



CRISTALV2.0 PACKAGE

A WELL VALIDATED CRITICALITY SAFETY CALCULATION PACKAGE

The CRISTAL package is devoted to criticality safety calculation for safety enhancement and criticality risk prevention. The CRISTAL V2 package was first released in 2014 and its latest version (2.0.3) is available at the OECD-NEA Database.

The CRISTAL V2.0.3 validation database has expanded its coverage and contains more than 3,100 experimental configurations of various fissile media, materials, geometries and neutron spectra representing configurations encountered in the fuel cycle.

The CRISTAL criticality safety package provides three different calculation routes to address all calculations needs for criticality safety assessments, from standards calculation to 3D full modeling of a scene. The different routes are:

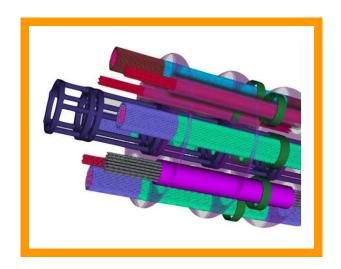
- a multi-group deterministic route (M.D.) based on multi-group cross-sections using APOLLO2 Sn calculations,
- a multi-group Monte Carlo route (M.M.C.) based on the APOLLO2 and MORET 5 codes,
- a point-wise Monte Carlo route (P.W.M.C.) using the TRIPOLI-4® code,

A criticality standard calculation route, based on iterative APOLLO2 Sn calculations is also available in the package.

All these calculation routes use the cross-sections library CEAV5.1.2 generated by the same processing tool based on the JEFF-3.1.1 evaluation. In the framework of the CRISTAL project, the calculation sequences were optimized on a criterion of computing time minimization while providing accurate results.

The CRISTAL package is based on a modular architecture and relies on extensively validated neutron transport codes for criticality safety applications. The link between the calculation codes is ensured by the LATEC workbench that allows, via an abstraction level, to generate all CRISTAL input files, including material composition and geometrical description, and the use of validated calculation sequences with the support of

library procedures APROC and APROC_CRISTAL (CEA). The workbench has undergone many upgrades in order to most efficiently address the user's needs through the four calculation routes available within the package.



ABSTRACT

The CRISTAL package is made of three main calculation routes: the APOLLO2-Sn deterministic route, the APOLLO2-MORET 5 multigroup Monte-Carlo industrial route and the continuous energy TRIPOLI-4® Monte-Carlo route. This package is generally used by the French criticality-safety practitioners (IRSN, CEA and industry) for projects in France and abroad. A first version of CRISTAL V2.0.3 has been sent to the NEA databank. In support of this delivery, it was decided to deliver a validation report that is the object of the present technical report. This report is based on a limited set of benchmarks representative of the validation files for each of the three calculation routes. It should be noted that some results have already been communicated to the international community in the **ICSBEP Handbook**













The CRISTAL V2 Project is a French collaborative project since 2008. The development, verification and validation processes are carried out in a joint project between the IRSN (Institut de Radioprotection et de Sûreté Nucléaire), the Energies Division of the Commissariat à l'Énergie Atomique et aux Énergies Alternatives (CEA/DES) in collaboration with Orano, Framatome and EDF (Électricité de France).

Although the CRISTAL criticality calculation package CRISTAL V2 is developed by IRSN and CEA, the CRISTAL project involves many people from IRSN, CEA, Orano Group, Framatome and EDF.

The authors would thus like to thank all people from IRSN, CEA, Orano Group, Framatome, and EDF, contributing to the CRISTAL project. Whether it be in the different working groups or as daily user, all the feedback is helpful and allows us to make the package still better.

.

TABLE OF CONTENTS

1.	INTRODUCTION	6
2.	THE CRISTAL PACKAGE	7
3.	EXPERIMENTAL VALIDATION METHODOLOGY	8
4.	LIST OF SELECTED EXPERIMENTS	10
5.	RESULTS AND DISCUSSION	15
	5.1 COMPARISON TO EXPERIMENTS	15
	52 CODE TO CODE COMPARISON	19
	APOLLO2-Sn compared with TRIPOLI-4	19
	APOLLO2-MORET 5 compared with TRIPOLI-4	19
6.	CONCLUSION	29
7.	REFERENCES	30

1. INTRODUCTION

The CRISTAL V2 package is commonly used by criticality safety experts in France. It embeds three calculation routes:

- two multi-group and fast computing routes (APOLLO2-Sn and APOLLO2-MORET 5) that are dedicated to standards
 calculations and 3D cases,
- and one continuous energy route (TRIPOLI-4®), more cpu time consuming, allowing to estimate the bias of multi-group routes.

The CRISTAL V2 package is the result of a long-term collaboration between IRSN, CEA and the French industry in order to meet domestic needs. In 2018, CRISTAL has been made available for the first time to international community through the NEA databank.

This report to give some fundamental elements on the experimental validation of the CRISTAL V2 package for a set of benchmarks modeled with the three calculation routes [4].

The list of selected experiments has been determined on the basis of experiments for which results are available in the ICSBEP Handbook [5] with the APOLLO2-MORET route (mainly for CRISTAL V1 release).

After giving some explanations on the characteristics and objectives of the three calculation routes and the validation methodology, the comparison between calculated k_{eff} and benchmark ones will be presented, and the main tendencies will be reported. Moreover, we will give some insight on the performance of the multi-group routes from comparison with the TRIPOLI-4® continuous energy route.

2. THE CRISTAL PACKAGE

The CRISTAL package, dedicated to criticality calculations, includes codes, calculation procedures and nuclear data libraries.

In its V2.0 version, the CRISTAL package is composed of three routes using the nuclear data library CEAV5.1.2 based on the European JEFF-3.1.1 evaluation [1].

- The multi-group routes, called respectively « standard route » and Sn route, are composed of the deterministic APOLLO2 code, with its associated library CEA5.1.2 at 281 energy groups derived from the JEFF-3.1.1 evaluation and the multi-group Monte Carlo MORET 5 code. An APOLLO2-Pij calculation (method of probability collisions) allows calculating self-shielded cross sections, which can be used, either for an APOLLO2-Sn calculation with a collapsing of cross sections in 20 energy-groups or for a MORET 5 calculation.
- The continuous energy route called is composed of the Monte Carlo continuous energy TRIPOLI-4® (release 4.8) code and the JEFF-3.1.1 based CEAV5.1.2 library.

The LATEC workbench allows automatic generation of the APOLLO2, APOLLO2-MORET 5 and TRIPOLI-4® input decks taking into account the recommended calculation schemes for APOLLO2 code [2].

Table 1 gives the releases for the different codes and libraries used in the standard route of the CRISTAL V2.0.3 package.

Table 1: Codes and libraries used in the V2.0.3 release

Codes/Libraries	V2.0.3 Version
LATEC workbench	1.5
APOLLO2 Code	2.8-3.C
APROC	2.8-3.C
APROCRISTAL	V2.0
CEA V5 library	1.2
MORET 5 code	B.1
TRIPOLI-4® code	8

In this report and in figures and tables, the APOLLO2-Sn route will be designated by AP2Sn, the APOLLO2-MORET 5 route will be designated by AP2M5 and the TRIPOLI-4®route will be designated by T4.

3. EXPERIMENTAL VALIDATION METHODOLOGY

The experimental validation leans on the comparison of calculation results to experimental values. The observed differences are then interpreted and potentially transposed to real studied configurations. Hence it is crucial that the experimental validation database is as much as possible representative of all fissile media and configurations encountered in nuclear installations and transports [3].

The ICSBEP Handbook [5] being a well-known source of relevant experimental data for criticality safety, this report uses the same nomenclature based only on physical-chemical characteristics of fissile media. This nomenclature is structured in three parts XXX-YYY-ZZZ following the nature of the fissile medium (XXX), its physical characteristics (YYY) and the energy spectrum (ZZZ). Table 2 presents the syntax adopted (example, LEU-COMP-THERM for UO₂ rods enriched at 4.5 % in water).

Fissile medium (XXX)		Physical characteristics (YYY)		Spectrum (ZZZ)	
PU	Plutonium	MET	Metal	FAST	Fast
LEU	Lowly enriched uranium	COMP	Compounds (UO ₂)	INTER	Intermediate energy
HEU	HEU Highly enriched uranium		Solution	THERM	Therma
IEU	Intermediate enriched uranium	MISC	Others	MIXED	Mixed
233U	²³³ U				
MIX	Uranium and Plutonium				
SPEC	Special isotopes				

Table 2: Classification of ICSBEP benchmarks

An experiment is classified as "fast" if the percentage of fissions occurring at an energy higher than 100 keV exceeds 50 %.

An experiment is classified as "intermediate" if the percentage of fissions occurring at an energy comprised between 100 keV and 0.625 eV exceeds 50 %.

An experiment is classified as "thermal" if the percentage of fissions occurring at an energy lower than 0.625 eV exceeds 50 %.

An experiment is classified as "mixed" if more than 50 % of the fissions do not occur in any one of the three previously defined energy ranges.

The results tables (see section 5) use for each experiment:

- the keff of the calculation performed with CRISTAL V2.0: it is the value of the multiplication factor obtained with the V2.0 version of the CRISTAL package (APOLLO2-Sn, APOLLO2-MORET 5 and TRIPOLI-4® routes) for the experiment of interest,
- the standard deviation of keff calculated by the Monte Carlo MORET 5 or TRIPOLI-4®code: σ_{MC},

These results tables provide for each experiment:

the C-E: it is the difference between the keff calculated with a given route of the CRISTAL package (version 2.0) and the benchmark k_{eff} [5]. This value is given in **pcm** (10⁻⁵) in the tables.

The calculation-experiment differences are recognized as significant if it is higher than the uncertainty margins, that is to say if:

$$|C - E| > ts \times \sigma_{comb}$$

with:

- ts, the broadening coefficient, set to 3, corresponding to a confidence interval of 99,8 % for a normally distributed
- σ_{comb} , the combined uncertainty of the Monte Carlo calculation and the experimental uncertainty :

$$\sqrt{\sigma_{calc}^2 + \left(\frac{\sigma_{exp}}{x}\right)^2} = \sigma_{comb}$$

with:

- σ_{calc} , the Monte Carlo standard deviation of MORET 5 or TRIPOLI-4[®],
- σ_{exp} , the k_{eff} uncertainty given in the ICSBEP report,
- x, the broadening coefficient used to estimate the uncertainty on benchmark keff (1, 2, or 3) in the ICSBEP. In some cases the broadening coefficient is not defined in the benchmark, then it is assumed to be equal to 1. In this document x is always equal to 1.

LIST OF SELECTED EXPERIMENTS

The experiments have been chosen to cover a wide range of energy spectra and fissile media encountered in criticality safety practical cases. For most selected cases, keff results computed with previous releases of the CRISTAL package are reported in the ICSBEP handbook [5].

The list of selected cases is given in Table 3.

Table 3: List of selected cases

Experiment	Case	Description
LAPERINIENT	HST-001-001	Description
	HST-001-001	
	HST-001-002	
	HST-001-004	
	HST-001-005	
HEU-SOL-THERM-001	HST-001-006	Minimally reflected cylinders of highly enriched solutions of uranyl nitrate
	HST-001-007	
	HST-001-008	
	HST-001-009	
	HST-001-010	
	HST-002-001	
	HST-002-003	
HEU-SOL-THERM-002	HST-002-007	Concrete reflected cylinders of highly enriched solutions of uranyl nitrate
	HST-002-011	g., ,,,,,,,,,
	HST-002-013	
	HST-006-001	
	HST-006-002	
	HST-006-003	
	HST-006-004	
	HST-006-005	
	HST-006-006	
	HST-006-007	
	HST-006-008	
HEU-SOL-THERM-006	HST-006-009	Experiments with boron-poisoned highly enriched uranyl nitrate solution
	HST-006-010	
	HST-006-011	
	HST-006-022	
	HST-006-023	
	HST-006-024	
	HST-006-025	
	HST-006-026	
	HST-009-001	
HEU-SOL-THERM-009	HST-009-002	Water-reflected 6.4-liter spheres of enriched uranium oxyfluoride
302 303	HST-009-003	solutions

Experiment	Case	Description
	HST-009-004	
	LCT-005-001	
	LCT-005-002	
	LCT-005-003	
	LCT-005-004	
	LCT-005-005	
	LCT-005-006	
	LCT-005-007	
LELL COMP THERM OOF	LCT-005-008	Enriched uranium dioxide fuel rods in water containing dissolved
LEU-COMP-THERM-005	LCT-005-009	gadolinium
	LCT-005-010	
	LCT-005-011	
	LCT-005-012	
	LCT-005-013	
	LCT-005-014	
	LCT-005-015	
	LCT-005-016	
	LCT-007-001	
	LCT-007-002	
	LCT-007-003	
	LCT-007-004	
LEU COMAD TUEDAM OOZ	LCT-007-005	Webser well-stand 4.730 at 6/ provide advancional district final and amount
LEU-COMP-THERM-007	LCT-007-006	Water-reflected 4.738-wt.%-enriched uranium dioxide fuel-rod arrays
	LCT-007-007	
	LCT-007-008	
	LCT-007-009	
	LCT-007-010	
	LCT-041-001	
	LCT-041-002	
LEU-COMP-THERM-041	LCT-041-003	Storage arrays of 3%-enriched LWR assemblies: the CRISTO II experiment in the EOLE reactor
	LCT-041-004	in the Local reactor
	LCT-041-005	
	LMSCT-001-001	
	LMSCT-001-002	
LEU-MISC-THERM-001	LMSCT-001-003	Stacy heterogeneous cores: a 60-cm-diameter tank containing 5%-enriched UO ₂ fuel rods in 6%-enriched uranyl nitrate solutions, water-reflected
	LMSCT-001-004	002 fuer rous in 0%-enficied drang mitrate solutions, water-reflected
	LMSCT-001-005	
	LMSCT-002-001	
	LMSCT-002-002	
LELL BAICO THERSA COS	LMSCT-002-003	Stacy: a 60-cm-diameter tank containing 5%-enriched UO ₂ fuel rods (2.1-
LEU-MISC-THERM-002	LMSCT-002-004	cm square lattice pitch) in 6%-enriched uranyl nitrate solutions, unreflected
	LMSCT-002-005	<u> </u>
	LMSCT-002-006	
LEU-SOL-THERM-002	LST-002-001	174 liter spheres of low enriched (4.9%) uranium oxyfluoride solutions

Experiment	Case	Description
	LST-002-002	
	LST-002-003	
	LST-004-001	
	LST-004-029	
	LST-004-033	
LEU-SOL-THERM-004	LST-004-034	Stacy: water-reflected 10%-enriched uranyl nitrate solution in a 60-cm- diameter cylindrical tank
	LST-004-046	diameter cymunical tank
	LST-004-051	
	LST-004-054	
	LST-007-014	
	LST-007-030	
LEU-SOL-THERM-007	LST-007-032	Stacy: unreflected 10%-enriched uranyl nitrate solution in a 60-cm- diameter cylindrical tank
	LST-007-036	diameter cymidical tank
	LST-007-049	
	LST-008-072	
LEU-SOL-THERM-008	LST-008-074	Stacy: 60-cm-diameter cylinders of 10%-enriched uranyl nitrate solutions
	LST-008-076	reflected with concrete
	LST-008-078	
	LST-009-092	
LEU-SOL-THERM-009	LST-009-093	Stacy: 60-cm-diameter cylinders of 10%-enriched uranyl nitrate solutions reflected with borated concrete
	LST-009-094	renected with borated contrete
	LST-010-083	
LELL COL THERM 010	LST-010-085	Stacy: 60-cm-diameter cylinders of 10%-enriched uranyl nitrate solutions
LEU-SOL-THERM-010	LST-010-086	reflected with polyethylene
	LST-010-088	
	MCT-011-001	
	MCT-011-002	
MIV COMP THERM 011	MCT-011-003	Water reflected mixed plutenium uranium evide (20 ut % nu) ninc
MIX-COMP-THERM-011	MCT-011-004	Water-reflected mixed plutonium-uranium oxide (20 wt.% pu) pins
	MCT-011-005	
	MCT-011-006	
	MMSCT-001-106	
	MMSCT-001-107	
	MMSCT-001-109	
	MMSCT-001-110	
	MMSCT-001-111	
MIX-MISC-THERM-001	MMSCT-001-112	Mixed oxide fuel-pin lattice in plutonium-uranium nitrate solution
	MMSCT-001-113	
	MMSCT-001-114	
	MMSCT-001-115	
	MMSCT-001-116	
	MMSCT-001-117	
MIX-MISC-THERM-002	MMSCT-002-001	
INITA-INITAC-1 HERINI-UUZ	MMSCT-002-002	

Experiment	Case	Description
	MMSCT-002-003	Mixed Oxide RAPSODIE fuel pin arrays moderated by dilute plutonium
	MMSCT-002-004	nitrate solution (9.89, 10.07, OR 19.6 g Pu/l) and reflected by water
	MMSCT-002-005	
	MMSCT-002-006	
	MMSCT-002-007	
	MMSCT-002-008	
	MMSCT-002-009	
	MMSCT-002-010	
	MMSCT-002-011	
	MMSCT-002-012	
	MMSCT-004-001	
	MMSCT-004-002	
MIX-MISC-THERM-004	MMSCT-004-003	Water-reflected triangular-pitched lattice of mixed oxide fuel rods
WIIX-WIISC-TTILKWI-004	MMSCT-004-004	immersed in plutonium / uranyl nitrate solution containing gadolinium
	MMSCT-004-005	
	MMSCT-004-006	
PU-MET-FAST-001	PMF-001-001	Bare sphere of plutonium-239 metal (4.5 at.%. 240Pu, 1.02 wt.% Ga)
PU-MET-FAST-002	PMF-002-001	240 Pu JEZEBEL: bare sphere of plutonium-239 metal (20.1 at.% 240 Pu, 1.01 wt.% Ga)
PU-MET-FAST-024	PMF-024-001	Polyethylene-reflected spherical assembly of 239PU(δ , 98%)
	PST-001-001	
	PST-001-002	
DU COL TUEDA 004	PST-001-003	Water reflected 44.5 inch dispersion sub-curs of physical increases callitings
PU-SOL-THERM-001	PST-001-004	Water-reflected 11.5-inch diameter spheres of plutonium nitrate solutions
	PST-001-005	
	PST-001-006	
	PST-002-001	
PU-SOL-THERM-002	PST-002-003	Water-reflected 12-inch diameter spheres of plutonium nitrate solutions
	PST-002-007	
	PST-003-001	
PU-SOL-THERM-003	PST-003-003	Water-reflected 13-inch diameter spheres of plutonium nitrate solutions
	PST-003-006	
	PST-004-002	
	PST-004-003	
DIL COL TUEDM 004	PST-004-005	Water-reflected 14-inch diameter spheres of plutonium nitrate solutions,
PU-SOL-THERM-004	PST-004-006	0.54% to 3.43% 240pu
	PST-004-008	
	PST-004-011	
DII COI THEBRA COF	PST-005-001	Water-reflected 14-inch diameter spheres of plutonium nitrate solutions,
PU-SOL-THERM-005	PST-005-005	4.05% and 4.40% pu240

Experiment	Case	Description
	PST-005-007	
PU-SOL-THERM-006	PST-006-002	Water-reflected 15-inch diameter spheres of plutonium nitrate solutions
	PST-023-001	
	PST-023-002	
	PST-023-003	
	PST-023-004	
	PST-023-005	
	PST-023-006	
	PST-023-007	
	PST-023-008	
	PST-023-009	
	PST-023-010	
	PST-023-011	
	PST-023-012	
	PST-023-013	
	PST-023-014	
	PST-023-015	
	PST-023-016	
PU-SOL-THERM-023	PST-023-017	Plutonium (33.89% and 4.23% 240 Pu) nitrate solutions in two water-
10 301 111211111 023	PST-023-018	reflected cylindric concentric tanks
	PST-023-019	
	PST-023-020	
	PST-023-021	
	PST-023-022	
	PST-023-023	
	PST-023-024	
	PST-023-025	
	PST-023-026	
	PST-023-027	
	PST-023-028	
	PST-023-029	
	PST-023-030	
	PST-023-031	
	PST-023-032	
	PST-023-033	
	PST-023-034	

5. RESULTS AND DISCUSSION

The APOLLO2-MORET 5 (AP2M5) comparison results are reported with a Monte Carlo standard deviation of 0.00050. The TRIPOLI-4® (T4) comparison results are reported with a Monte Carlo standard deviation lower than 0.00050.

The C-E results are reported for each code and the difference between deterministic codes and the TRIPOLI-4® continuous energy code are given to assess the calculation scheme effect.

5.1 COMPARISON TO EXPERIMENTS

The (calculation – benchmark) keff differences are reported in Figure 1 to Figure 6. The red dotted lines correspond with the experimental uncertainties at the 3σ level. The treatment of uncertainties is detailed in section 3.

A good agreement between the calculated keff and the benchmark keff is obtained for all codes for LEU-SOL-THERM, HEU-SOL-THERM, LEU-COMP-THERM, MIX-MISC-THERM, PU-MET-FAST and PU-SOL-THERM series. However, some discrepancies are noticed for very few cases:

- MIX-MISC-THERM-001-117,
- MIX-MISC-THERM-002,
- LEU-COMP-THERM-007-002,
- LEU-COMP-THERM-005-15 and -16.

Regarding LEU-COMP-THERM-007-002 case, significant discrepancy can be outlined for the APOLLO2-Sn route.

Regarding LEU-COMP-THERM-005 series, significant discrepancies are noticed for cases 15 and 16 and for each route.

Regarding LEU-MISC-THERM, there is a general trend to overestimate keff for multigroup routes APOLLO2-Sn and APOLLO2-MORET 5, the agreement being better for TRIPOLI-4®. This comparison between the standard route and the continuous energy route highlights the impact of the multigroup approximation.

At least, calculated keff and benchmark keff of MIX-MISC-THERM benchmarks are roughly in good agreement. However, APOLLO2-Sn keff results of MIX-MISC-THERM-001-117 and MIX-MISC-THERM-002 are slightly overestimated.

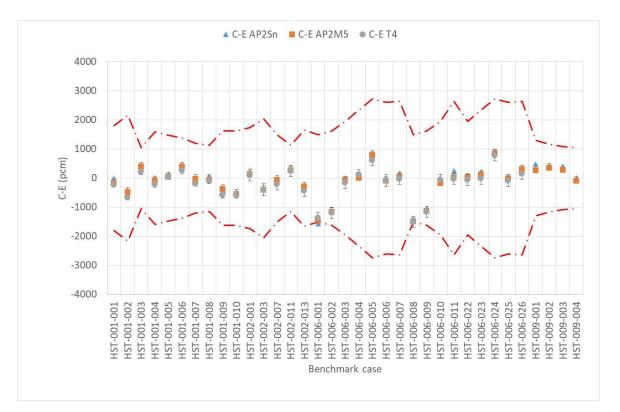


Figure 1 : C-E results for HEU-SOL-THERM experiments.

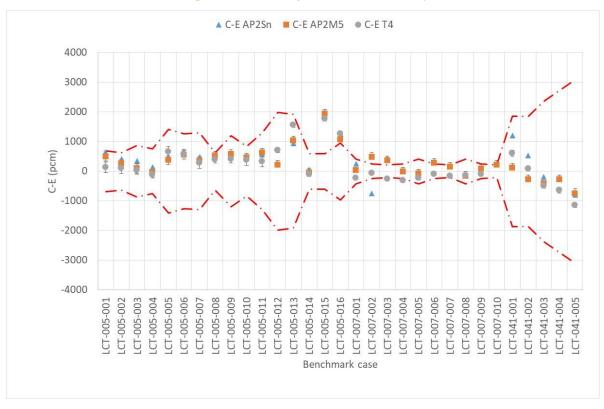


Figure 2: C-E results for LEU-COMP-THERM experiments.

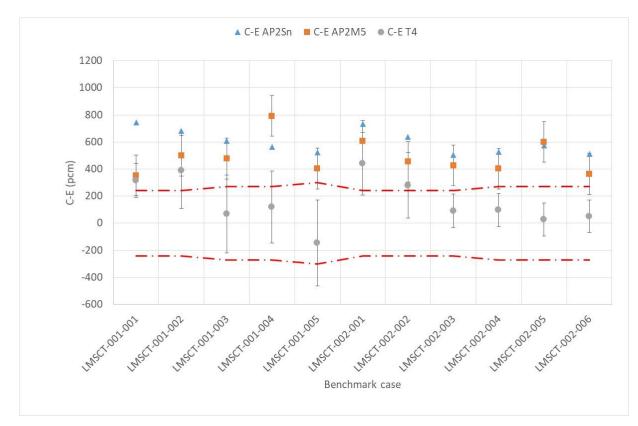


Figure 3: C-E results for LEU-MISC-THERM experiments.

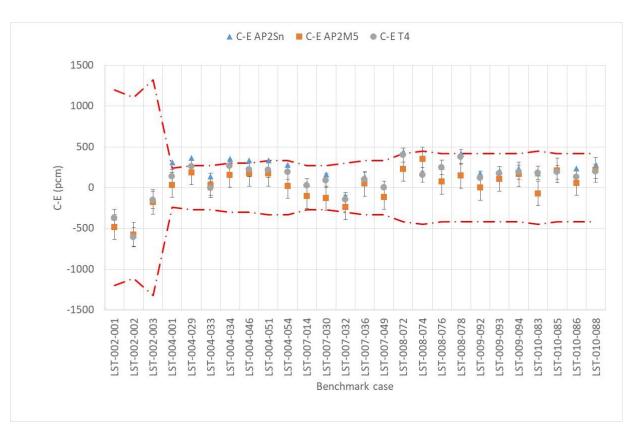


Figure 4: C-E results for LEU-SOL-THERM experiments.

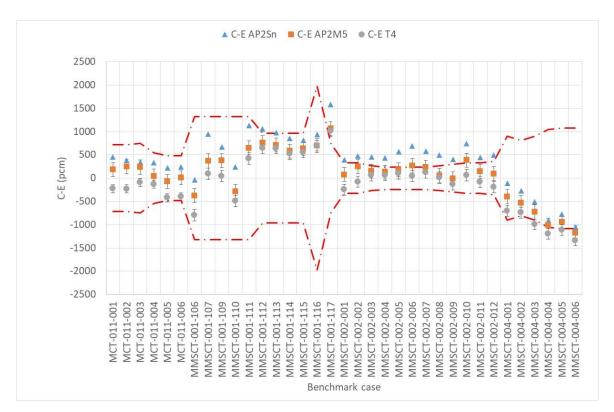


Figure 5: C-E results for MIX-COMP-THERM and MIX-MISC-THERM experiments.

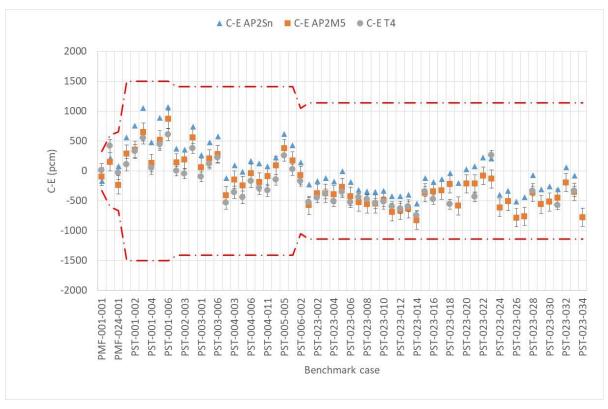


Figure 6: C-E results for PU-MET-FAST and PU-SOL-THERM experiments.

5.2 CODE TO CODE COMPARISON

The code-to-code keff differences (C-C in the figures) are reported in Figure 7 to Figure 12. Each multi-group route (APOLLO2-Sn or APOLLO2-MORET 5) is compared to the continuous energy route TRIPOLI-4®code.

Error bars on the Monte-Carlo differences between results are provided with a 3o. These error bars reflect the square root of the sums in quadrature of the Monte Carlo standard deviations of the codes.

Finally, they are no significant keff differences between the multi-group routes and the TRIPOLI4® route for homogeneous media (solutions, powders...) whereas some slightly significant keff differences are observed for heterogeneous media (assemblies, dissolvers, ...).

APOLLO2-Sn compared with TRIPOLI-4

For HEU-SOL-THERM and LEU-SOL-THERM benchmarks, there is no significant difference between APOLLO2-Sn and TRIPOLI-4® results, meaning that the calculation scheme effect is insignificant.

For LEU-COMP-THERM benchmarks, a calculation scheme effect can be pointed out for LEU-COMP-THERM-007, LEU-COMP-THERM-005 (except cases 5, 6 and 10), and LEU-COMP-THERM-041 series.

For LEU-COMP-THERM-007, there is a tendency to overestimate keff that depends on the moderation ratio.

For LEU-COMP-THERM-041, APOLLO2-Sn overestimates keff by 450-600 pcm. The multigroup treatment of nuclear data as well as their homogenization and collapsing of cross sections in 20 energy groups structure are responsible for these tendencies.

For LEU-MISC-THERM, we can see a significant calculation scheme effect between multi-group routes and the continuous energy TRIPOLI-4® route. This effect is due to the multi-group treatment of cross sections and to the collapsing of cross sections for the APOLLO2-Sn calculation route.

For MIX-COMP-THERM and MIX-MISC-THERM, there is an overestimation ranging from about 200 pcm to 800 pcm for the APOLLO2-Sn route. This calculation scheme effect is due to the multi-group treatment of cross sections, homogenization and collapsing of cross sections in the APOLLO2-Sn calculation route.

For PU-SOL-THERM benchmarks, APOLLO2-Sn overestimates keff for PST-001 and PST-004 to PST-006 (340 to 500 pcm). Cases 4, 5, 6, 18 and 21 of PU-SOL-THERM-023 are overestimated by 170 pcm to 370 pcm; case 23 is underestimated by -200 pcm.

PU-MET-FAST-001 and -002 benchmarks are slightly underestimated (-200 pcm).

APOLLO2-MORET 5 compared with TRIPOLI-4

For HEU-SOL-THERM and LEU-SOL-THERM benchmarks, there is no significant difference between APOLLO2-MORET 5 and TRIPOLI-4® results, meaning that the calculation scheme effect is insignificant.

For LEU-COMP-THERM benchmarks, a calculation scheme effect can be pointed out for LEU-COMP-THERM-007, LEU-COMP-THERM-005 (cases 1, 5, 11, 12, 13), and LEU-COMP-THERM-041 series.

For LEU-COMP-THERM-007, there is a tendency to overestimate keff that depends on the moderation ratio.

For LEU-COMP-THERM-041, APOLLO2-MORET 5 underestimates keff by 350-500 pcm when compared to TRIPOLI-4 for case 1 and 2. Cases 4 and 5 are overestimated by around 400 pcm with APOLLO2-Sn. The multigroup treatment of nuclear data as well as their homogenization are responsible for these tendencies.

For LEU-MISC-THERM, we can see a significant calculation scheme effect between APOLLO2-MORET 5 routes and the continuous energy TRIPOLI-4® route from 300 pcm to 670 pcm, except for cases 1 and 2 of LEU-MISC-THERM-001 and LEU-MISC-THERM-002. This effect is due to the multi-group treatment of cross sections for the multi-group route.

For MIX-COMP-THERM-011, there is an average +400 pcm difference between APOLLO2-MORET 5 and TRIPOLI-4®results.

For MIX-MISC-THERM-001, there is a significant overestimation of APOLLO2-MORET 5 for cases 106, 107, 109, 110 and 111.

For MIX-MISC-THERM-002, there is a significant overestimation of APOLLO2-MORET 5 for cases 1, 2 and 10 to 12.

For MIX-MISC-THERM-004, there is a significant overestimation of APOLLO2-MORET 5 for cases 1 to 3.

The calculation scheme effect is due to the multi-group treatment of cross sections and homogenization of cross sections in the APOLLO2-Pij calculation.

For PU-MET-FAST and PU-SOL-THERM benchmarks, APOLLO2-MORET 5 and TRIPOLI-4® are quite in a good agreement, except for a few cases. For instance, cases 18 and 23 of PU-SOL-THERM-023 are overestimated by 300-400 pcm. PU-SOL-THERM-001-006, PU-SOL-THERM-002-003, PU-SOL-THERM-004-011, PU-SOL-THERM-005-001 are slightly overestimated by 200-300 pcm.

PU-MET-FAST-002-001 is slightly underestimated by -260 pcm.

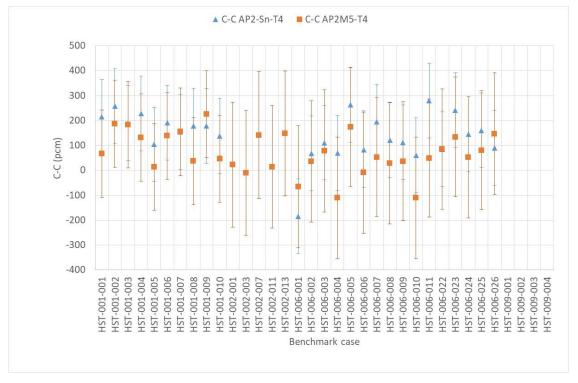


Figure 7: Code to code comparison for HEU-SOL-THERM experiments.

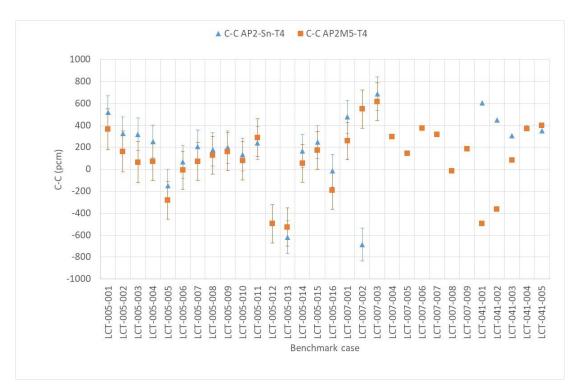


Figure 8: Code to code comparison for LEU-COMP-THERM experiments.

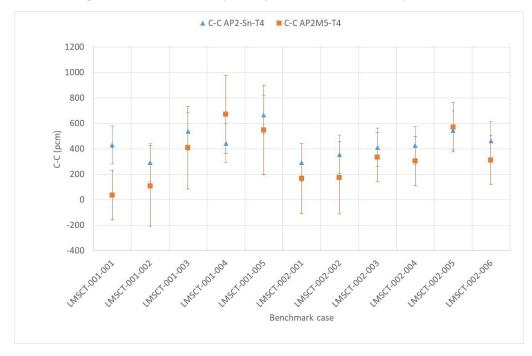


Figure 9: Code to code comparison for LEU-MISC-THERM experiments.

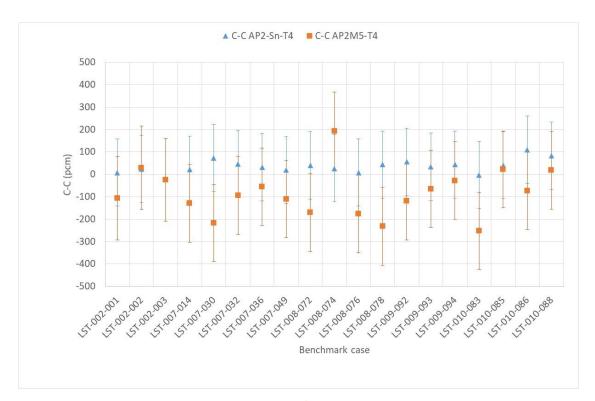


Figure 10: Code to code comparison for LEU-SOL-THERM experiments.

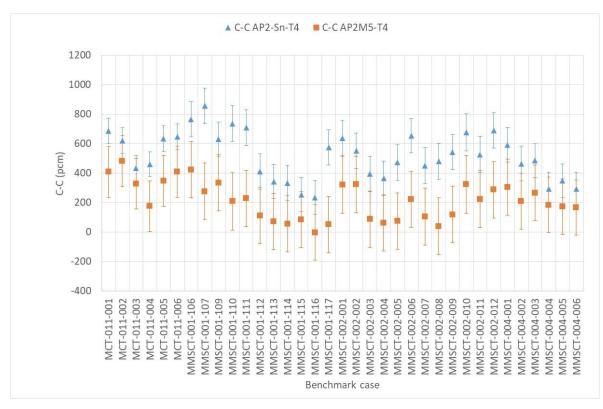


Figure 11: Code to code comparison for MIX-COMP-THERM and MIX-MISC-THERM experiments.

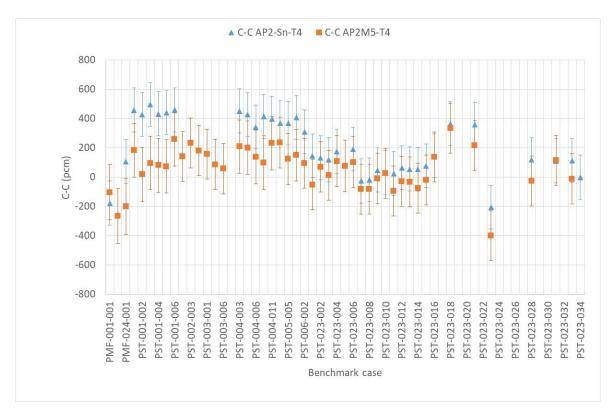


Figure 12: Code to code comparison for PU-MET-FAST and PU-SOL-THERM experiments.

Table 4: Results of the CRISTAL V2.0.3 validation

Identifier	Case	C-E (Sn)	C-E (AP2M5)	C-E (T4)	AP2M5-T4	AP2Sn-T4
	1	-8	-157	-224	67	216
	2	-412	-483	-670	187	258
	3	398	391	208	183	190
	4	9	-87	-219	132	228
	5	136	46	32	14	104
HEU-SOL-THERM-001	6	454	401	263	138	191
	7	-37	-36	-191	155	154
	8	78	-62	-100	38	178
	9	-417	-370	-596	226	179
	10	-457	-549	-595	46	138
	1		130	107	23	
	3		-414	-403	-11	
HEU-SOL-THERM-002	7		-64	-205	141	
	11		260	246	14	
	13		-295	-443	148	
	1	-1563	-1445	-1379	-66	-184
	2	-1126	-1158	-1194	36	68
	3	-50	-83	-161	78	111
	4	182	1	112	-111	70
	5	873	783	610	173	263
	6	-1	-91	-83	-8	82
	7	173	30	-23	53	196
HELL SOL THERM OOG	8	-1390	-1482	-1511	29	121
HEU-SOL-THERM-006	9	-1046	-1123	-1159	36	113
	10	-3	-174	-63	-111	60
	11	249	18	-31	49	280
	22	23	24	-61	85	84
	23	226	119	-15	134	241
	24	924	831	779	52	145
	25	60	-21	-101	80	161
	26	238	295	148	147	90
	1	481	265			
HEU-SOL-THERM-009	2	441	340			
TIEO SOL-THENIVI-003	3	409	289			
	4	6	-102			
LEU-COMP-THERM-041	1	1210	111	606	-495	604

Identifier	Case	C-E (Sn)	C-E (AP2M5)	C-E (T4)	AP2M5-T4	AP2Sn-T4
	2	538	-275	87	-362	451
	3	-188	-412	-495	83	307
	4	-263	-274	-645	371	382
	5	-795	-746	-1146	400	351
	14	44	-106	23	-129	21
	30	163	-128	89	-217	74
LEU-SOL-THERM-007	32	-100	-241	-147	-94	47
	36	134	47	102	-55	32
	49	17	-113	-2	-111	19
	72	439	229	399	-170	40
1511 CO1 TUEDA 1000	74	184	351	157	194	27
LEU-SOL-THERM-008	76	257	73	249	-176	8
	78	422	147	378	-231	44
	92	173	-2	117	-119	56
LEU-SOL-THERM-009	93	206	107	172	-65	34
	94	236	164	192	-28	44
	83	179	-71	181	-252	-2
15U COL TUEDA A 040	85	230	211	189	22	41
LEU-SOL-THERM-010	86	240	57	130	-73	110
	88	283	218	200	18	83
	106	-32	-373	-797	424	765
	107	950	369	92	277	858
	109	676	379	44	335	632
	110	246	-281	-490	209	736
	111	1132	652	423	229	709
MIX-MISC-THERM-001	112	1059	760	647	113	412
	113	979	710	636	74	343
	114	858	582	525	57	333
	115	811	641	556	85	255
	116	936	699	700	-1	236
	117	1588	1064	1012	52	576
	1	391	75	-247	322	638
	2	476	248	-76	324	552
	3	460	152	64	88	396
AAIV AAICO TUEDAA 003	4	433	131	67	64	366
MIX-MISC-THERM-002	5	575	177	102	75	473
	6	698	269	44	225	654
	7	580	232	127	105	453
	8	494	52	12	40	482

Identifier	Case	C-E (Sn)	C-E (AP2M5)	C-E (T4)	AP2M5-T4	AP2Sn-T4
	9	410	-12	-132	120	542
	10	741	387	62	325	679
	11	444	141	-83	224	527
	12	497	95	-193	288	690
	1	-110	-399	-704	305	594
	2	-275	-531	-741	210	466
MALV MAICC THERMA COA	3	-507	-726	-993	267	486
MIX-MISC-THERM-004	4	-906	-1014	-1199	185	293
	5	-768	-944	-1117	173	349
	6	-1049	-1176	-1344	168	295
PU-MET-FAST-001	1	-167	-94	10	-104	-177
PU-MET-FAST-002	1	215	151	416	-265	-201
	1	-227	-575	-524	-51	147
	2	-166	-380	-450	70	134
	3	-117	-372	-386	14	119
	4	-178	-395	-505	110	177
	5	-5	-271	-348	77	193
	6	-183	-423	-526	103	193
	7	-317	-523	-442	-81	-25
	8	-342	-554	-474	-80	-18
	9	-345	-552	-544	-8	49
	10	-334	-487	-514	27	30
	11	-420	-689	-595	-94	25
	12	-419	-661	-633	-28	64
	13	-394	-633	-600	-33	56
PU-SOL-THERM-023	14	-543	-823	-748	-75	55
	15	-119	-366	-346	-20	77
	16	-182	-340	-478	138	146
	17	-137	-328			
	18	-39	-219	-555	336	366
	19	-200	-583			
	20	28	-214			
	21	77	-216	-434	218	361
	22	229	-81			
	23	212	-133	266	-399	-204
	24	-399	-615			
	25	-335	-509			
	26	-514	-784			
	27	-440	-759			

Identifier	Case	C-E (Sn)	C-E (AP2M5)	C-E (T4)	AP2M5-T4	AP2Sn-T4
	28	-66	-361	-335	-26	119
	29	-306	-559			
	30	-255	-518			
	31	-307	-453	-569	116	112
	32	64	-192			
	33	-76	-351	-339	-12	113
	34		-775			
	1	655	501	137	364	518
	2	424	257	96	161	328
	3	347	93	29	64	318
	4	147	-37	-107	70	254
	5	506	375	656	-281	-150
	6	643	564	573	-9	70
	7	488	352	281	71	207
	8	583	530	402	128	181
LEU-COMP-THERM-005	9	605	568	407	161	198
	10	519	463	386	77	133
	11	574	621	333	288	241
	12		215	711	-496	
	13	940	1034	1560	-526	-620
	14	67	-45	-98	53	165
	15	2017	1940	1769	171	248
	16	1253	1074	1266	-192	-13
	1	257	36	-221	257	478
	2	-750	483	-65	548	-685
	3	430	356	-259	615	689
	4		-19	-315	296	
	5		-87	-231	144	
LEU-COMP-THERM-007	6		284	-90	374	
	7		152	-163	315	
	8		-157	-142	-15	
	9		87	-99	186	
	10		213			
	1	746	353	315	38	431
	2	682	499	389	110	293
LEU-MISC-THERM-001	3	607	477	67	410	540
	4	566	792	120	672	446
	5	524	404	-145	549	669
LEU-MISC-THERM-002	1	734	607	440	167	294

Identifier	Case	C-E (Sn)	C-E (AP2M5)	C-E (T4)	AP2M5-T4	AP2Sn-T4
	2	638	454	280	174	358
	3	505	427	92	335	413
	4	526	403	98	305	428
	5	576	600	28	572	548
	6	514	363	50	313	464
LEU-SOL-THERM-002	1	-367	-482	-375	-107	8
	2	-582	-576	-605	29	23
	3		-176	-152	-24	
MIX-COMP-THERM-011	1	460	181	-228	409	688
	2	389	248	-234	482	623
	3	341	237	-93	330	434
	4	330	45	-132	177	462
	5	217	-72	-419	347	636
	6	244	8	-403	411	647
PU-MET-FAST-024	1	76	-233	-32	-201	108
PU-SOL-THERM-006	2	142	-74	-169	95	311
	1	563	289	104	185	459
PU-SOL-THERM-001	2	761	352	333	19	428
	3	1052	651	554	97	498
	4	484	133	51	82	433
	5	888	521	447	74	441
	6	1068	866	608	258	460
PU-SOL-THERM-002	1	378	139	-3	142	381
	3	358	189	-46	235	404
	7	739	559	377	182	362
PU-SOL-THERM-003	1	264	58	-99	157	363
	3	478	205	118	87	360
	6	580	281	223	58	357
PU-SOL-THERM-004	2	-121	-409	-531	122	410
	3	96	-148	-357	209	453
	5	-14	-241	-443	202	429
	6	168	-37	-175	138	343
	8	132	-184	-284	100	416
	11	76	-92	-324	232	400
PU-SOL-THERM-005	1	228	94	-143	237	371
	5	624	379	255	124	369
	7	432	173	23	150	409

6. CONCLUSION

This report gives some views on the validation of the CRISTAL V2.0.3 package for a set of benchmarks of the ICSBEP handbook [5].

CRISTAL package has been validated on a wide range of applications cases corresponding to the use of criticality-safety practitioners.

A general good agreement between the calculated keff and the benchmark keff is obtained for each route for HEU-SOL-THERM, LEU-SOL-THERM, PU-MET-FAST and PU-SOL-THERM series. The JEFF-3.1.1 evaluation of nuclear data does not contribute to significant biases in the thermal and fast energy ranges.

An overall quite good agreement is also observed for LEU-COMP-THERM series without absorbers and metallic reflectors surrounding the assembly of UO₂ rods and without vacant rods in the assembly.

The homogenization and multi-group treatment of cross section seem correctly addressed.

For UO2 assemblies with absorbers and metallic reflectors, a significant bias was identified in connection with the multigroup treatment of nuclear data.

TRIPOLI-4 calculations could be used as check-calculations for such configurations as well as for configurations with heterogeneities (vacant rod positions).

Regarding LEU-MISC-THERM and MIX-MISC-THERM, there is a general trend to overestimate keff for multigroup codes, the agreement between the benchmark keff and the calculated one being better for TRIPOLI-4®.

7. REFERENCES

- [1] A. SANTAMARINA, D. BERNARD, P. BLAISE, M. COSTE, A. COURCELLE, T.D. HUYNH, C. JOUANNE, P. LECONTE, O. LITAIZE, S. MENGELLE, G. NOGUERE, J-M. RUGGIERI, O. SEROT, J. TOMMASI, C. VAGLIO, J-F. VIDAL, The JEFF-3.1.1 Nuclear Data Library JEFF Report 22 Validation Results from JEF-2.2 to JEFF-3.1.1, NUCLEAR ENERGY AGENCY, ISBN 978-92-64-99074-6
- [2] F. DAMIAN, A. COLLIN, N. GERARD-CASTAING, C. JOUGLARD, A. ZOIA, Validation of APOLLO2 toward Monte Carlo TRIPOLI-4 throughout irradiation: transposition of the process on critical fuel assembly configurations, PHYSOR 2018
- [3] J.M. GOMIT, I. DUHAMEL, Y. RICHET, A. ENTRINGER, C. MAGNAUD, F. MALOUCH, C. CARMOUZE, CRISTAL v2: new package for criticality calculations, NCSD2022, Anaheim, USA
- [4] J J.M. GOMIT, C. CARMOUZE, B. COCHET, N. LECLAIRE, F. DAMIAN, A. ENTRINGER, E. GAGNIER, CRISTAL-V2/NDP_V2.0/B, CRISTAL V2.0 Package. Principles and Validation Domain, CRISTAL-V2 Project team 2016 July
- [5] NEA Nuclear Science Committee International Handbook of Evaluated Criticality Benchmark Experiments NEA/NSC/DOC (95)03 – September 2021

Keywords:

CRISTAL, criticality calculation, safety, validation

Tables and illustration table

Illustrations

Figure 1 : C-E results for HEU-SOL-THERM experiments	16
Figure 2: C-E results for LEU-COMP-THERM experiments.	16
Figure 3: C-E results for LEU-MISC-THERM experiments.	17
Figure 4: C-E results for LEU-SOL-THERM experiments.	17
Figure 5: C-E results for MCT and MIX-MISC-THERM experiments	18
Figure 6: C-E results for PMF and PU-SOL-THERM experiments.	18
Figure 7: Code to code comparison for HEU-SOL-THERM experiments.	20
Figure 8: Code to code comparison for LEU-COMP-THERM experiments.	21
Figure 9: Code to code comparison for LEU-MISC-THERM experiments.	21
Figure 10: Code to code comparison for LEU-SOL-THERM experiments.	22
Figure 11: Code to code comparison for MIX-COMP-THERM and MIX-MISC-THERM experiments	22
Figure 12: Code to code comparison for PU-MET-FAST and PU-SOL-THERM experiments	23
Tables	
Table 1 : Codes and libraries used in the V2.0.3 release	
Table 2 : Classification of ICSBEP benchmarks	
Table 3: List of selected cases	10
Table 4: Results of the CRISTAL V2.0.3 validation	24

IRSN

Nuclear Safety Division

CRISTAL PROJECT

Number: CRISTAL/NT/2024-1

E-mail

cristal@irsn.fr

Report number

Report IRSN 2024-00100 All rights reserved CRISTAL Project / IRSN Februrary 2024



31, avenue de la division Leclerc 92260 Fontenay-aux-Roses RCS Nanterre B 440 546 018

MAIILNG ADRESSE

B.P 17 92260 Fontenay-aux-Roses Cedex PHONE

+33 (0)1 58 35 88 88

WEBSITE

www.irsn.fr

Email

contact@irsn.fr

● @IRSNFrance