WPEC - SG45: procedure for the validation of IRSN criticality input decks

LECLAIRE Nicolas
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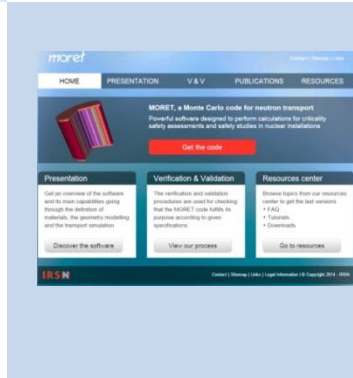1. **IRSN calculations with MC codes**

2. **Validation database**

3. **Procedure**

   a) **Construction of input decks**

   b) **Data relating to chemical data**

   c) **Geometry and simulation options**

   d) **Verification – check lists**

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IRSN calculations with MC codes

Use of CRISTAL criticality package

- 3 calculation routes:
    - APOLLO2-MORET 5
        - Using the APOLLO2 deterministic code for the generation of homogenized, self-shielded cross sections and flux with p_{ij} method
        - MORET 5.B.1 for the 3D transport calculation
            - » Used by criticality safety assessment teams
            - » Used by criticality safety practitioners outside IRSN
            - » Used by research and development team: validation of CRISTAL
    - APOLLO2-Sn: 1D or 2D calculation
    - TRIPOLI-4: continuous energy 3D transport calculation (reference route)

Use of the MORET 5 continuous energy code for research

- Along with JEFF-3.1.1, JEFF-3.2, ENDF/B-VII.1… at ACE format
    - Homemade processing using the GAIA 1.1 tool based on NJOY2016.03
- By research and development teams
    - Testing last nuclear data libraries: JEFF-3.3, ENDF/B-VIII.0
    - Use of sensitivity capability in relation with GLLSM in MACSENS and TSURFER

Validation database
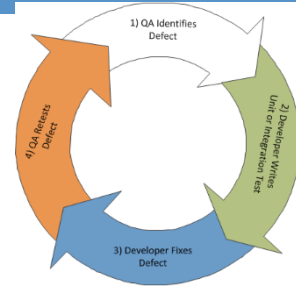
CRISTAL package APOLLO2-MORET 5 route

- More than 2200 experimental cases
  - Various criticality safety applications covering the whole management of fuel cycle
  - In keeping with other codes from CRISTAL package (APOLLO2-Sn and TRIPOLI-4): maximum of common cases

MORET 5 continuous energy code

- More than 1200 experimental cases for criticality issues
  - Some in common with APOLLO2-MORET 5
  - Data of interest: mainly k_{eff}
- Ever growing database for reactor physics applications
  - Data of interest: k_{eff}, reaction rates, kinetics parameters, fluxes, …

Under QA procedure

- Independent review of input decks saved on Gforges platform
  - Signature by author and reviewer of check-list

Construction of input decks

▌ **Name of the input deck follows ICSBEP nomenclature**
  - Ex: PU-SOL-THERM-022-d.c01: solution of plutonium nitrate in thermal energy spectrum, series 22, case 1 and detailed model
    - Differentiation between detailed and simplified model
    - Number of case in a series consistent with what is given in section 3 of ICSBEP Handbook

▌ **Cartridge describing the configuration**
  - Chemical and geometrical characteristics, category with respect to the validation database ordering (POWDER, METAL, SOLUTION, LATTICE...`
  - Benchmark k_{eff} and associated uncertainty (1σ, 2σ, 3σ?)
  - Name of laboratory
  - Simplifications: missing isotopes?
  - Review number of ICSBEP
  - Writer and reviewer, company, date of review, signature

```
**********************************************
*                                            *
*              I.R.S.N/SNC                    *
*            APOLLO2  MORET 5                 *
*                                            *
**********************************************
*                                            *
*            PU-SOL-THERM-022                 *
*                 VALDUC                      *
*              ICSBEP volume 1                *
*                révision 0                   *
*                 case 1                      *
*         CATEGORIE : SOLUTION                *
**********************************************
*        PU(NO3)4   C(PU) = 152 g/l           *
*      75 % 239PU - H+ = 3.85 N               *
*         REFLECTEUR EAU (20 cm)              *
*         diamètre externe = 50 cm            *
* keff(exp) = 1.0000 +/- 0.00229  (1 sigma)   *
**********************************************
* writer: N. LECLAIRE  reviewer. G. POULLOT   *
**********************************************
```

▌ **Input decks APOLLO2-MORET 5**
  - Many comments to make clear what the geometry is

Data relative to chemical media

▌Corresponding to section 3 of benchmark

▌If natural isotope, use natural if available

▌If missing isotopes in the library, it is recommended to forget it and not to replace it by another one unless an equivalence in terms of reaction rates has been proved

▌If natural isotope split into isotopes, use the isotopes

▌Indicate when isotopes are omitted

▌Chemical link to model the thermalization S(α,β)
  ▪ H-H_2O, D-D_2O, Be-BeO, Zr-ZrH, H-ZrH

Geometry and Simulation options

Geometry Review
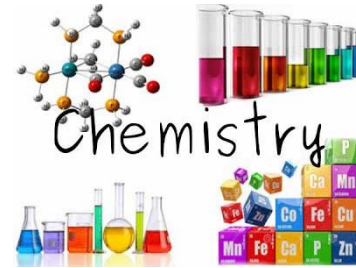
▌ Specify if detailed or simplified model

▌ Description of geometry based on section 3

▌ If missing data, look at section 1

▌ Give explicit description in the comments for each volume

▌ Simulation options
  - Number of neutrons per batch must not be under-estimated
    - At least 10000 neutrons for small criticality geometry
    - Up to 100000 neutrons for reactor physics geometry
    - Number of batch depends of the target Monte Carlo standard deviation
    - In MORET, the MC standard deviation is chosen so that the combined standard deviation does not exceed by 10% the experimental uncertainty
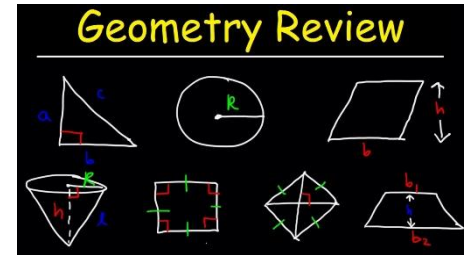
Verification

▌ Can be done either on the printed version of the input deck or on electronic version with a comparison tool
- Corrections to be made indicated on printed version
- Signature and date of verification of the reviewer
- Comments of the author after verification and signature

▌ In paralell, a check list is created
- First part filled by the author
  - Description of the benchmark
- Second part filled by reviewer
  - Calculated k_{eff} and MC standard deviation
  - Platform on which calculation has been launched
  - Simulation options
    – Number of neutrons per batch, number of batches, Chi2 test
    – Eliminate transient by removing 100 first steps
  - Position of sources

▌ Electronic and paper version of input decks transmitted to validation database manager

Check List

To be filled by the author								
Name of series								
Category								
Case n°								
Reference of description								
N° + Revision date	Revision X of							
Author								
Date								
Reviewer								
Experimental k_{eff}								
Δ experimental								
Δ experimental / σ experimental								
Known confidence interval?								

Check List

To be filled by reviewer of the benchmark								
Procedure respected? PSN-EXP/SNC/2016-406								
Cartridge filled correctly?								
Name of files?								
Calculation route								
Platform								
Calculated k_{eff}								
σ **calculation**								
Simulation criteria								
Number of batches MINI > 150?								
Number of neutrons per batch								
Apparent convergence								
Khi 2 test: 6/6 ?								
Consistent estimators?								
σ**(calcul) < 0,458 x** σ**(experimental) ?**								
Consistent between cases								
Position of sources?								
Remarks								
DATE AND SIGNATURE AUTHOR:				**DATE AND SIGNATURE REVIEWER:**				

Classification in validation database

Under Gforges: management of configurations

- Various validation database: CRISTAL V2.0, CRISTAL V1.2
- Date of modifications

Various folders

- INPUT DECK
- LISTING
- GRAPH
- RESUME
- OUTPUT.XML

Base de Qualification

Index of /CRISTAL.V2.0/JDD

File ▲	Rev.	Age	Author
Parent Directory			
DISSOLVEURS/	98	4 years	leclaire
INTERACTION/	109	3 years	leclaire
JDD/	98	4 years	leclaire
METAL/	109	3 years	leclaire
POUDRES/	106	3 years	leclaire
RESEAUX/	108	3 years	leclaire
SOLUTION/	98	4 years	leclaire
SPEC/	98	4 years	leclaire
U233/	98	4 years	leclaire
applet_resources/	106	3 years	leclaire
Copie de secours de modele_rapport-qualif-restreinte-13-02.wbk	104	3 years	leclaire
Copie de secours de modele_rapport-qualif-restreinte-14-05-ID.wbk	106	3 years	leclaire
HST-poison.xlsx	106	3 years	leclaire
Qualification-06-02-2014.xlsx	99	4 years	leclaire
Qualification-result.xlsx	98	4 years	leclaire
V1-2-V2-0.xlsx	106	3 years	leclaire
complement-metalliques.docx	99	4 years	leclaire
list-keff-exp.csv	98	4 years	leclaire
metalliques.xlsx	104	3 years	leclaire
modele_rapport-qualif-restreinte-10-12.docx	98	4 years	leclaire
modele_rapport-qualif-restreinte-13-02.docx	104	3 years	leclaire

Tree classification in each folder

- Type of medium: 8 categories: powder, lattice, solution, dissolvor, SPEC, U233, metal, interaction …
  - ICSBEP identifier
    - » Case Number
    - » Input

Flowchart

Le·rédacteur·:¶
- → élabore·(ou·corrige)·les·jeux·de·données·(jdd)¶
- → lance·les·calculs¶
- → renseigne·la·check-list¶
- → transmet·au·vérificateur·la·check-list,·les·jdd·aux·formats· informatique·et·papier,·et·la·description·du·benchmark¶

Le·vérificateur·:¶
- → vérifie·la·conformité·des·jdd·au·descriptif·du· benchmark¶
- → vérifie·la·check-list¶

Les·jdd·et·la·check-list·sont-ils·validés·par·le·vérificateur?¶

NON¶

OUI¶

Le·rédacteur·(ou·le·vérificateur)·transmet·au·responsable·de· l'archivage·informatique·de·la·base·de·qualification·:¶
- → les·jdd·au·format·informatique¶
- → la·check-list¶

Le·responsable·de·l'archivage·informatique·de·la·base·de· qualification·:¶
- → vérifie·la·check-list¶
- → relance·les·calculs¶
- → vérifie·la·conformité·des·résultats·à·la·check-list¶

Les·jdd·et·la·check-list· sont-ils·conformes·à·la· procédure?¶

NON¶

OUI¶

Les·fichiers·jdd·et·résultats·sont·ajoutés·à·la·base·de·qualification· informatique.¶
Les·jdd·au·format·papier·validés·sont·transmis·au·responsable·de· l'archivage·papier·de·la·base·de·qualification.¶

Thanks for your attention!!

Questions ??