working Party is acting on this experience to avoid similar delays and discussions in the future.

A reference value that is supported by several methods, each based on appropriate validation, should have a smaller uncertainty than most benchmarks. A target uncertainty in $k_{eff}$ of each reference value is a standard deviation of 0.001. It is important to note that the evaluations and the evaluated reference values in this report are for demonstration purposes only. The values are not even preliminary best-estimates. The values will often be close to the true values, but further validation, independent verification, improvement of evaluation methods and discussion are needed.

The results clearly show that bias corrections from a good selection and evaluation of criticality safety benchmarks can reduce the spread of results from direct calculations (raw data). Considering that the bias corrections are based on linear interpolation, while the relations are non-linear, the agreements between different methods are sometimes remarkable. In other cases, the selection or availability of benchmarks for validation is clearly not adequate.

Many discrepancies have been identified. Most of them have been resolved. Errors, sometimes large enough to make “safe” values critical, have been identified in handbooks and methods. The methods used to determine nuclide densities need further verification. The limitations when applied to areas outside the solubility ranges need to be better documented and understood. The specifications for hydrated nitrate reference systems should have covered the concentration range between the solubility limit and the crystal form. Critical values for the reference parameters at crystal density are important.

## Conclusions

Availability of high-quality products such as the modern calculation methods (codes, cross-sections and utilities), validation sources and validation evaluation tools has made the prospect of obtaining a consensus on reference values more feasible than many participants realised when the study started in 1998. The best of the reference values can be converted to benchmarks, after some additional work and confirmation by more evaluators and reviewers.

It is likely that serious errors in methods, new or old, or in the use of the methods can be found. Validation using a limited number of benchmarks, with interpolation between, is not sufficient. Verification of the capabilities of each method, not only at optimum conditions but at all conditions that the method may be applied to, is essential.

The comparison of validated results and the evaluation of discrepancies in contributed reference values have demonstrated that the differences are more often due to inadequate use of methods, inadequate determination of nuclide densities, editorial mistakes, etc. than they are due to cross-section errors. An important reason for this is that the cross-section biases can be corrected for, using appropriate verification against criticality safety benchmarks.

# INTRODUCTION

Nuclear criticality safety during operations, transport and storage of fissionable materials requires reliable information. Elaborate evaluations of credible systems and sophisticated methods to model the neutron transport in those systems are often justified to assure criticality safety, without causing other unacceptable hazards or side-effects. However, validated reference values for simple systems are valuable for many purposes. Critical values for well-specified, water-moderated and water-reflected systems are examples of such reference values.

Previous OECD/NEA studies on nuclear criticality safety demonstrate the importance of validation. These include [107-109] involving spent LWR fuel transport, large arrays and dissolution of fuel. Later OECD/NEA studies on burnup credit are not exceptions, but the lack of benchmarks based on public critical experiments has made validation more difficult.

Correctly determined reference values are physical constants, if all specifications are given. The main purpose of this report is to describe initial efforts to establish reference values. Potential applications of such values include establishment of safety limits, validation of calculation methods, emergency preparedness and response. It is important to realise that the selected limiting reference values are not necessarily limiting under other conditions (reflection, moderation, temperature, etc.).

Several criticality safety handbooks have been published [14-28] to provide data and safety principles for the design, safety evaluation and licensing of operations, transport and storage of fissionable materials. The data often comprise not only critical values, but also subcritical limits and safe values. The values and limits in each handbook must be used with consideration of the limitations of the handbook, whether they are clearly specified or not. Determination of subcritical limits or safe values is outside the scope of the study. Determination of a reference value that gives a specific $k_{eff}$ value such as 0.95 would not be outside the scope of the study. To call it safe or a recommended limit would be. The Expert Group has clearly expressed that it is not an objective to recommend values; the application of the reference values is left to the user.

Subcritical limits and safe values sometimes differ because the safety criteria and definitions differ in different organisations. However, handbook reference values for well-specified and identical systems should be in agreement, within uncertainties caused by the methods (codes, data and validation) applied. This is of specific importance as safe values often are based on reference values.

The study, see also scope and objectives in Appendix A, consists of several steps, each vital for its success. A first step is to select and define the reference systems. A second step is to collect existing and new values for the reference systems. A third step is to use existing or new validation of methods to correct for any remaining biases and to estimate uncertainties. A fourth step is to consider all contributions in an effort to determine a single best-estimate reference value for each system. Based on this information, discrepancies in published handbooks and in other contributed results can be identified and, hopefully, explained. Finally, potential future tasks should be discussed and conclusions need to be drawn.

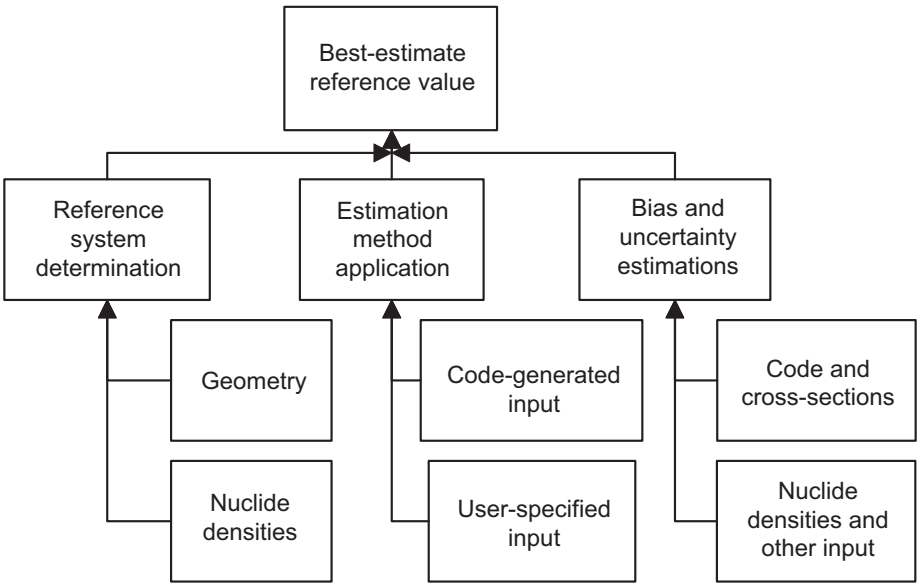
## BEST-ESTIMATE REFERENCE VALUES

The type of reference value covered by this report is a physical constant for a well-defined reference system containing fissile material. Selected reference systems (applications) include water-moderated and water-reflected masses, volumes, cylinders and slabs as well as concentrations and moderations of various materials under specified conditions. Other reference systems consist of benchmark specifications. Each unique reference system has a unique reference value associated with a specific reference parameter. The reference parameters for applications include fissile element mass, volume, cylinder diameter, slab thickness, concentration and moderation. For benchmarks, the most common reference parameter is $k_{eff}$.

The requested reference values refer to mass, geometry or concentration controlled critical systems. The reference parameters for mass and geometry control are minimised with optimum homogeneous and uniform mixtures of the fissile material with water. For concentration control, the systems are expected to be infinite and the fissile element concentration or the moderation ratio keeps the system exactly critical. The specifications for soluble materials were not sufficiently clear. They referred to solutions but the intention was probably to cover a mixture of the material, whether soluble or not, with water. It should have been solution within the solubility range and a mixture of the crystal form and the saturated solution above the solubility limit.

A reference value is determined from three sources: The determination of the system specifications, the application of a suitable estimation method and finally the bias-correction. Each source contributes to uncertainties in the final value. Figure 1 shows a simplified chart with required input preparation, calculations and bias-correction due to various error sources.

**Figure 1. Best-estimate reference values, error sources and validation**



The system specifications may be given explicitly or implicitly. Explicitly means that materials, geometry and all other system data are fixed and given. Implicitly means that some data need to be derived by the contributor, based on some general specifications. An example is the specification of optimum water-moderation. Optimum conditions determined by different evaluators will vary. The conditions are determined both by the optimisation method and by the input data (including nuclide density correlation "laws" and cross-sections). This process introduces biases and uncertainties.

A benchmark contains simplified geometry and material specifications compared with the experimental configuration. A bias correction and an uncertainty are estimated for the benchmark to account for known and unknown deviations between the benchmark and the experiment. The validation process involves additional material and geometry biases and uncertainties due to the actual modelling of the benchmark. In some cases, there are no such additional biases and uncertainties.

Each code or code system has a number of built-in features and options, including defaults that may be changed by the user. The input data can come from various sources. Whether they come directly from the code system itself or are user-supplied, they need to be tested in various combinations. Further, they need to be tested with the code system to be used for determining the reference value of interest. This is often referred to as verification. Overall validation of the method is treated as a separate issue. Validation of each user's application of the method is also important.

A bias-correction is necessary to obtain a best-estimate reference value, which is the major objective of the study. To obtain a bias-correction, it is necessary to have some benchmarks to validate the method (code and data). Appropriate determination of biases and uncertainties can be complicated but is necessary to get credible results. A bias-correction can be positive, negative or zero. Each benchmark has an associated unique reference value.

Even for a benchmark based on a critical experiment, the reference value is tied to the benchmark model of the experiment and not directly to the experiment itself. There may be several benchmark models of the same experiment. The true reference value for a benchmark may not be known accurately. A best-estimate reference value for a benchmark is connected with an uncertainty.

The selection of benchmarks and the evaluation of the results should probably be different for reference value and for safe value determinations. Different weights can be given to each benchmark. Outliers ("odd" results) and complicated systems may be completely left out of the database for reference value determinations. However, all data should be considered in the uncertainty evaluation required to establish safe values. Validation of a method for safety application should be made with typical user input data. Validation for best-estimate purposes should involve more accurate calculations.

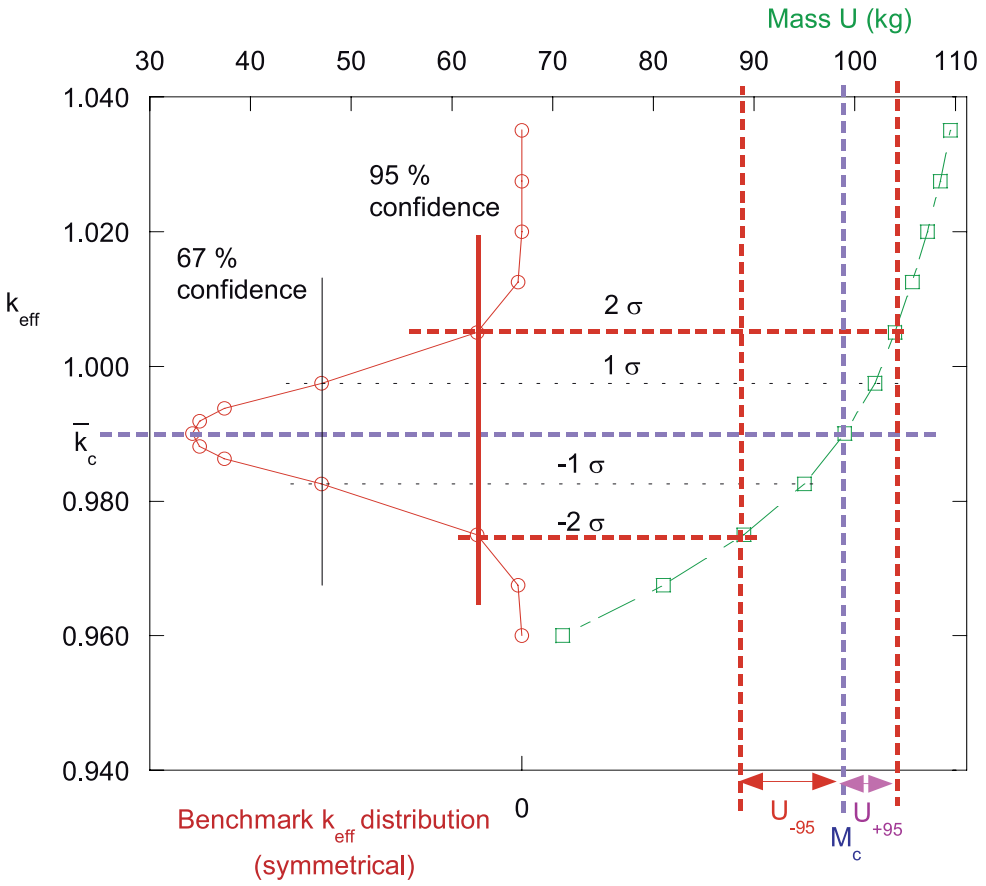
A simplified view of the procedure for determining a reference value (minimum critical mass) is shown in Figure 2. It is based on a compilation of benchmark results on the left side, with the average used as a bias and a standard deviation as a measure of uncertainty. The distribution is assumed to be symmetrical around the mean. On the right, at least three calculations of systems close to the requested reference value (minimum critical mass), are used to generate a curve showing $k_{eff}$ as a function of the actual mass.

The curve is normally curved (!), not a straight line. The bias-corrected estimate of criticality $\overline{k}_c$ is transferred to the right side, giving the best-estimate $M_c$ of the reference value. The uncertainties in the reference value are derived in the same way. The curved line means that the positive and negative reference value uncertainties $U_{-95}$ and $U_{+95}$ are different when the $k_{eff}$ uncertainties are identical. This is seen in Appendix G for the method EMS-S4X-238 (original EMS contribution). If $k_{eff}$ complies with a

normal distribution, the reference value will not. The reverse is also true; if a reference parameter complies with a normal distribution, $k_{eff}$ will not.

It is easy to see in Figure 2 that a normal (Gaussian) distribution of $k_{eff}$ leads to non-symmetric levels of confidence of the reference value. The figure indicates an uncertainty corresponding to the lower limit of the 95% level of confidence almost twice as large as the upper limit uncertainty. It is not a question of $\pm \sigma_m$. The best-estimate critical mass $M_c$ is 99 kg, the upper limit ($M_c + U_{+95}$) is 104 kg and the lower limit ($M_c - U_{-95}$) is 89 kg. Other statistical background information is given in Appendix B, Appendix M and [92].

**Figure 2. Estimation of minimum critical mass and its uncertainties**



## FISSIONABLE REFERENCE SYSTEMS

All the selected fissionable materials are also fissile. The large number of systems selected during the first year of the study was probably more motivated by practical safety interests than by physics and numerical considerations.

The fissionable materials include only two actinide elements, uranium and plutonium, and they are not mixed. The uranium isotopes are $^{235}U$ and $^{238}U$ and the mass percentages of $^{235}U$ in the total uranium are 100, 20, 5, 4 and 3. The plutonium isotopes are $^{239}Pu$, $^{240}Pu$, $^{241}Pu$ and $^{242}Pu$ and the isotope distributions, with each isotope mass percentage of total plutonium given in that order[1], are 100/0/0/0, 95/5/0/0, 80/10/10/0, 90/10/0/0, 80/15/5/0 and 71/17/11/1. The compositions are sorted according to total fissile nuclide ($^{239}Pu$ and $^{241}Pu$, with $^{241}Pu$ weighted higher for equal sums) fractions.

The four chemical structures are uranium dioxide ($UO_2$), uranyl nitrate hexahydrate (UNH or $UO_2(NO_3)_2+6H_2O$), plutonium dioxide ($PuO_2$) and plutonium nitrate pentahydrate (PuNH or $Pu(NO_3)_4+5H_2O$). The plutonium valence is thus four. The valence number three for plutonium and the corresponding composition $Pu(NO_3)_3+5H_2O$ is possible in real applications.

The fissile materials and geometries are not specified completely. Water in optimum fractions has to be added to the small oxide particles and hydrated nitrate crystals. The resulting mixtures and solutions are considered homogeneous and uniform (the same concentrations everywhere). Homogeneous here means that the fissionable material surface is not concave anywhere (no point on the surface can be "seen" from any other non-neighbour point on that surface).

Theoretical densities of both oxides and hydrated nitrates must be considered. The issue of realism in the dioxide/water mixtures and in the solution/crystal densities is left to the evaluator but needs to be considered. Mixtures of saturated solutions with hydrated nitrate crystals may be realistic under certain conditions. Mixtures of dioxide powder with water at optimum conditions are not always stable, the dioxide powder will settle to the bottom of the system. The evaluator should note if the conditions are not credible; e.g. the solution being above the saturation level or even above the crystal density.

The credibility issue must not hide the purpose of the study: to determine physical constants. There must be only one correct value for each reference system. For solutions, the solubility limits and the crystal densities can be considered as physical (or chemical) constants. The range in between was not properly specified at the beginning of the study. A reasonable approach is to assume a mixture of the saturated solution and the crystal (precipitation). IRSN uses this assumption in its extended isopiestic method [39-41, 60, 89].

The systems are either fully water-reflected or infinite.

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[1] Trailing zeros are sometimes skipped, e.g. 100 instead of 100/0/0/0, 90/10 rather than 90/10/0/0, etc.

## SOURCES FOR REFERENCE VALUES

The best-estimate reference values (physical constants), the major purpose of the study, are obtained by evaluation of validated results from different sources. Some are published in handbooks and in other literature while others have been determined by participants to support the study.

The reported results are not always best-estimate values. They may have been calculated using the best available or best validated methods at a certain time but without bias corrections. They may be used safely if the combinations of biases and uncertainties are small, compared with the safety margins added before application.

Calculation results without bias corrections are separated from those with corrections. New or revised bias-corrections can be applied later, without recalculations.

Each source of reference values is listed in Table 1. More detailed descriptions are supplied in Appendix C. There may be additional methods used for odd cases. The specification of each method may vary slightly in the text, tables and figures but the format should be reasonably consistent.

There may be other handbooks and published results that can be used to determine a single best-estimate value for each reference system.

**Table 1. Sources for critical values**

| Source id. | Reference | Handbook or New calculation | Method (code+data) | Bias correction |
|---|---|---|---|---|
| ARH-600 | [14] | Handbook | | |
| DIN | [15]-[18] | Standards | | |
| EMS-S1K-27 | This report | New calculations | SCALE 1, K5[1]+ 27 lib | |
| EMS-S4X-238 | [29] | New calculations | SCALE 4, XSD[2]+238 lib | Yes, rough[3] |
| EMS-M5-E50 | This report | New calculations | MCNP5+ENDF/B 5.0 | Yes |
| EMS-M5-E5F | This report | New calculations | MCNP5+ENDF/B 5.F[4] | Yes |
| EMS-M5-E62 | This report | New calculations | MCNP5+ENDF/B 6.2 | Yes |
| EMS-M5-E66 | This report | New calculations | MCNP5+ENDF/B 6.6 | Yes |
| EMS-M5-E68 | This report | New calculations | MCNP5+ENDF/B 6.8 | Yes |
| EMS-M5-E7P | This report | New calculations | MCNP5+ENDF/B 7P | Yes |
| EMS-M5-F22 | This report | New calculations | MCNP5+JENDL 3.2 | Yes |
| EMS-M5-F30 | This report | New calculations | MCNP5+ JENDL 3.3 | Yes |
| EMS-M5-J32 | This report | New calculations | MCNP5+JEF 2.2 | Yes |
| EMS-M5-J33 | This report | New calculations | MCNP5+JEFF 3.0 | Yes |
| EMS-S5X-238 | This report | New calculations | SCALE 5, XSD[2]+ 238 lib | Yes |
| EMS-S5X-27 | This report | New calculations | SCALE 5, XSD[2]+ 27 lib | Yes |
| EMS-S5X-44 | This report | New calculations | SCALE 5, XSD[2]+ 44 lib | Yes |
| EMS-S5K-238 | This report | New calculations | SCALE 5, K5a[2]+ 238 lib | Yes |
| EMS-S5K-27 | This report | New calculations | SCALE 5, K5a[2]+ 27 lib | Yes |
| EMS-S5K-44 | This report | New calculations | SCALE 5, K5a[2]+ 44 lib | Yes |
| GRS-HzK-98 | [19] | Handbook | | |
| GRS-M4-E50 | [31] | New calculations | MCNP – E5 Lib | |
| GRS-S4X-44 | [31] | New calculations | SCALE – 44 Lib | |
| IPPE-84 | [20] | Handbook | KRAB-1+ABBN-78 | |
| IPPE-ABBN93 | [35] New | New calculations | XSD or K5A+ABBN93a | Yes |
| IRSN-CrV0-20 | [39]-[41] | New calculations | CRISTAL V0 | |
| IRSN-CrV1-172 | [43] | New calculations | CRISTAL V1 | |
| IRSN-DTF-78 | [21] | Handbook | DTF-IV, literature? | |
| IRSN-DTF-96 | SEC/DI/96.16 | Internal report | DTF-IV, literature? | |
| JAERI-H-88 | [22] | Handbook (transl) | JACS | Yes, rough[3] |
| JAERI-H-99 | [23], [24] | Handbook (transl) | JACS | Yes, rough[3] |
| NUPEC | [51] | New calculations | SCALE 44 Lib | |
| ORNL-S4X-238 | [52] | New calculations | SCALE 238 Lib | |
| Serco-Mk8-F22 | [55], [56] | New calculations | MONK 8A, -B, JEF 2.2 | Yes[5] |

[1] SCALE 1 with KENOV (not Va), Modified 1985 for IBM PC AT (Intel 80286) with 640 kb RAM.

[2] XSD stands for XSDRNPM while K5a stands for KENOVa.

[3] EMS-S4X-238 and JAERI validations are not focused on the current applications, based on "old" validation.

[4] As E50 except that the .55c set is used for $^{239}$Pu. "F" stands for Final.

[5] SERCO validation and to some extent all EMS validations are also quite rough, not being very focused.

## EVALUATION OF BEST-ESTIMATE VALUES AND UNCERTAINTIES

During the final evaluation, it was decided to add more methods. MCNP5 and a wide selection of continuous energy cross-sections (ENDF/B releases 5.0, 6.2, 6.6 and 6.8, JEF 2.2 as well as JENDL3.2 and 3.3) were used (even more were available but not used). Release 1.30 of MCNP5 was obtained late November 2004 together with preliminary ENDF/B-VII cross-sections. JEFF 3.0 cross-sections were contributed in December 2004 by OECD/NEA (Dr. Yolanda Rugama).

SCALE 5 was released recently, unfortunately without new cross-sections. Revised calculations with the 238-group library as well as new calculations with the 27- and 44-group libraries were carried out. Reference values were calculated using both KENOVa and XSDRNPM/S for all applications and with the three mentioned cross-section libraries. This simplifies verification of XSDRNPM results.

IPPE originally had contributed results from a 1984 handbook. During the final evaluation, IPPE added results using a more recent method based on XSDRNPM and ABBN93a cross-sections.

The contributions from the participants are summarized in Appendix G. The methods used by each participant to calculate critical values as well as validation and, in some cases, bias corrections and uncertainties are described in Appendix C, for EMS and IPPE also in Appendix I. The validation methods vary between the participants, as does the quality of the bias corrections.

Appendix D contains calculated sensitivities for changes in $k_{eff}$ ($\Delta k$) due to a small change in each of the selected parameters mass, volume, cylinder diameter, slab thickness and concentration. They can be used to obtain the $\Delta k$ values corresponding to different calculated or best-estimate critical values. The small $k_{eff}$ changes used to derive the sensitivities are usually less than 0.005, but there is no consistency. The sensitivities are not linear. There is no single value that could be used to get accurate corrections for the different biases found for different methods. An appropriately determined curve would be the best way to handle this problem.

Reported results that are not corrected for biases can be very useful if they are supported by separate validation reports or conclusions. Calculation results from different contributors based on identical or almost identical methods are also valuable. They reduce the potential for human error and indicate the sensitivity of the method to users.

Often, the variations of the calculation results can be attributed mainly to the basic evaluated nuclear cross section library. Such observations simplify comparisons of calculated values, e.g. during independent verification of safety evaluations, and may support improvements of the basic cross sections.

An effort has been made during the evaluation of the contributed values to select suitable benchmarks for verification (Appendix E). Typical criteria are simple systems, preferably with water moderation and water reflection, and low uncertainties in the benchmarks. Later, in Appendix H, the similarities between applications and benchmarks are evaluated using more sophisticated methods (SCALE 5 TSUNAMI-IP). EALF values for all applications are shown in Table I1.

The selected benchmarks were calculated with all the EMS methods as well as with the recent IPPE-ABBN93 method. The results, as well as some preliminary trends, are given in Appendix F.

IPPE benchmark results were obtained using the same cross-sections as in the applications. XSDRNPM has been reported to give essentially the same results as the Monte Carlo code KENOVa when the same cross-sections and appropriate convergence, mesh and angular quadrature input are applied.

SCALE 5 and the new TSUNAMI sequences were used to calculate the similarity indices $c_k$, $E_{sum}$ and G related to the applications and the benchmarks. In addition, an index $R_{en}$ was defined to display EALF ratios for benchmarks related to applications. The results are summarised in Appendix H. Additional $R_{en}$ values, unrelated to benchmarks ("mathematical"), were inserted for information. The lack of benchmark EALF values near the application EALF is sometimes very obvious. This is easy to recognize when $R_{en}$ curves with only benchmark points are compared with $R_{en}$ curves with additional "mathematical" points. Comparisons of the TSUNAMI-IP indices to $R_{en}$ show that EALF is indeed a useful trending parameter for these systems.

The benchmark uncertainties and the TSUNAMI indices were used to select sub-sets of benchmarks for verification of different applications. Appendix I contains bias determinations for the EMS and IPPE methods applied to the different applications.

Serco has also submitted bias-corrected results based on MONK calculations and large sets of benchmarks. The JAERI handbook results are validated, but the validation range appears to be too wide to be reliable for reference value determination and there are not so many reference values. The benchmarks supporting the JAERI handbook are also quite old, lacking the bias and uncertainty information available in the ICSBEP Handbook. The "raw" data were not directly available (though the biases are published in the JAERI Handbook). A decision was made to base the best-estimate values on averages of bias-corrected Serco MONK, IPPE ABBN93, EMS-SCALE5+238, EMS-MCNP5+ENDF/B-7P (or -68), EMS-MCNP5+JEFF3.0 and EMS-MCNP5+JENDL-3.3 results.

These best-estimate reference values are intended for demonstration only. They are dominated by EMS methods. The associated EMS evaluation and validation results are correlated since they are based on identical geometry and nuclide density input data. However, the demonstration is considered valuable since any detected biases can be corrected easily for all the methods. It is apparent from some comparisons of bias-corrected reference values that the bias-correction has not worked out very well. However, often the opposite is true; the bias-corrections have been successful in reducing the spread of results, indicating some quality.

It is repeated that total bias-corrections and uncertainties need to cover not only cross-section and code-related biases and uncertainties but also those from nuclide density determinations. Very late during the evaluation (March 2005) a comparison of nuclide density methods was carried out with very interesting results for solutions (Appendix K). Some of the previously selected base methods for best-estimate determination now had to be completely removed; the density methods were not adequate. The IRSN extended isopiestic method turned out to be the only credible source for some values. The IPPE ABBN93 method is credible near the crystal density.

The best-estimates are included in Tables 2 to 5. The precision corresponds to a $k_{eff}$ precision between 0.0001 and 0.001. The uncertainties are very subjective and no effort has been made to separate upper and lower limits of confidence. Even so, at this time, this compilation of reference values may be the best source available anywhere.

**Table 2. Demonstration reference values for $UO_2$**

| Fissile material | Parameter | Reference value | Expanded standard uncertainty (95)[1] | Comments |
|---|---|---|---|---|
| $U(100)O_2$ | Mass (kg U) | 0.798 | 0.010 | |
| | Volume (litre) | 4.35[2,3] | 0.10 | |
| | Cylinder diam. (cm) | 12.47[2] | 0.06 | |
| | Slab thickness (cm) | 3.45[2] | 0.10 | |
| | Concentr. (g U/l) | 12.18 | 0.20 | |
| | Moderation H/U | 2137 | 34 | |
| $U(20)O_2$ | Mass (kg U) | 5.22 | 0.10 | |
| | Volume (litre) | 10.78 | 0.40 | |
| | Cylinder diam. (cm) | 17.97 | 0.20 | |
| | Slab thickness (cm) | 7.24 | 0.30 | |
| | Concentr. (g U/l) | 64.0 | 0.7 | |
| | Moderation H/U | 409.0 | 5.0 | |
| $U(5)O_2$ | Mass (kg U) | 37.0 | 1.0 | |
| | Volume (litre) | 27.78 | 0.70 | |
| | Cylinder diam. (cm) | 25.65 | 0.30 | |
| | Slab thickness (cm) | 12.17 | 0.30 | |
| | Concentr. (g U/l) | 285.7 | 2.5 | |
| | Moderation H/U | 89.6 | 0.7 | |
| $U(4)O_2$ | Mass (kg U) | 55.4 | 1.5 | |
| | Volume (litre) | 35.7 | 0.9 | |
| | Cylinder diam. (cm) | 28.25 | 0.50 | |
| | Slab thickness (cm) | 13.77 | 0.20 | |
| | Concentr. (g U/l) | 370.6 | 3.0 | |
| | Moderation H/U | 68.7 | 0.6 | |
| $U(3)O_2$ | Mass (kg U) | 99.6 | 1.8 | |
| | Volume (litre) | 53.5 | 1.0 | |
| | Cylinder diam. (cm) | 32.66 | 0.40 | |
| | Slab thickness (cm) | 16.61 | 0.21 | |
| | Concentr. (g U/l) | 522 | 5 | |
| | Moderation H/U | 47.8 | 0.5 | |

[1] Subjective and simplified. Upper and lower limits could be quite different.

[2] A correction has been made since the theoretical density for $U(100)O_2$ is 10.84 and not 10.96 g/cm$^3$.

[3] A small negative bias correction, -0.03 litre, was made to this value, since the optimum geometry is not a sphere for this material and reflection. Substantially larger biases may be observed if the same spherical assumption is made for some under-moderated systems not included in this study [103].

**Table 3. Demonstration reference values for UNH**

| Fissile material | Parameter | Reference value | Expanded standard uncertainty (95)[1] | Comments |
|---|---|---|---|---|
| U(100)NH | Mass (kg U) | 0.826 | 0.012 | |
| | Volume (litre) | 6.71 | 0.40 | |
| | Cylinder diam. (cm) | 14.95 | 0.50 | |
| | Slab thickness (cm) | 5.48 | 0.35 | |
| | Concentr. (g U/l) | 12.23 | 0.50 | |
| | Moderation H/U | 2109 | 83 | |
| U(20)NH | Mass (kg U) | 6.13 | 0.10 | |
| | Volume (litre) | 16.30 | 1.20 | |
| | Cylinder diam. (cm) | 21.00 | 0.40 | |
| | Slab thickness (cm) | 9.29 | 0.25 | |
| | Concentr. (g U/l) | 64.8 | 1.0 | |
| | Moderation H/U | 397.1 | 6.2 | |
| U(5)NH | Mass (kg U) | 75.4 | 3.0 | |
| | Volume (litre) | 80.7 | 8.0 | |
| | Cylinder diam. (cm) | 37.9 | 1.6 | |
| | Slab thickness (cm) | 20.04 | 0.70 | |
| | Concentr. (g U/l) | 312.5 | 5.3 | |
| | Moderation H/U | 76.2 | 1.4 | |
| U(4)NH | Mass (kg U) | 144 | 7 | |
| | Volume (litre) | 136 | 15 | |
| | Cylinder diam. (cm) | 45.4 | 1.7 | |
| | Slab thickness (cm) | 25.05 | 0.85 | |
| | Concentr. (g U/l) | 417 | 10 | |
| | Moderation H/U | 55.1 | 1.5 | |
| U(3)NH | Mass (kg U) | 469 | 40 | |
| | Volume (litre) | 370 | 50 | |
| | Cylinder diam. (cm) | 64.8 | 3.5 | |
| | Slab thickness (cm) | 37.5 | 2.2 | |
| | Concentr. (g U/l) | 629 | 7 | |
| | Moderation H/U | 33.6 | 1.3 | |

[1] Subjective and simplified. Upper and lower limits could be quite different.

**Table 4. Demonstration reference values for $PuO_2$**

| Fissile material | Parameter | Reference value | Expanded standard uncertainty (95)[1] | Comments |
|---|---|---|---|---|
| $Pu(100/0/0/0)O_2$ | Mass (kg Pu) | 0.510 | 0.018 | |
| | Volume (litre) | 1.151 | 0.033 | |
| | Cylinder diam. (cm) | 7.68 | 0.10 | |
| | Slab thickness (cm) | 1.721 | 0.060 | |
| | Concentr. (g Pu/l) | 7.28 | 0.30 | |
| | Moderation H/Pu | 3636 | 190 | |
| $Pu(95/5/0/0)O_2$ | Mass (kg Pu) | 0.621 | 0.018 | |
| | Volume (litre) | 1.236 | 0.040 | |
| | Cylinder diam. (cm) | 7.95 | 0.11 | |
| | Slab thickness (cm) | 1.934 | 0.070 | |
| | Concentr. (g Pu/l) | 7.88 | 0.09 | |
| | Moderation H/Pu | 3360 | 123 | |
| $Pu(80/10/10/0)O_2$ | Mass (kg Pu) | 0.686 | 0.036 | |
| | Volume (litre) | 1.288[2] | 0.042 | |
| | Cylinder diam. (cm) | 8.04[2] | 0.12 | |
| | Slab thickness (cm) | 1.912[2] | 0.070 | |
| | Concentr. (g Pu/l) | 8.16 | 0.09 | |
| | Moderation H/Pu | 3250 | 115 | |
| $Pu(90/10/0/0)O_2$ | Mass (kg Pu) | 0.754 | 0.027 | |
| | Volume (litre) | 1.307 | 0.040 | |
| | Cylinder diam. (cm) | 8.15 | 0.10 | |
| | Slab thickness (cm) | 2.066 | 0.025 | |
| | Concentr. (g Pu/l) | 8.56 | 0.25 | |
| | Moderation H/Pu | 3094 | 88 | |
| $Pu(80/15/5/0)O_2$ | Mass (kg Pu) | 0.874 | 0.042 | |
| | Volume (litre) | 1.367[2] | 0.042 | |
| | Cylinder diam. (cm) | 8.27[2] | 0.12 | |
| | Slab thickness (cm) | 2.096[2] | 0.090 | |
| | Concentr. (g Pu/l) | 9.09 | 0.25 | |
| | Moderation H/Pu | 2914 | 78 | |
| $Pu(71/17/11/1)O_2$ | Mass (kg Pu) | 0.907 | 0.050 | |
| | Volume (litre) | 1.413[2] | 0.054 | |
| | Cylinder diam. (cm) | 8.37[2] | 0.13 | |
| | Slab thickness (cm) | 2.104[2] | 0.080 | |
| | Concentr. (g Pu/l) | 9.28 | 0.35 | |
| | Moderation H/Pu | 2859 | 104 | |

[1] Subjective and simplified. Upper and lower limits could be quite different.

[2] Includes a correction. The theoretical density for $PuO_2$ with this isotope distribution is not 11.46 g/cm .

**Table 5. Demonstration reference values for PuNH**

| Fissile material | Parameter | Reference value | Expanded standard uncertainty (95)[1] | Comments |
|---|---|---|---|---|
| Pu(100/0/0/0)NH | Mass (kg Pu) | 0.524 | 0.020 | |
| | Volume (litre) | 7.36 | 0.50 | |
| | Cylinder diam. (cm) | 15.56 | 0.40 | |
| | Slab thickness (cm) | 5.67 | 0.30 | |
| | Concentr. (g Pu/l) | 7.33 | 0.20 | |
| | Moderation H/Pu | 3598 | 96 | |
| Pu(95/5/0/0)NH | Mass (kg Pu) | 0.639 | 0.030 | |
| | Volume (litre) | 10.78 | 0.50 | |
| | Cylinder diam. (cm) | 17.94 | 0.40 | |
| | Slab thickness (cm) | 7.18 | 0.30 | |
| | Concentr. (g Pu/l) | 7.93 | 0.20 | |
| | Moderation H/Pu | 3325 | 82 | |
| Pu(80/10/10/0)NH | Mass (kg Pu) | 0.707 | 0.040 | |
| | Volume (litre) | 12.18 | 0.50 | |
| | Cylinder diam. (cm) | 18.77 | 0.20 | |
| | Slab thickness (cm) | 7.61 | 0.30 | |
| | Concentr. (g Pu/l) | 8.19 | 0.20 | |
| | Moderation H/Pu | 3221 | 97 | |
| Pu(90/10/0/0)NH | Mass (kg Pu) | 0.777 | 0.040 | |
| | Volume (litre) | 13.42 | 0.50 | |
| | Cylinder diam. (cm) | 19.48 | 0.40 | |
| | Slab thickness (cm) | 8.11 | 0.30 | |
| | Concentr. (g Pu/l) | 8.59 | 0.20 | |
| | Moderation H/Pu | 3068 | 70 | |
| Pu(80/15/5/0)NH | Mass (kg Pu) | 0.905 | 0.040 | |
| | Volume (litre) | 15.42 | 0.50 | |
| | Cylinder diam. (cm) | 20.54 | 0.40 | |
| | Slab thickness (cm) | 8.75 | 0.30 | |
| | Concentr. (g Pu/l) | 9.15 | 0.20 | |
| | Moderation H/Pu | 2881 | 62 | |
| Pu(71/17/11/1)NH | Mass (kg Pu) | 0.948 | 0.040 | |
| | Volume (litre) | 15.83 | 0.50 | |
| | Cylinder diam. (cm) | 20.72 | 0.40 | |
| | Slab thickness (cm) | 8.89 | 0.30 | |
| | Concentr. (g Pu/l) | 9.31 | 0.25 | |
| | Moderation H/Pu | 2833 | 74 | |

[1] Subjective and simplified. Upper and lower limits could be quite different.

## COMPARISON OF CONTRIBUTED VALUES WITH BEST-ESTIMATE VALUES

The data in criticality safety handbooks, standards and guides are derived not only to support safe systems but also to allow efficient and fast evaluations. A non-conservative (non-pessimistic) value could be a safety problem if the bias and uncertainty are not taken into account. A conservative value could lead to inefficient operations and designs. A conservative value applied in one country could also lead to problems in transport licensing (multilateral approval is required). It is valuable for a reviewer to understand the causes of differences in the calculation results for the same system.

In an emergency situation, correct information may be more valuable than ever. Non-conservative values without known biases could cause a criticality accident due to bad decisions. Conservative values could lead to unnecessary worries, alarms, evacuations, stopped operations, bad publicity, etc. The JCO criticality accident response in Japan 1999 shows that, using a realistic system model and a validated calculation system, JAERI could be confident that the criticality excursion would end by removing the cooling water around the accident vessel, Conservatism, such as spherical geometry or excessive allowance for calculation uncertainty, could have prevented such a decision.

This study shows that deterministic codes need to be better validated. Some critical experiment specifications can be used to create benchmarks for deterministic codes but it is better to use the validated Monte Carlo results to create simple benchmarks, like the reference values in this report. The total uncertainty can be made smaller than for most experimental benchmarks.

Conclusions from comparisons between handbook and calculated results with appropriately determined best-estimate values for a limited set of fissile systems may be extended to more complicated systems containing similar fissile materials.

The reference values and uncertainties reported in the previous chapter are for demonstration only. Many values and uncertainties will be good, others not so good. They are based on subjective selections and evaluations of benchmarks, correlated inputs for benchmarks and reference system calculations, linear interpolation and extrapolation of non-linear relations, work carried out under time-pressure, insufficient time for review, etc.

The Figures 3 to 15 show total biases for all methods based on the best-estimate reference values in the previous section. The points are connected with lines to identify the method and not to show any trend between different reference systems. There are three charts for each material type. The first covers all contributed values, the second covers final evaluation values while the third is limited to "modern" and validated methods. The symbol for each method unfortunately changes between charts.

Each bias is calculated as the difference between the (bias-corrected when available) value in Appendix G and the value in Tables 2 to 5. The sum of the biases for the "major 6" bias-corrected values (cross-sections only!) used to determine the first best-estimate values is not always close to zero. The reason is that additional bias corrections due to density issues have been added to some reference values (Appendix L). For $U(100)O_2$ volume a bias correction of -0.03 litre was made since the optimum geometry is not a sphere.

**Figure 3. $UO_2$ reference values – Estimated total biases for contributed values**

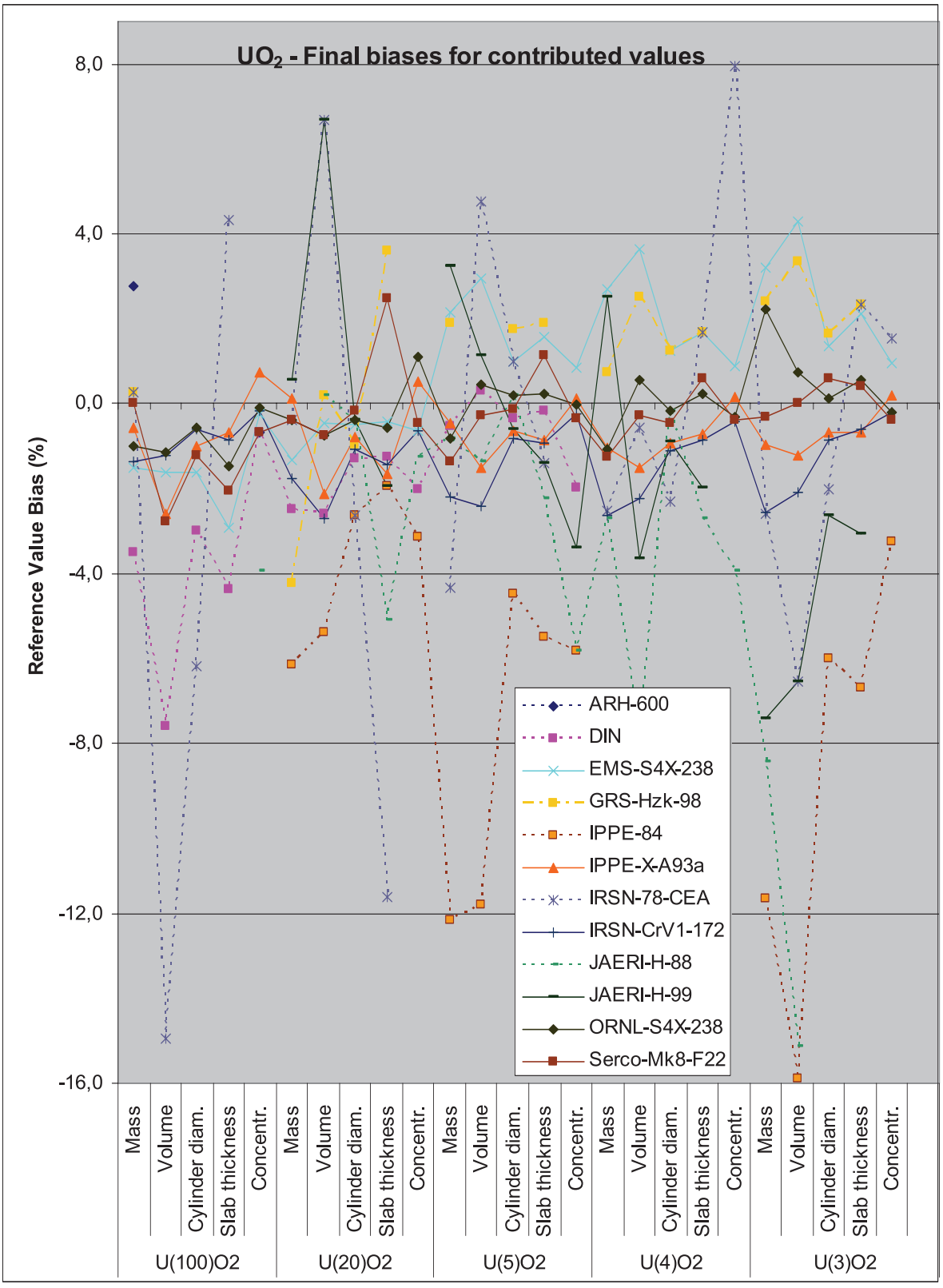


**Figure 4. $UO_2$ reference values – Estimated total biases for final evaluation values**

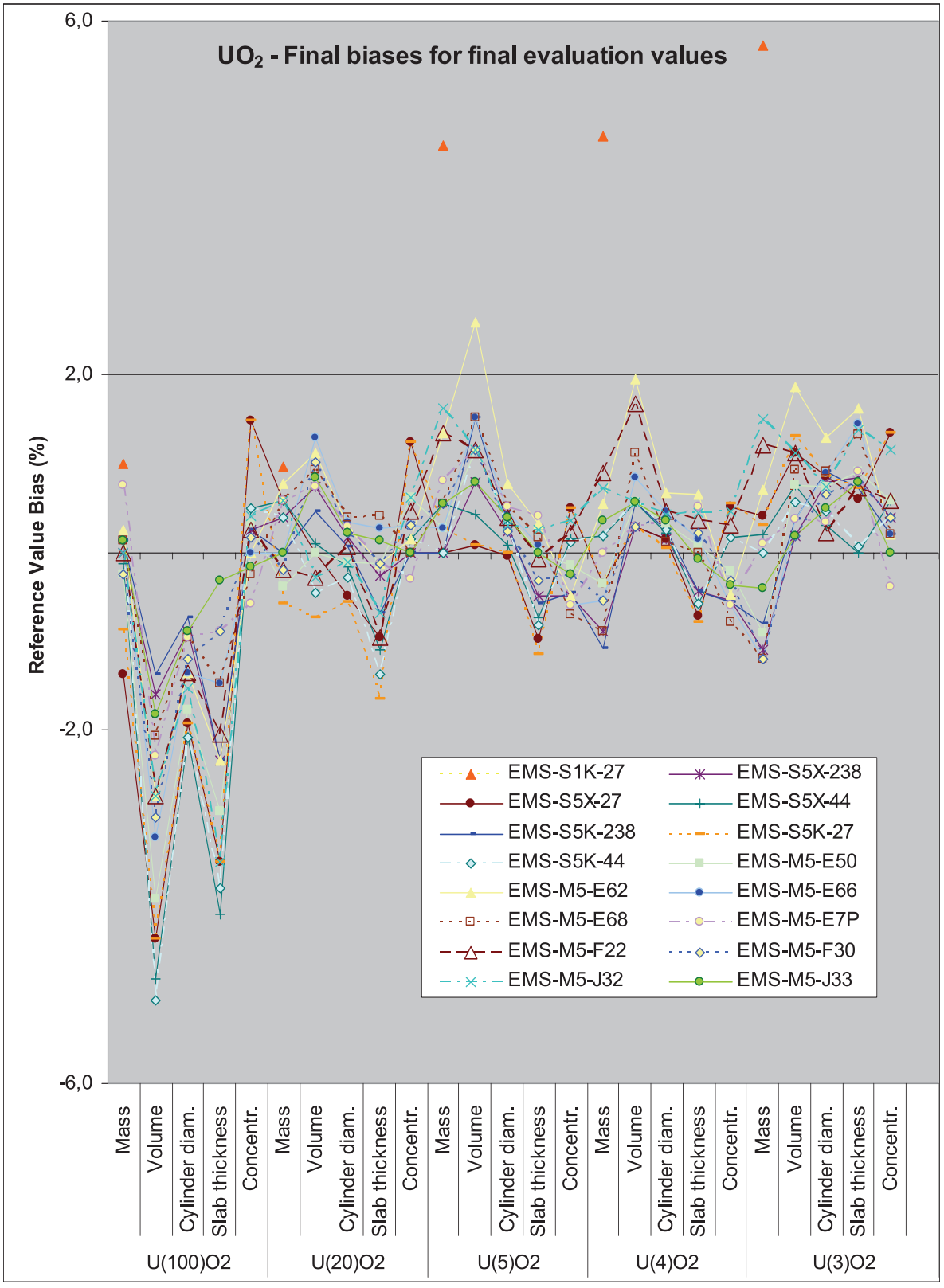


**Figure 5. $UO_2$ reference values – Estimated total biases for "modern" methods**

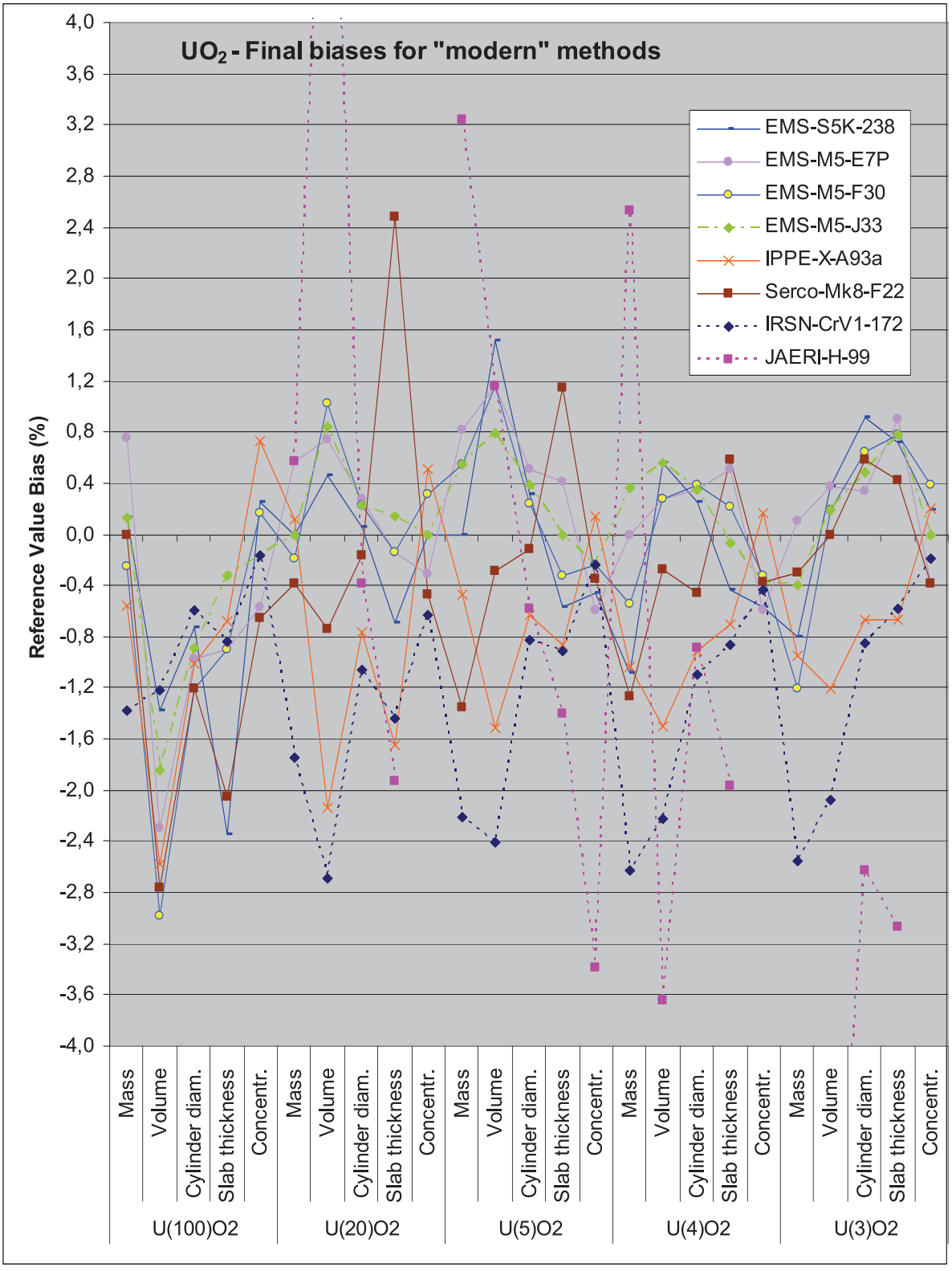


**Figure 6. UNH reference values – Estimated total biases for contributed values**

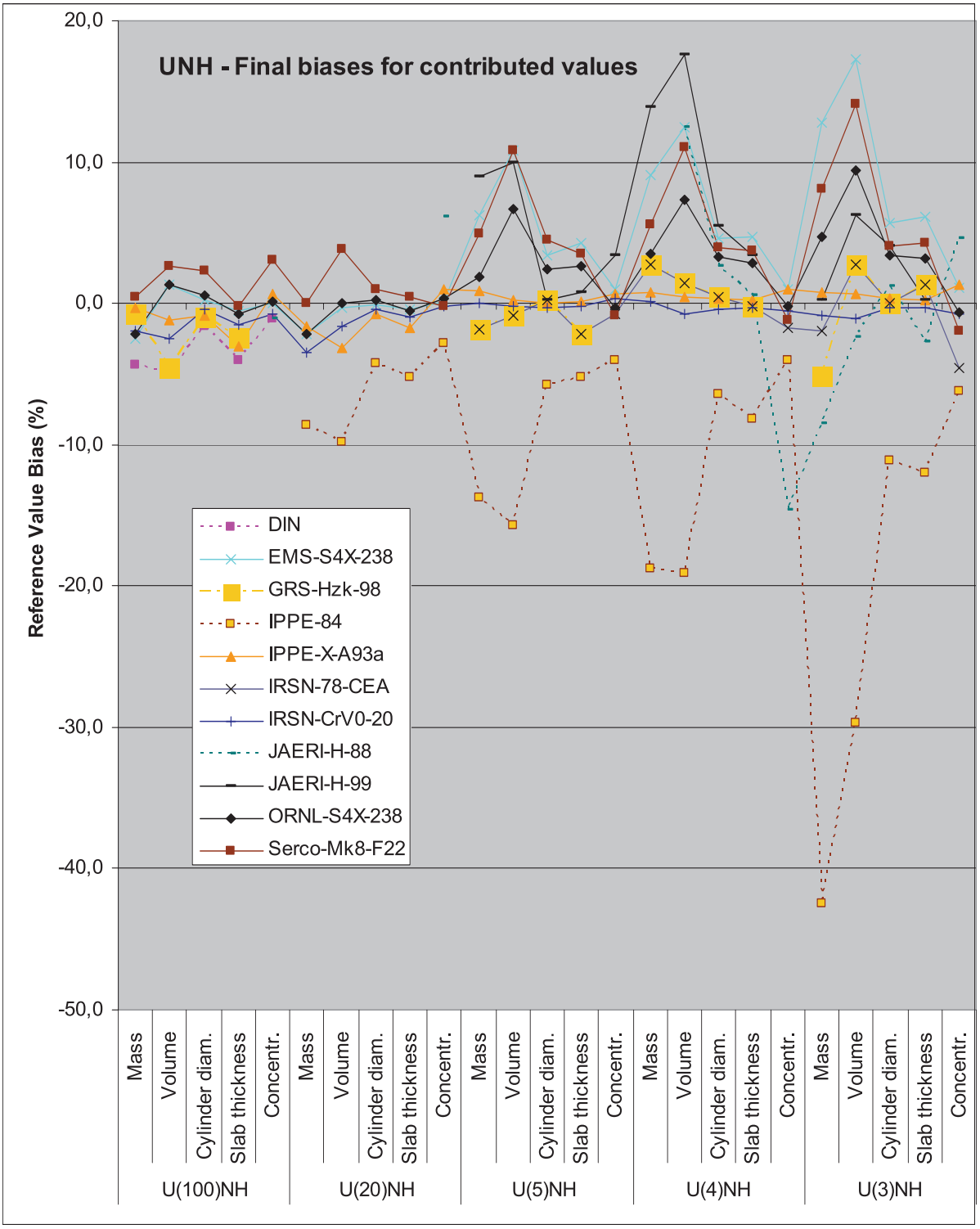


**Figure 7. UNH reference values – Estimated total biases for final evaluation values**

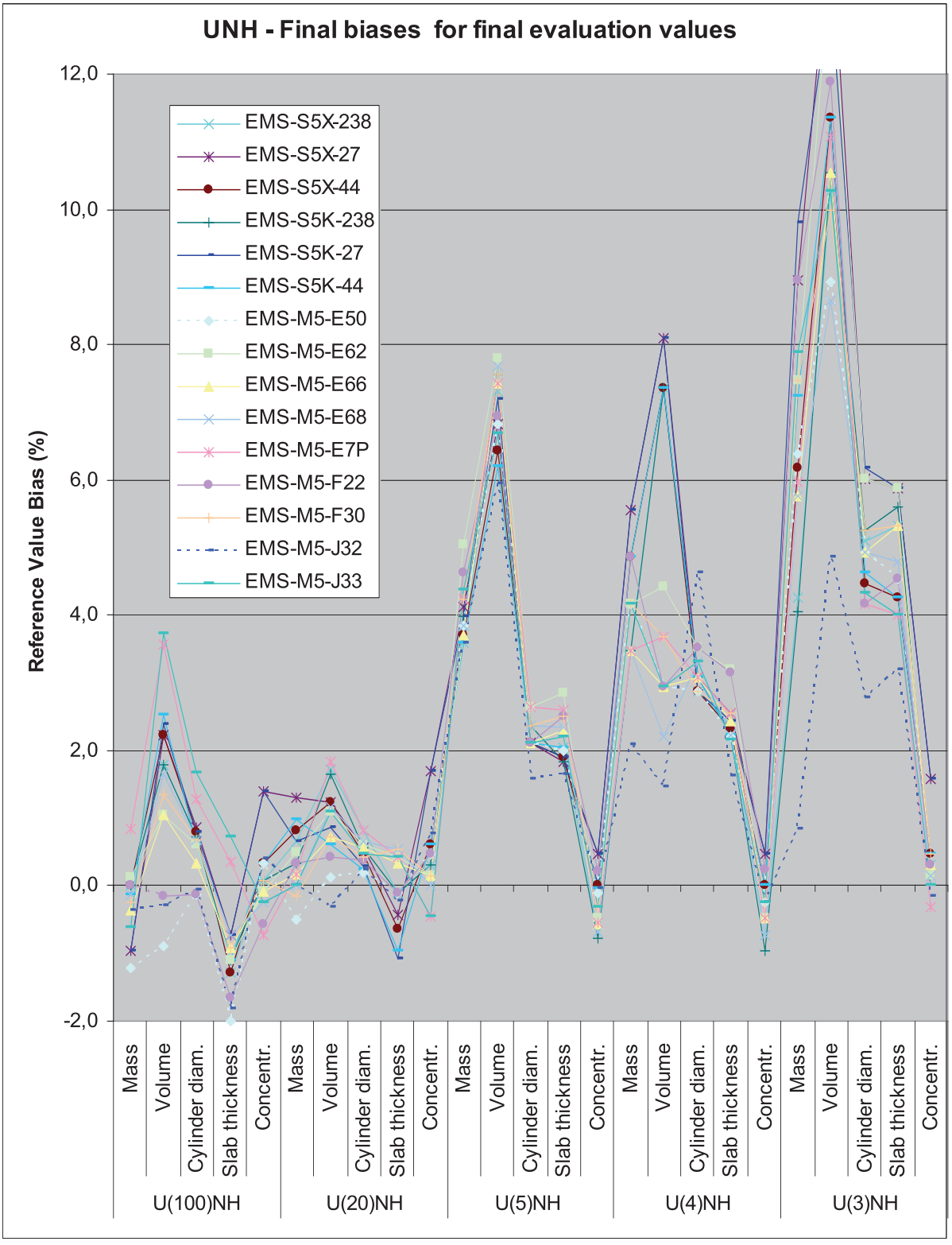


**Figure 8. UNH reference values – Estimated total biases for "modern" methods**

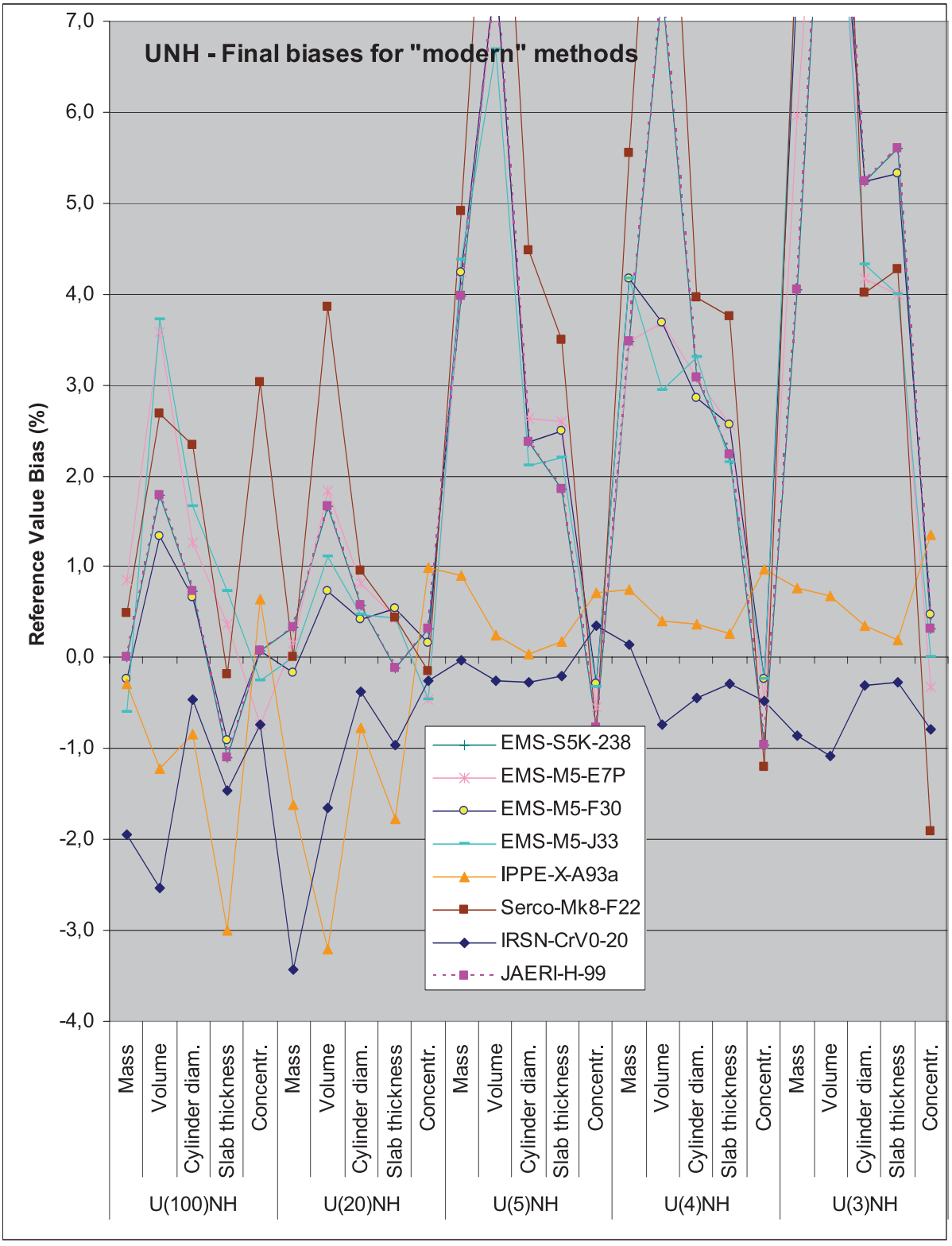


**Figure 9. $PuO_2$ reference values – Estimated total biases for contributed values**

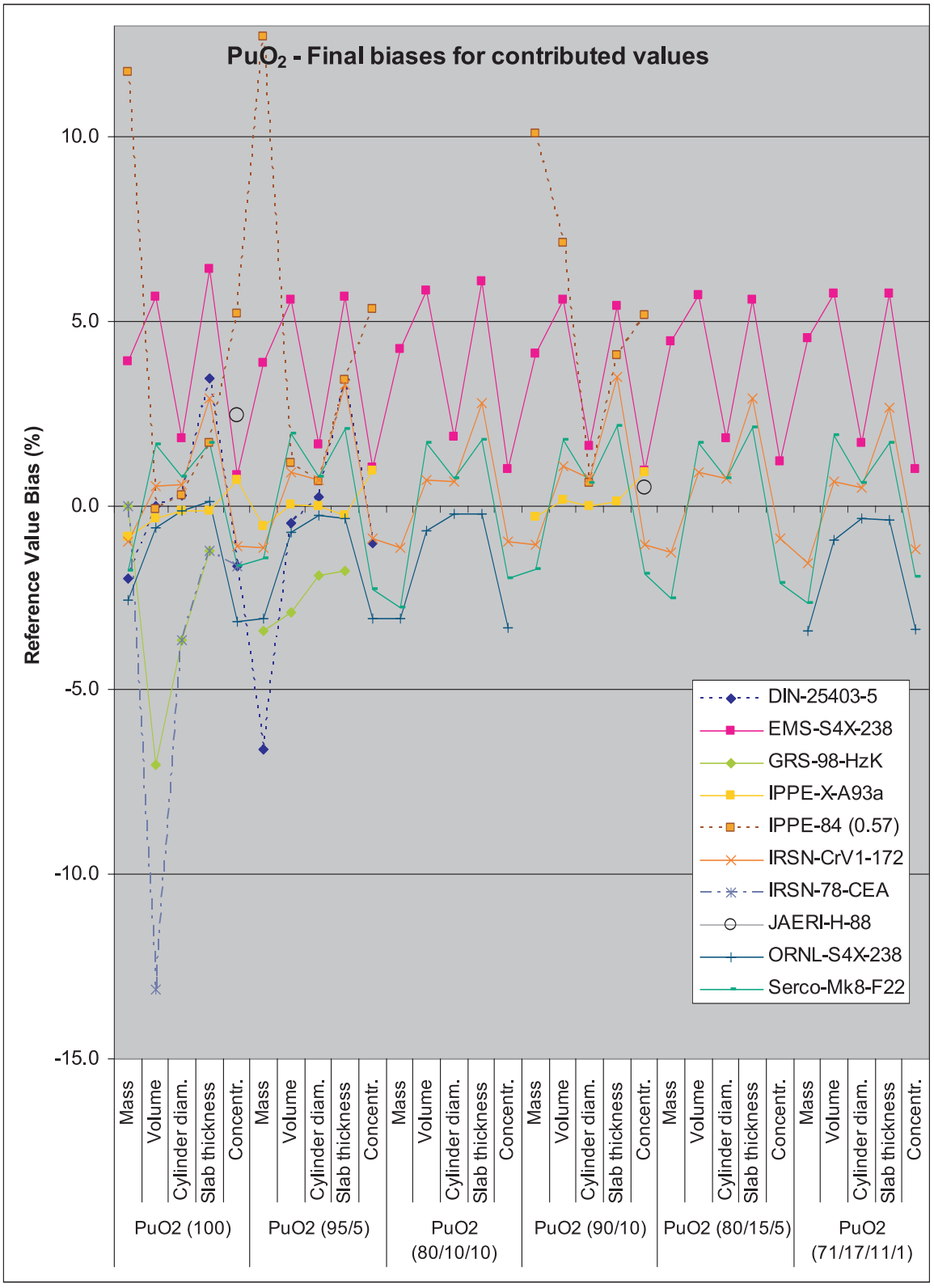


**Figure 10. $PuO_2$ reference values – Estimated total biases for final evaluation values**

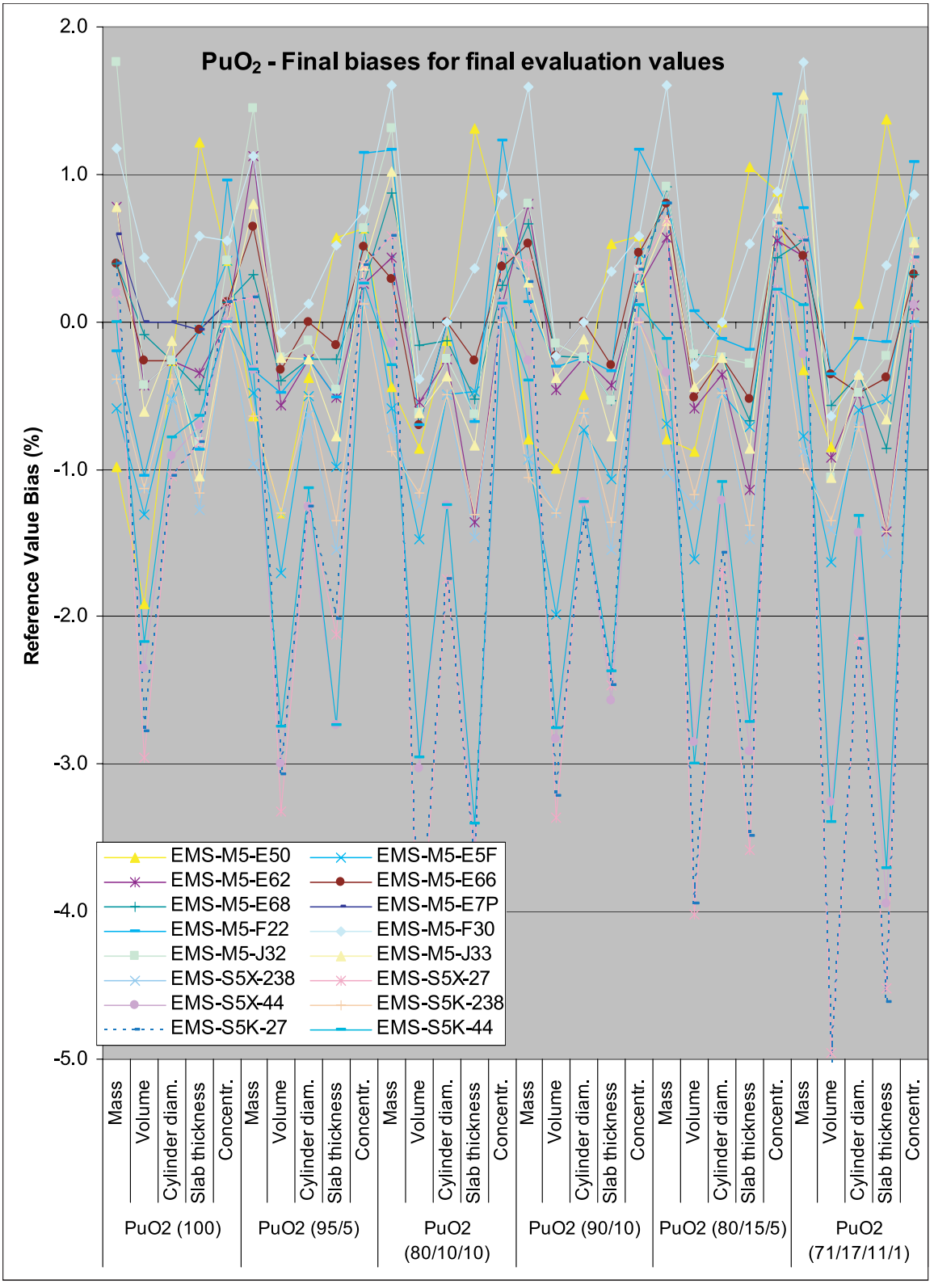


**Figure 11. $PuO_2$ reference values – Estimated total biases for "modern" methods**

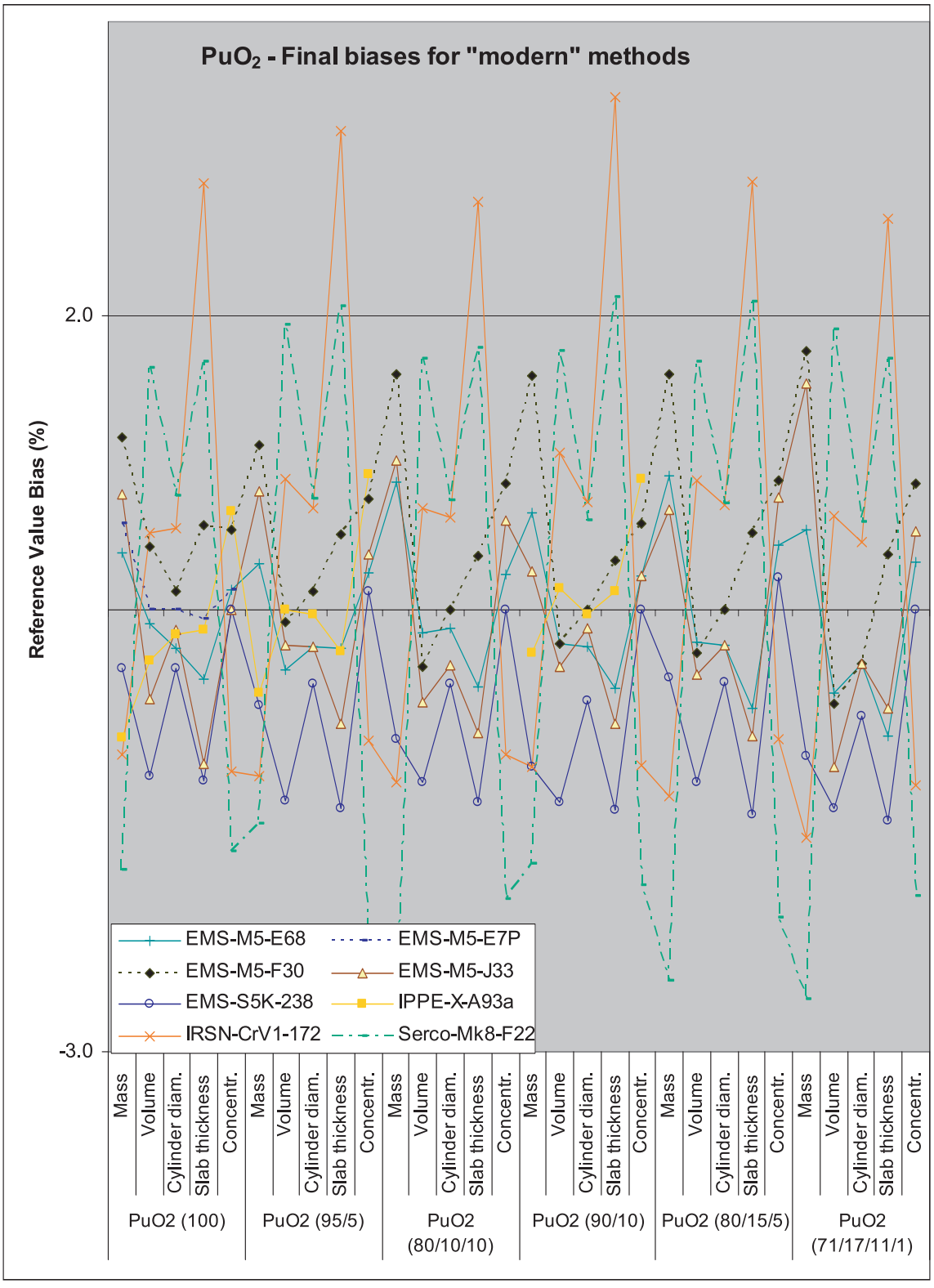


**Figure 12. PuNH reference values – Estimated total biases for contributed values**

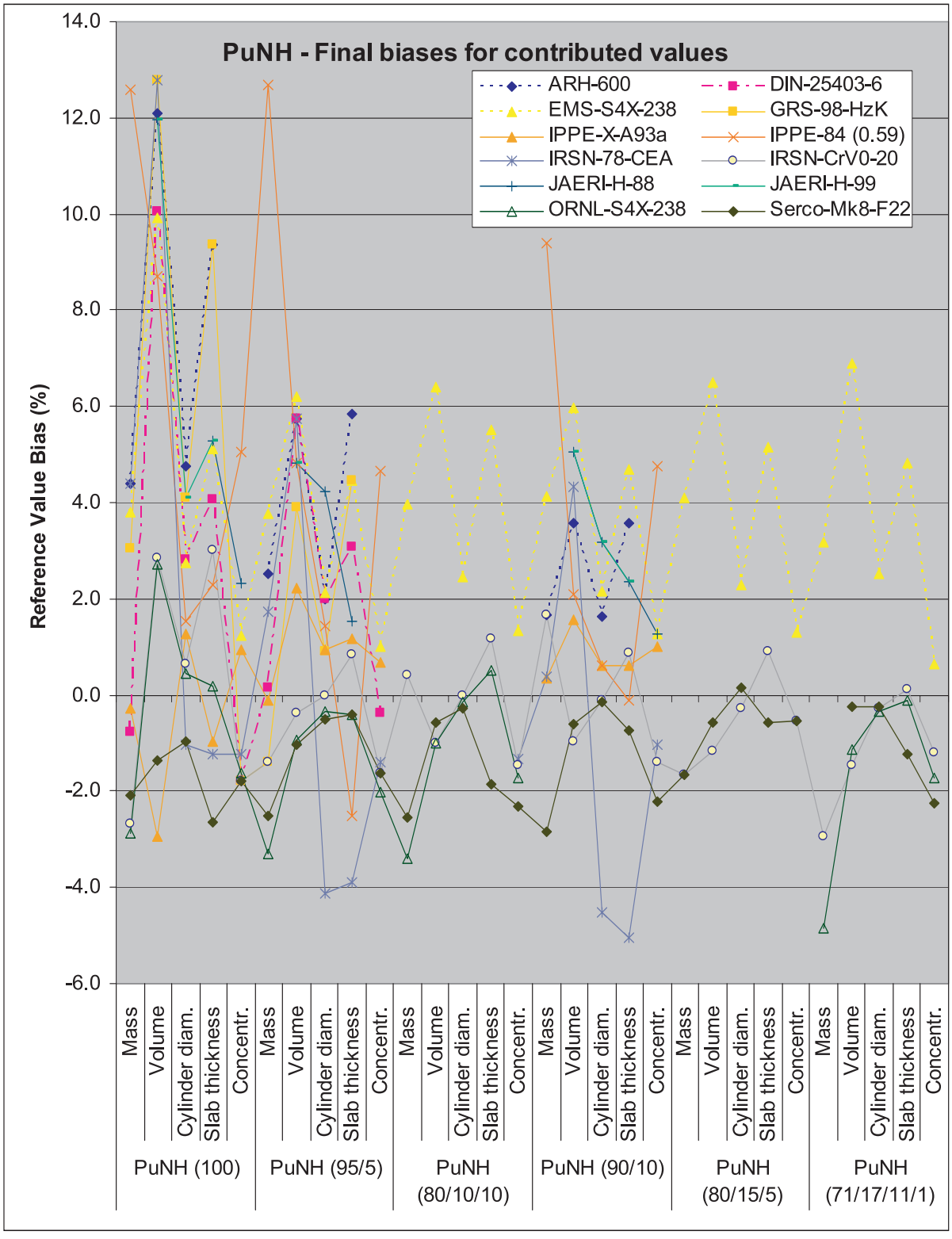


**Figure 13. PuNH reference values – Estimated total biases for final evaluation values**

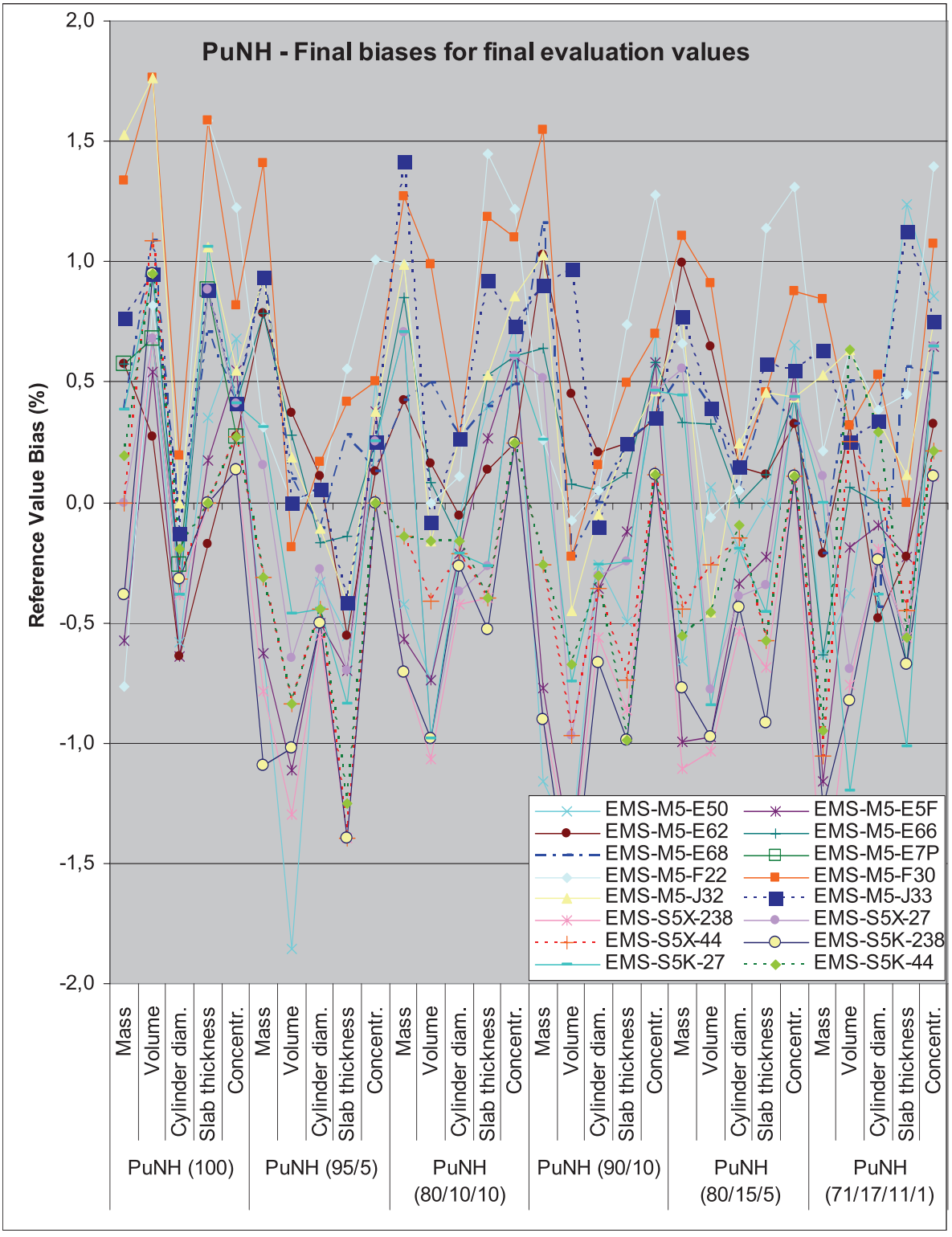
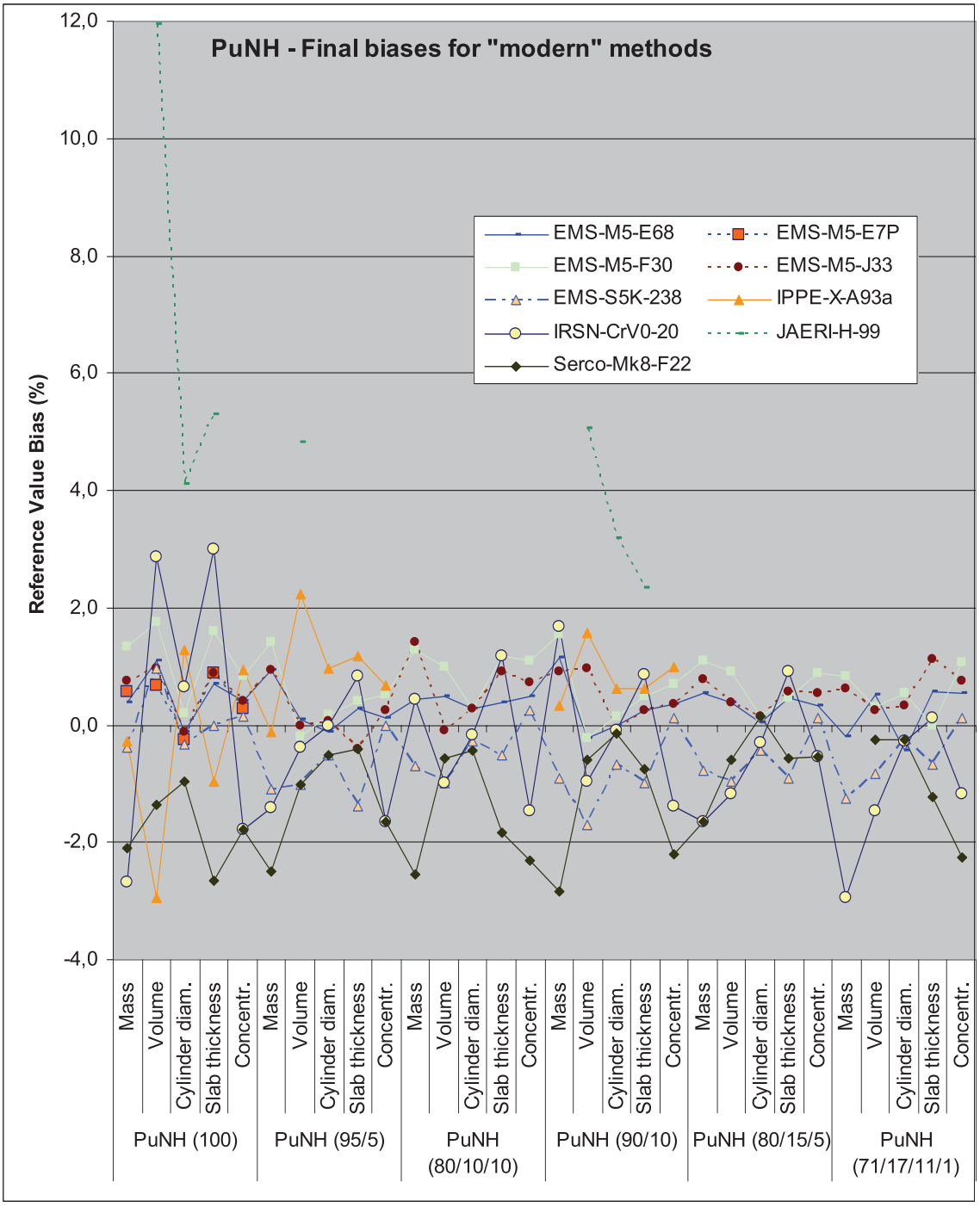


**Figure 14. PuNH reference values – Estimated total biases for "modern" methods**



# DISCUSSION OF THE RESULTS OF THE STUDY

The availability of a large number of evaluated high-quality benchmarks [68] made it reasonable to expect that a comparison of best-estimate results from validated methods would lead to quite close agreement. All the selected systems represent real operations and designs. Many criticality safety benchmarks cover similar fissile materials and moderations.

If the best-estimate values don't agree within reasonable uncertainty ranges, it could be a sign of inadequate validation. This was already clear during the selection of benchmarks; they are not sufficient for many reference systems. The evaluation of the validation results is very subjective.

Very late in the evaluation, comparisons of nuclide density methods were made. This is something that several contributors, in particular IRSN, had pointed out as a difficult area during the study. However, the main evaluator and report writer (EMS) had not previously been involved in such evaluations. The effort to compile conclusions from other participants in early 2005 turned out to be very complicated. The information was not very clear. Many contributors were busy with other projects, reducing the possibility for information exchange.

Some of the major experiences during the final evaluation from August 2004 until April 2005 are described below. The evaluation work and results were presented at the ANS Winter Meeting 2005 [104]. An early compilation and some evaluation of the Expert Group results can be found in a presentation at ICNC 2003 [61].

## Insufficient accuracy in deterministic code applications

Experience [29] from using the SCALE 4 deterministic code XSDRNPM/S showed early during the study that the default SCALE parameters were not sufficient to get accurate results for fast systems and for systems with thin slabs. The SCALE 5 results using XSDRNPM/S reported here have been confirmed with KENOVa calculations using the same cross-section libraries. The preliminary SCALE 5 results were not as accurate. For slabs, a finer mesh was required. For spheres in particular, but also for cylinders and maybe for slabs, increased (from 8 up to 64) orders of angular quadrature were required.

Preliminary IRSN CRISTAL calculations for fast system slabs and to some extent also for volumes (spheres) and cylinders showed that the default parameters (including cross-sections) for thermal systems were not sufficient. This has been recognised by IRSN; the results were preliminary and not intended as best-estimate values. If used in safety applications, the errors would have been large and underestimating $k_{eff}$.

IPPE, in their 1984 Handbook [20], made it very clear that the methods were not rigorous. However, the IPPE validation was sufficient to point out errors and uncertainties. In many cases, the errors were cancelling each other. The results from the 1984 IPPE handbook are often deviating significantly from the best-estimate results in this report.

## Correlations between reference values

There are many correlations between the reference values. The calculation codes and cross-sections are not always independent even if they are developed or processed at different sites. The benchmarks are not independent. The nuclide density methods are not independent for each reference system or for each contribution. The input data for calculations of reference values are not independent. Statistical evaluations of outputs, biases and uncertainties are not independent.

A surprising correlation between values in the handbooks GRS-Hzk-98 [19] and IRSN-DTF-78 [21] seems to have been found. Figure 6 shows that 11 out of 12 GRS and IRSN values are identical for UNH with low-enriched uranium. The twelfth value was changed by GRS at a later time. The methods documented in the handbooks are very different and this agreement is not a coincidence.

All of the correlations involve errors and uncertainties. An example is the EMS input for MCNP5 calculations, using different cross-section libraries for the same reference system. Geometry and material specifications are identical, only the cross-section identifiers vary. The material specifications are identical to those used by EMS for SCALE 5 calculations. Comparing preliminary results, it was obvious for one reference system, U(100)NH slabs, that the differences between MCNP5 and SCALE 5 results were not credible. Checking the input, it was noticed that a comment "c" character in front of the thermal scattering data input line (MT) for MCNP5 was inadvertently retained. The system is moderated by water and this line should be present. Correcting the input for all 18 cases (2 each for 9 cross-section libraries) made the results consistent with SCALE 5 and other results.

## Contributed values include "raw data" and bias-corrected estimate values

A complication in comparing the contributed results is that they are not suitable for direct comparison. Results that are taken directly from the code output are considered as "raw data". In such cases it is valuable to have separate validation documentation that can be used to understand the differences to other results, including best-estimate results. Validation for some handbook values may not be so clear, but the methods used to derive them are normally documented and will help in explaining differences to values from other sources.

At least three different types of verification can be identified. The first type, used to determine values in the Japanese Handbooks and by EMS in the original SCALE 4.4 contribution, is based on evaluation of a very large number of benchmarks based on critical experiments. This is a very rough method since the benchmarks are of different quality and of widely varying applicability to the system being evaluated. Further, the validation is not complete since determination of nuclide densities and other input specifications is not covered. The ORNL contribution, as finally approved for publication [52], contains a reference to the same verification report [78] as used in the EMS SCALE 4.4 contribution [29]. Since the "raw data" from EMS compares very well with the ORNL values, ORNL and EMS values should be seen as obtained using the same method and confirming each other.

The second type, applied by IRSN for CRISTAL, focuses on overall criticality safety validation of the method, including nuclide densities. Accurate determination of biases and uncertainties for each application type is not published since they are considered adequately small related to criticality safety margins.

The third type, as has been attempted in the final evaluation by EMS and partly in contributions by Serco, is based on more detailed weighting of benchmarks and is intended to cover all bias and uncertainty contributions. IPPE contributed verification results and information that allowed a verification of this type during the final evaluation.

## Documentation, source documents, references

It is very important that the source documents are available for checking of information. There are many cases of discrepancies between reported values or methods and the information in the source documents. Sometimes various information sources inside a document are inconsistent as well. Important but unclear information in a published reference should be clarified in a later publication.

The IRSN contributions, publications and presentations [39-41, 60, 89] on the advantage of the isopiestic law compared with a former (1968) ARH-600 law for PuNH systems, as implemented in the pre-processor CIGALES, may at first not be easy to understand. These works pointed out that the density law formerly used by IRSN could lead to a $k_{eff}$ underestimation up to 3.4%. The problem was known since 1987. IRSN was aware of the 1972 revision of the ARH-600 method, based on a volume addition principle. However, IRSN preferred to wait for the development of an approach based on physical considerations that could take into account higher actinides, high concentrations (> 600 g/l) and high acidities. This development eventually resulted in the extended isopiestic law.

The caution against use of the 1968 ARH-600 PuNH density method is valid. Besides the IRSN use of it in some earlier codes, it may have been used in other safety analyses that are still applied. However, it has been confirmed that some sources, including the IRSN 1978 Standard de Criticité [21] as well as SCALE releases before version 5, are based on the 1972 revision of ARH-600 and do not cause the problems described by IRSN.

## Input data for benchmarks

In safety applications, it is a common understanding that the validation of methods should be made with input that is representative of normal use of the methods. That is not a good idea for best-estimate determinations, as requested here. The uncertainties should be reduced as much as possible. EMS has used input for verification of 16 methods (10 based on MCNP5 and 6 on SCALE 5) on input data from the ICSBEP Handbook [68]. Considering the lack of time and resources, this introduces much less uncertainties than if independent input data had been generated. However, some input examples from the ICSBEP Handbook may have significant errors and this may influence the bias-corrections for some systems.

A serious input error introduced in the 2004 version of the ICSBEP Handbook [68] was discovered during this verification work. The thermal plutonium benchmark set Pu-ST-022 contains 18 individual benchmarks. Nine are without neutron poisons, nine have such poisons. Only the first nine, the “clean” benchmarks were used here. The sample MCNP 4 results in the Handbook were surprisingly low, not consistent with other results using the ENDF/B-V cross-section library. A check of the sample input showed that a simple editorial mistake had caused an incorrect material composition for air (lots of cadmium). This is similar to the EMS input mistake mentioned above, under correlations. These benchmarks (Pu-ST-022) had been used in EMS verification before the 2004 issue.

The Pu-ST-022 benchmark documentation in the 2004 edition of the ICSBEP Handbook is a re-evaluation of the 1996 version, mainly giving reviewed uncertainties. There were also some problems with the MCNP sample input and results. The 2004 edition had new “printed” (pdf) sample input but kept the old sample input file on the CD. The corrections seem to give very small $k_{eff}$ changes. Further efforts should be made to check the MCNP 5 verification against this benchmark series. During the review of this report, the 2005 edition of the ICSBEP Handbook was released. The mentioned problem has been solved, together with some other improvements for Pu-ST-022.

The sample input data and results in the ICSBEP handbook are very valuable to the criticality safety community. It gives us something to compare our own calculations with. It makes it easier to improve the Handbook by finding input mistakes and editorial errors. However, the Handbook input data and sample results are not intended for direct safety applications. They are not reviewed as closely as the benchmark specifications.

## Reference system specifications

The study started without specifications of which reference systems to be evaluated. They were introduced during the first two, maybe even three years of the study. Now it seems as if the specifications for the hydrated nitrate systems were not sufficiently clear. The intention was certainly to cover all credible mixtures of the hydrated nitrate crystals with water. However, the reference to solutions is misleading. The crystallised theoretical density material is not a solution. It is homogeneous, uniform and sufficiently realistic for consideration in a safety application. The concentration range between saturation of the solution (solubility limit) and the crystal form was not well defined.

It would have been better if the specifications had expressed clearly that a mixture of saturated solution and crystals needed to be considered. Also, results at crystal density should have been requested even if they are not the minimum values (they are still very important reference values).

## Theoretical densities involving actinides with different isotope distributions

The Japanese handbook [24] clearly informs the reader that the theoretical density for $UO_2$ varies, depending on the enrichment $^{235}U$. In connection with work on criticality properties of all actinide nuclides [95], EMS used this information to determine theoretical densities for other nuclides than that for which the original density was specified for. The simple basis is that the material structure of a specific element, and thus its atomic density, doesn't depend on the mass of the isotope. The atomic number densities remain the same, independent of the isotope. This automatically leads to different theoretical densities for different isotopic distributions – e.g., for $UO_2$, the density with natural uranium is 10.96 g/cm$^3$ while it becomes 10.84 g/cm$^3$ if all uranium consists of $^{235}U$.

It seems as if all contributions, except the IRSN CRISTAL values, have been based on a fixed $UO_2$ theoretical density of 10.96 g/cm$^3$. For fast systems involving $U(100)O_2$, this introduces a bias. A correction was determined, based on SCALE 5 calculations. For plutonium systems, the correction is smaller since they are dominated by the isotope $^{239}Pu$, for which the $PuO_2$ theoretical density 11.46 g/cm$^3$ has been used by most contributors. An exception is IPPE who has used 11.44 g/cm$^3$ in their recent contributions with ABBN93 cross-sections. The overestimation of the minimum critical volume is about 4 ml, or going from 1.148 to 1.144 litres. This is not much in safety applications. For this evaluation of best-estimate values such differences are significant. It is about 0.4% which is the total uncertainty (one standard deviation) quoted for the MONK 8B contribution from Serco.

## Nuclide density methods

A more thorough investigation of the density methods used in different contributions was made very late during the evaluation (end of February, March 2005). At this time it had already been discovered that SCALE 5 had problems with densities above solubility and gave seriously incorrect information about the crystal density.

All contributions, except the IRSN extended isopiestic method, for UNH with uranium having low $^{235}U$ enrichment involve dubious density methods. The systems at crystal densities are not calculated correctly, except for the IRSN method and the IPPE simple mixing (no solution) method. This is basically a user problem and not a method problem. However, the information given in SCALE (in particular SCALE 5) output about the crystal density is not correct.

The solution equations should not be used above the solubility limits. The Pitzer method, as used in SCALE 5, is not intended for direct calculation of concentrations above the solubility limit [54]. It replaced a method (ARH-600) in earlier versions that also was limited to the solubility range but was commonly applied to higher concentrations.

Sometimes the applicability ranges, as stated by method developers, are even more restricted than the soluble range. The IRSN extended method combines a solution method (the isopiestic law) with crystals in a homogeneous, uniform mixture. That appears to be a reasonable method for covering the whole range of concentrations.

Also below the solubility limits, the different methods vary significantly. It was too late to start validation work of the various methods in March 2005. Instead, the IRSN isopiestic method has been used as a reference when the best-estimate reference values have been determined.

JAERI informed the Expert Group in August 2004 that a new mixture model gives higher H/U than the Moeken model adopted for the previous calculations for UNH in the Japanese Handbook and its associated Data Collection. The information from Serco on the method used to get densities for MONK also appears to demonstrate some weaknesses (non-conservative).

## Benchmark accuracies

The selection of benchmarks for bias and uncertainty estimation is very important. Traditional trending against some parameter such as H/X ratio, average fission energy or energy corresponding to average lethargy of neutrons causing fission (EALF) are often useful for simple systems like the ones included in this study. Enrichment $^{235}U$ is also a likely trending parameter. During the evaluation of this study, the new techniques in SCALE 5, TSUNAMI-IP [79, 86-88] were also taken advantage of (see Appendix H).

Information about the similarities of benchmarks to applications is very important. However, equally (?) important to the weighting of benchmarks is the accuracy of the benchmarks. A single benchmark with an uncertainty of 0.001 in $k_{eff}$ has the same statistical weight as nine independent benchmarks, each with an uncertainty of 0.003 in $k_{eff}$. Many benchmarks have much larger uncertainties.

## Criticality Safety Handbooks

The various handbooks are very valuable to criticality safety specialists. However, each handbook contains errors and uncertainties. Several have been discovered or demonstrated during this study and during the final evaluation. Even the most recent one, the Japanese Handbook version 2 [24], contains a serious error. The minimum critical mass for $U(20)O_2$ is given in the Handbook and in the first contribution to the study as 7.43 kg $^{235}U$. This is about 40% too high. JAERI is aware of the problem (simple mistake) and a new value has been contributed to this study. The error has been published by JAERI, e.g. see [105].

## Validation for Safety or Best-estimate evaluations

The traditional methods for safety verification have not been very useful in determining bias-corrections for the requested reference values. The ORNL validation report [78] used by EMS in 2001 [29] and referred to by ORNL [52] covers a wide range of systems. The uncertainties appear large enough to cover incorrect bias-corrections. A similar problem also appears to be the case for the verification and bias-corrections used to determine the values in the Japanese Handbooks.

## Fissionable material reactivity comparison

The preliminary classification of the order of plutonium isotope distributions was based on the fraction of fissile plutonium isotopes as opposed to fissionable-only isotopes in the total plutonium element. When the fissile fractions were equal, the $^{241}$Pu isotope was weighted higher than $^{239}$Pu.

When all results have been compiled and evaluated, the reactivity classification worked, except for one reference system. A water-reflected Pu(80/10/10)$O_2$ critical slab is thinner than a water-reflected Pu(95/5)$O_2$ critical slab. For identical materials in sphere and cylinder forms, the opposite conclusions can be drawn about the corresponding reference values.

This experience demonstrates some of the complications that can be expected when reactivity equivalency is applied.

## Uncertainties – Combinations, distributions, credibility

The fact that the uncertainties in the estimated reference values are much more subjective than the reference values themselves is pointed out in this report and was pointed out during a presentation of the draft report at the WPNCS meeting in September, 2005. It was stressed that the report is a result of early work on a study that is expected to continue. To use “objective” statistical propagation methods now in order to determine uncertainties would probably give less credible results than the subjective values given. Verifications of various components of the methods used to obtain the reference values may be more or less credible, but the model used to obtain combined uncertainties is not. Appendix S and also Appendix M cover some of the problems.

Optimisation of moderation is a contributor to the total uncertainty. In some cases this optimisation uncertainty is essentially zero and definitely not normally distributed. Such cases involve theoretical density for volume, cylinder and slab systems of U(100)$O_2$ and all $PuO_2$ as well as U(3)NH. The optimum is almost definitely solid materials at theoretical density. If there is any uncertainty in any value, the optimum density is not higher than the theoretical density. This issue is not reflected in the subjective uncertainty estimates for U(3)NH in Table 3. It should be possible to determine the volume, cylinder and slab values more accurately for U(3)NH than for U(4)NH and U(5)NH.

# RECOMMENDATIONS FOR FURTHER WORK

The study should be completed by striving for a consensus on best-estimate reference values and uncertainties. This is covered by the scope and objectives for the work reported here. As stated frequently during the first part of the study, the values are physical constants. Their accuracies depend on the availability of benchmarks (for overall criticality safety validation and for verification of cross-sections, nuclide densities, etc.), of quality methods and on quality evaluation techniques. Such efforts fit very well in the structure of the OECD/NEA and with efforts carried out by other international organisations such as IAEA and ISO.

Clearer specifications of the hydrated nitrate reference systems are needed. It is suggested that the solubility limit is stated, when possible. The crystal density should be specified and reference values for this state should be evaluated, whether they correspond to minimum critical values or not. Theoretical densities for all compositions should be specified, including influences of isotopic variations. A minimum critical value for concentration, under many additional constraints, corresponds to a maximum critical moderation atomic ratio H/X, with few additional constraints. The H/X atomic ratio is a better reference parameter than concentration in $g/cm^3$ and should be determined.

The large spread in results for some reference systems indicates that the validation process can be improved significantly. There are many benchmarks that were not included because they appeared to be complicated. However, the complications may not necessarily invalidate them from supporting the evaluation of the selected reference systems.

A complete validation is necessary. This means that benchmarks on nuclide densities are needed. As already pointed out by IRSN, the ICSBEP Handbook often contains sufficient information to expand the current benchmarks to include nuclide density determination based on chemical data.

Modern tools for criticality safety assessment should be used in the work. Further, the work may also lead to suggestions to code developers for additional output information to support the user. An example of useful information is the specification of EALF values in SCALE 5 (XSDRNPM/S and KENOVa) and in MCNP5. Use of the new TSUNAMI and SMORES sequences in SCALE 5 as well as options in other methods could lead to suggestions for additional information in the code output.

The issue of $k_{eff}$ versus reference parameter relationships should be discussed. The curves can be approximated using various equations. The $k_{eff}$ versus spherical radius proposed by Rombough [96] is an example. Statistical evaluation methods and uncertainty distributions may also be studied. The issue of $k_{eff}$ correlations when input parameters are independent could easily be demonstrated.

A database of calculated values of $k_\infty$ for all actinide nuclides as well as for many compositions would be easy to compile and valuable for many purposes. Different reflectors are already included in the scope and objectives of the current study.

The concept of “minimum critical values” is too limited even for the past study (H/X ratios are maximum critical values) and should be replaced by “reference values”, see also Appendix N.

# CONCLUSIONS

As in previous studies on comparisons of criticality safety methods by OECD/NEA Expert and Working Groups, appropriate validation is a necessary key to success. To determine the requested reference values, the traditional method of validation against benchmarks based on critical experiments is not sufficient. Such validation is only partial, like a verification of computer codes and cross-section data. It is obvious that a complete validation requires benchmarks to test nuclide density determination methods. Some of the ICSBEP Handbook benchmarks can be extended for that.

It was not a surprise to find that some of the older data in criticality safety handbooks appear to have large errors, some underestimating $k_{eff}$. It was more surprising to find that modern tools seem to be insufficiently validated or documented to warn users about lacking support for certain applications. Deterministic calculations of fast systems require special verification of cross-sections and of input parameters. Hydrated actinide nitrate densities, outside the soluble ranges, that were calculated quite well in a previous version caused SCALE 5 to give seriously incorrect information to the user. Potential consequences of changes to a successful method always need to be checked carefully.

Many discrepancies have been identified and resolved. Most of them have been corrected during the study, without publication. Published incorrect values should be corrected in a public report. Besides the SCALE 5 hydrated nitrate density problem, some others should be mentioned. IRSN has reported that the plutonium nitrate density law applied up to the year 2000 in the graphical user interface CIGALES (generates nuclide atom densities) caused serious underestimation in $k_{eff}$, increasing with plutonium concentration. This old IRSN density method was based on a 1968 release of the ARH-600 handbook. This release may also have been used by other organisations in safety analyses that are still applied. However, the equation was corrected in a 1972 revision of the ARH-600 handbook and this is the method used in SCALE before release 5. A very serious error for the $U(20)O_2$ minimum critical mass in the Japanese Handbook [24] was noticed during the evaluation and has been corrected by JAERI. The critical and safe masses in the Handbook are overestimated by 40%.

One of the reasons for slow progress has been that several participants have not been convinced that the determination of best-estimate reference values is feasible for criticality safety applications. It is clearly included in the scope and objectives. Hopefully, this report demonstrates that it is feasible.

Selection of benchmarks for the final evaluation was made using accuracy and simplicity as primary indicators. A single benchmark with a $k_{eff}$ uncertainty of 0.0010 should be weighted as high as ten independent benchmarks, each with a $k_{eff}$ uncertainty of 0.0031. Similarity indices based on the SCALE 5 TSUNAMI sequences as well as on energy corresponding to average lethargy of neutrons causing fission (EALF) seem to work quite well. For some of the reference values, the verification appears very successful while the opposite seems true for other reference values.

A comparison of nuclide densities for nitrate solutions showed surprising variation, even within the soluble range of actinide concentrations. The IRSN work on the extended isopiestic law as reported to the Group has been valuable to support this report.

A solid (theoretical density) Pu(80/10/10)$O_2$ critical slab is thinner than a solid Pu(95/5)$O_2$ critical slab when both are water-reflected. This may seem surprising since the opposite is true for sphere and cylinder reference values for the same materials and reflection.

A compilation of calculated values ("raw data") without support from validation is not very meaningful on its own. The scope of the study is primarily focused on the physical constants, the reference values, and after that on the performance of calculation methods and handbooks. Using the established reference values, the discrepancies in results reported from different methods and handbooks can be evaluated. Also the general performances of common methods and handbooks are of interest to the criticality safety community.

The Expert Group early agreed that the results of the evaluation, when agreed upon, should be in the form of reference values and not as recommended values. It is up to the user to determine how to apply the values. This was confirmed in an enquiry during the 2004 meeting.

The final best-estimate reference values reported are for demonstration only. They are not even preliminary values. This conclusion applies even more to the uncertainties. There may still be correlated errors that could lead to significant changes. The evaluation of best-estimate reference values is subjective. A consensus on the values has not been requested since it would take considerable time and require additional resources and evaluations. The procedure leading to the determination of each reference value should be clear enough to explain the value and to support improvements.

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## *Appendix A*
## SCOPE AND OBJECTIVES[1]

*Scope*

Basic minimum critical values are important physical constants needed for assessing safety margins in criticality and are used for licensing. The scope of the expert group is to compile minimum critical values of $^{235}U/^{238}U$-, Pu-, MOX-, and $^{233}U$-systems. Homogeneous systems with uniform distribution of the fissile material will be covered. Discrepancies in the data will be identified and an explanation of discrepancies sought.

*Objectives*

Under the guidance of the Working Party on Nuclear Criticality Safety, the expert group will:

- collect data from different countries, including a short description of the methods used to achieve the data;
- identify discrepancies and propose explanations;
- address effects of engineering data, of density formulae, reflector materials;
- provide technical input to the International Community, e.g. ISO;
- supply a general reference for criticality safety analyses that use/include minimum critical values.

[1] The formal "Scope and objectives" as published on the OECD/NEA/NSC www page

## *Appendix B*
## TERMINOLOGY

The terminology is included for the purpose of this report and is limited to a few concepts that are important to nuclear criticality safety, have caused discussion and even confusion during the study or are not clearly defined in international glossaries, guides and standards.

*Actinides*

It is convenient to refer to actinides as a group of elements rather than to list them. The reference systems in this report are limited to uranium and plutonium. The benchmarks include other actinides. The actinide group consists of 14 elements starting with atomic number 90 and finishing with number 103. Actinium (89) is not an actinide. Nuclides like $^{235}U$ and $^{239}Pu$ are often referred to as actinides but they are actinide nuclides.

*Atomic number density*

The density of a nuclide is often specified in number of atoms per barn-cm ($10^{-24}$ $cm^3$). The determination of such atomic number densities is very important to get good reference values. A computer code system may convert other input specifications into atomic number densities.

*Best-estimate value*

At a certain time and for a given purpose, this value is the most accurate estimation available to the publisher or to the contributor. By definition this means that there was no bias in the value that was known to or assumed by the publisher or contributor. The uncertainties should be specified separately.

*Bias*

A bias is the difference between a calculated or measured result and a best-estimate result. It can be a constant or a function of one or more parameters. A bias is an error, also referred to as a systematic error, with an estimated ("known") sign and magnitude. This error should not be confused with the systematic effect (sometimes, but not in this report, also called systematic error). Biases can be correlated to each other. The determination of a bias usually leads to an uncertainty in the bias. This bias uncertainty often results in a systematic effect.

*Bias correction*

A bias correction is used in this report to obtain a best-estimate value from a calculation, measurement or other procedure. In this case, it has the same value as the bias but with a reversed sign. In other applications, e.g., criticality safety analysis, the bias correction is more open to judgment and need. The bias is considered a fact while the bias-correction in safety applications can be made more or less conservative.

*Critical system*

A system of fissionable and other materials that, through fission and other processes caused by free neutrons, produces as many neutrons as are lost (absorption and leakage).

*Critical value*

A critical value is a parameter value that, under specified material and geometry constraints, determines a critical system. This value is a physical constant, a "reference value".

*Cross-sections for neutrons*

A neutron cross-section for a nuclide or material gives the probability for a reaction between a free neutron and the nuclide or material. The cross-section is dependent on the energy of the neutron, the properties of the nuclide and the environment of the nuclide (material properties, temperature). The cross-sections are evaluated from measurements and theoretical models.

*EALF – Energy corresponding to average lethargy of neutrons causing fission*

This parameter is considered more useful than the average energy causing fission since the importance of thermal neutron fissions is clearer. The EALF value is an average and will not always be a clear indicator of the neutron physics of the system. It could be like comparing the average colour of the rainbow with the colour of a mud pool. However, EALF has been found to be useful in many cases. Some computer codes include EALF in the output.

*Eta – $\eta$*

A function defined as the ratio of produced to absorbed neutrons for a certain fissionable nuclide, element, compound, solution or mixture. The function is dependent on neutron energy but integral (total energy range or limited energy ranges) values may be of use as well. The JANIS 2.1 code [71] is useful in generating charts of this parameter.

*Fissile*

A fissile nuclide is a fissionable nuclide that can be fissioned by slow neutrons. The distinction between fissile and non-fissile (as between many other adjectives such as soft/hard, good/bad, homogeneous/heterogeneous, etc.) depends on the application. In nuclear criticality safety, the fissile property is usually related to the support for criticality when some water is present or added to the system. In some criticality safety applications, special moderators such as graphite, beryllium and deuterium may need to be considered in the definition of fissile. Natural uranium is a fissile material in some applications but can be neglected as a criticality safety hazard in the absence of other fissile materials and large quantities of special moderators.

*Fissionable*

A fissionable nuclide can be fissioned by a free neutron at some energy. In criticality safety applications, this energy needs to be credible during handling, storage and transport operations. A fissionable element, material, system, etc. contains sufficient quantities and concentrations of fissionable nuclides for the neutron-induced fission process to be considered significant. A fissionable nuclide does not necessarily support criticality on its own. As with the fissile concept, the definition of fissionable is application-dependent.

*Handbooks and other reference value compilations*

Values given in handbooks and other sources are used for various purposes. Safety handbooks may use different approaches than other handbooks. Different criteria may be used to derive and present the values, even when they have the same "label". This should be understood when a value from a handbook is used together with methods or values from other sources.

*Human error*

Human error is used here loosely as a category to cover deviations between the documented information and the real facts and which lie outside the reported accuracy claims. These claims may not always be obvious but should be available in some form. Many of the discrepancies requested in the scope of this work can be referred to this category. Human errors range from editorial errors to fundamental flaws in established theories and methods.

*$K_\infty$ and $k_{eff}$*

See neutron multiplication factor.

*Maximum critical value*

One or more parameters are optimized while other conditions are fixed to give a maximum critical value for a specified parameter. An example is the maximum critical atomic moderation ratio H/X, where X corresponds to a fissionable nuclide or element.

*Minimum critical value*

One or more parameters are optimized while other conditions are fixed to give a minimum critical value for a specified parameter. Examples are critical mass and dimensions assuming that the water moderation is optimized. The minimum critical mass is normally expected to have the shape of a sphere but the optimum shape needs to be verified.

*Neutron multiplication factor, $k_{eff}$ and $k_\infty$*

The effective neutron multiplication factor, $k_{eff}$ is a system property determined by a converged self-generating neutron flux distribution. $K_{eff}$ is an eigenvalue needed to make the "amplitude" of the distribution constant. The infinite neutron multiplication factor $k_\infty$ is a fissionable material or unit property determined for an infinite material or array of identical units. $K_{eff}$ is related to the neutron flux through a complex relation, the neutron transport equation, and can't be generally modelled as a sum or product of independent variables. Each system has a single value of $k_{eff}$. A single value of $k_{eff}$ corresponds to many systems; the value itself is not necessarily a sufficient indicator of the system properties. The reactivity effect of multiple parameter changes to the system are not determined by individual reactivities but by the combined effect of system parameter and neutron flux changes.

For critical and near-critical systems, $k_{eff}$ may be defined and measured as the ratio between produced (excluding fixed sources) and lost (absorption and leakage) neutrons. For other systems, the evaluator needs to introduce or select neutrons to comply with the converged flux distribution. The criticality safety properties for such systems are not necessarily indicated by the real neutron flux and multiplication. The eigenvalue model gives information about such properties.

*Random effect*

If a value changes between evaluations, consistently with a certain probability distribution, the variation may be considered to give a truly random effect for each evaluation. If there is a trend that applies to several evaluations, the trend becomes a systematic effect for the evaluations. It is essential for some evaluations to separate random and systematic effects of each component of the combined uncertainty and to combine them separately.

*Reactivity*

Reactivity is a change in $k_{eff}$. It is used here as the absolute $k_{eff}$ change, without normalisation. The unit mk the reactivity multiplied by 1 000, is used in many tables. This is the intended accuracy for the requested reference values. One mk is also used to determine the number of significant digits. Reactivities in the same system are correlated through the neutron flux. Reactivities are not equivalent to reaction rates or reaction rate changes. E.g. ratios of the individual nuclide absorptions to the total absorptions are not equivalent to the ratios of the individual nuclide absorption reactivities to the total absorption reactivity.

*Reference values*

A value that corresponds to clearly defined conditions and is used in criticality safety applications. The exact specifications may not always be given. In this study, the optimization procedure contributes to the total bias and uncertainty. Maximum and minimum critical values, $k_{\infty}$, etc., are examples of reference values.

*Safe values*

A safe value is associated with a special operation or type of operation involving fissionable materials. The magnitude of the value does not necessarily in itself inform about the safety margin or even if the operation is safe or unsafe.

*Sensitivity*

The sensitivity is a change of a variable due to a small variation in a parameter. An example is the change in $k_{eff}$ that corresponds to a small change in the material mass. “Small” is not defined but is related to the validity range of the relationship. A linear sensitivity has a smaller range of validity than a more complicated relationship. A combined change based on several sensitivities need to comply with the same principle; the total change should be within the validity range for each sensitivity.

*Statistical distributions – Normal, Gaussian*

Input parameters are often assumed to be known with some uncertainty based on a normal or Gaussian probability distribution. It is very unlikely that the corresponding $k_{eff}$ uncertainties have the same distribution, unless the uncertainties are very small. An example is the steel thickness of plates between fuel assemblies in water. Assume that the thickness uncertainty complies with a Gaussian distribution. There is often a plate thickness for which $k_{eff}$ increases, whether it is increased or reduced. For other input parameter uncertainties, the $k_{eff}$ relationships are not linear. The EMS contribution from 2001 reports reference value uncertainties based on $k_{eff}$ uncertainties (Gaussian distribution). The positive and negative $k_{eff}$ limits of confidence are not symmetrical.

*Systematic effects (but not systematic errors or uncertainties)*

An uncertainty that represents a potential error that is common to more than one value or common to more than one evaluation of the same value has sometimes in the past been called a systematic error or systematic uncertainty. To be consistent with [94], it is now called just "an uncertainty". This uncertainty shall be included in the combined uncertainty for the calculation or measurement. However, the systematic effects of different components of each combined uncertainty need to be understood and combined properly when this is motivated.

Examples of systematic effects are calibration errors that remain unchanged between measurements and are not corrected for, a single calculation value that is applied to several operations or designs, validation uncertainties (not biases) determined from statistical evaluations, etc. The systematic effect can be dependent on time and other variables. It is important in assessing the safety of a facility with many operations or designs or of a particular design that is used in many operations. It is also important in assessing the cost of large uncertainties for such facilities or multiple uses of a design.

*Theoretical density*

The theoretical density is a maximum density based on pure material properties under conditions that are likely to be maintained in all credible environments. It is used to estimate densities in mixtures of materials. The sum of volume fractions of each material is normally assumed to be one. Void may then be considered as a material with a volume fraction. The nuclide densities in solutions are important in this study. They are often empirical.

*Uncertainty, single*

An uncertainty may be either a statistical result of calibration or validation, an allowance for unknown errors or a combination of both. It is separated from the bias, which has a known sign and a probable magnitude. There are many sources for uncertainties. The uncertainty is usually specified by a statistical measure, such as a confidence level or a standard deviation, often assuming a normal distribution of the probabilities. The uncertainty can lead to both random and systematic effects.

A large uncertainty can be converted to a bias and a smaller uncertainty using more resources (including more experiments or better evaluations of experiments). An uncertainty is thus a subjective view as seen by one evaluator. To another evaluator the uncertainty may be partially known (a bias), leaving only a smaller remaining uncertainty. A numerical rounding effect is a bias to the person who knows a higher precision and an uncertainty to the one who does not know. The effect can be systematic (multiple use) or random (single use).

*Uncertainty, combined*

The combined uncertainty may be derived from individual uncertainties in a procedure that needs to be validated in each case. The combination of uncertainties into a single combined uncertainty does not mean that each uncertainty can be forgotten. Evaluation of systematic effects requires consideration of each uncertainty. Independent uncertainties are described separately. The reason for this emphasis on uncertainties is that they are very important in the evaluation of critical experiments, of reference values and of safety of real systems.

*Uncertainties, independence*

For any system evaluated in this report (critical experiment benchmarks and reference value applications), there are no independent uncertainties in $k_{eff}$ or in the associated reference value, see Appendix M, Appendix S and [92]. All $k_{eff}$ uncertainties are correlated. The uncertainties of the input parameters may be independent but the uncertainties in $k_{eff}$ (and in the associated reference value) are not. An example based on a system with a metal plate in a fissile material shows this clearly. The input parameters are plate thickness and plate absorption cross-sections. The input parameter uncertainties are independent. If the plate thickness is smaller, the uncertainty in the absorption cross-sections will have a reduced effect on $k_{eff}$ (extreme: if the plate is not there at all, the cross-section uncertainty has no influence at all on $k_{eff}$). Similarly, if the absorption cross-section is much smaller than expected, due to less boron in the aluminium, the reactivity influence of the plate thickness is reduced (no boron at all may actually increase reactivity of the plate compared with water).

*Validation*

Validation of a value or a method involves evaluation of the total bias and uncertainties for a defined range of applications. The difference between validation and verification is dependent on the application of the method or the value. If the evaluation of the method or value is the overall purpose of a study, validation is correct. However, if the method or value is a part of a wider study, verification may be a more appropriate term for testing the accuracy and uncertainty in the method or value. It is thus not contradictory when a code developer refers to a validation report while the safety evaluator refers to the same document as a verification report. Sometimes the distinction is important and this report should be clear in such cases.

Validation for safety purposes should reflect the user influence on typical results. In this study of reference values, calculation method user influence on the results should be minimized.

*Verification*

Verification of a value or a method is more limited than validation. It relates to components of the method or a sub-range of the application range of the value. In some contexts, the distinction is not important and either term can be used. This report uses verification when it is clear that further verification of other overall method components is required to validate the requested reference values. The verification of the calculation method to obtain the best-estimate reference value can take advantage of non-standard and more resourceful options than what are normally applied by a user of the method.

# CD-ROM CONTENTS AND INSTRUCTIONS FOR USE

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