IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Enhancing nuclear safety

Procedure for Creating, Reviewing, and Submitting Input Files into the Benchmark Library

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OECD WebEx meeting

SG45

May 11, 2020

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Motivation and objectives

↳ Manage numerous criticality benchmarks input files generated, developed and maintained by various organizations

- Example in the US: MCNP (LANL), COG (LLNL), SCALE (ORNL)
- Example in Europe: MORET (IRSN)

- Standardize input file creation, review and maintenance
- Describe the procedure to follow in the creation of the input files and their integration in the experimental validation databases
- Describe the procedure on how to prepare and use of benchmarks for the validation of calculation routes
- Incorporate existing practices used by LANL with MCNP and also by IRSN with MORET (presented two years ago at SG45 meeting)
  - Review procedures

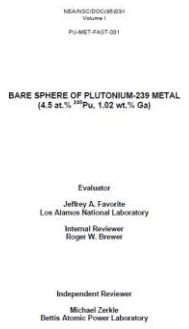
Creation of benchmark input files

Various steps

- Review benchmark description(geometry & materials)
- Model benchmark and create input files
- Verify input files and results
- Electronic archiving of input files and related documentation
- Create benchmark results report

Review the benchmark documentation

- Target: be consistent with the benchmark model described in the documentation (mainly section 3 of ICSBEP description)
- When there is doubt, consult detailed description of the ICSBEP benchmark (section 1)
- When an inconsistency is found between the two sections, it is allowed looking at the input files provided in the benchmark in order to solve the issue
  - Report such event to the authors of the benchmark description


NEA/NSC/DOC(95)03/I
Volume I
PU-MET-FAST-001

BARE SPHERE OF PLUTONIUM-239 METAL
(4.5 at.% ^{240}Pu, 1.02 wt.% Ga)

Evaluator
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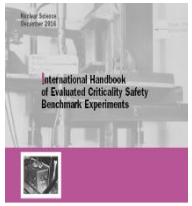
Los Alamos National Laboratory

Internal Reviewer
Roger W. Brewer

Independent Reviewer
Michael Zerkle
Bettis Atomic Power Laboratory

Model benchmarks

heu-met-fast-krusty-001-rev0-um.mcnp
heu-met-fast-001-001-simple-rev0.mcnp
leu-comp-therm-007-001-rev3.moret



Input file nomenclature

- Name: it should uniquely identify the benchmark
  - Freely chosen if not ICSBEP evaluation but ICSBEP preferred
    - ICSBEP identifier: heu-met-fast-001 (fissile/form/spectrum/series/case)
- Case number or name:
  - ICSBEP: case number as referenced in section 3 of the benchmark specification
  - If no case number are given (for instance, unique benchmark), then 1 is chosen
- **Optional model type:**
  - **In some benchmarks, two models (simplified/detailed) are proposed and this should be reflected in the input file name**
- **Revision number:**
  - **Should follow the ICSBEP revision number and be added whenever the benchmark specifications are modified**
    - **If first revision, rev0 is added to the end of input file identifier**
- Optional variant identifier:
  - Distinguish between options of the code (unstructured mesh in MCNP6)
- Name of code for which the input file is created (MCNP, SCALE, COG, MORET…)

Inter-comparison exercise

Model benchmarks

- Input file header
  - Calculation code name or calculation route
  - Name of organization that created it
  - Nomenclature (ICSBEP or other)
  - ICSBEP Handbook volume number **and revision number** (see inter-comparison exercise)
  - Optional model (simple/detailed) and variant type
  - Benchmark purpose
  - Benchmark aliases (pu-met-fast-002 is dirty jezebel)
  - Case number and/or experiment number (look at section 3 of ICSBEP document or document of benchmark selection)
  - Experiment multiplication factor and associated uncertainty with level of confidence
  - Other quantity of interest and associated uncertainty

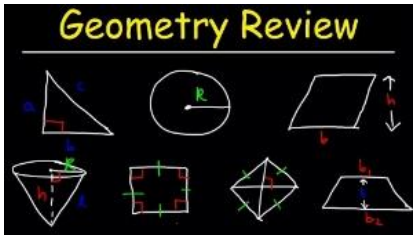
```
c file name : pu-met-fast-001-000-simple-rev4.mcnp
c
c organisation: lanl
c
c source : icsbep
c purpose : metal
c benchmark name : pu-met-sol-022
c benchmark alias : jezebel
c case : 0
c model type : simple
c revision : 4
c variant type : N/A
c code : mcnp
c
c type : effectiveMultiplicationFactor
c values : 1.000
c uncertainties : 0.00229
c
c type : effectiveDelayedNeutronFraction
c values : 0.00195
c uncertainties : 0.00010
```

Model benchmarks

Material composition

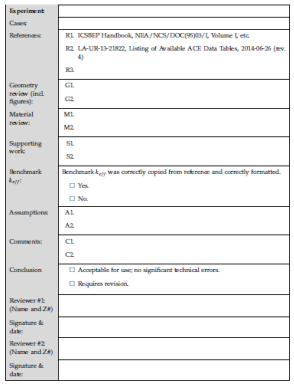
- Taken from benchmark specifications (section 3 of ICSBEP benchmark)
- No materials from other cases
- Same precision as in specifications
- Model chemical bonds between atoms using thermal scattering laws to take into account the effects of these bonds on the thermalization in the system
  - H_2O, CH_2, Be, O in BeO, Graphite, Fe, H in ZrH
- Natural elements if available, no decomposition in isotopes
- Policy for elements (and their isotopes) that are not available in the nuclear data libraries
  - Removed from the input file and atom density adjusted accordingly
- Policy for missing isotopes (in elements) in nuclear data libraries
  - Automatic procedure renormalizes the abundance (weight distribution on other isotopes) ➔ Indicate in the header of the input file ?
  - Default weight proportions **BUT** possibility to take them from a defined source (ICSBEP Handbook, other…)
- Case of H, C, N and O
  - User defined policy: H_1, C_{12}, N_{14}, O_{16} or O_{16} + O_{17}

Model benchmarks



- Geometry
  - Code default geometry specification
    - Constructive solid geometry for MCNP
  - Identical to the benchmark specifications (four decimal places prescribed in ICSBEP Handbook)
- Comments should be kept minimum (title, material name…)
- Calculation precision policy
  - Enough neutrons so that convergence can be achieved
  - Privilege the number of neutrons per batch to the number of batches
    - Feedback from Monte Carlo teams

Input file review



Experiment	
Case:	
References:	R1. ICSBEP Handbook, NEA/NCS/DOC(95)03/I, Volume I, etc. R2. LA-UR-13-21822, Listing of Available ACE Data Tables, 2014-06-26 (rev. 4) R3.
Geometry review (incl. figures):	G1. G2.
Material review:	M1. M2.
Supporting work:	S1. S2.
Benchmark k_{eff}:	Benchmark k_{eff} was correctly copied from reference and correctly formatted. ☐ Yes. ☐ No.
Assumptions:	A1. A2.
Comments:	C1. C2.
Conclusion	☐ Acceptable for use; no significant technical errors. ☐ Requires revision.
Reviewer #1 (Name and JM):	
Signature & date:	
Reviewer #2 (Name and JM):	
Signature & date:	

- Review of input files is mandatory
- Set in stone review procedures for each organization
  - LANL (MCNP), LLNL (COG), ORNL (SCALE), IRSN (MORET)
- Each organization is responsible for the review of its own input files and should apply its own review procedure
  - Based on the interaction between the author and a reviewer
- Check list should be filled by author and reviewer and transmitted for digital archive
  - Calculations run and follow procedures
    - Sufficient number of neutrons per cycle, good distribution within fissile volumes, consistence between all estimators of multiplication factor
  - Final input files run correctly
- Transmission of review documents to people in charge of validation database and people responsible for archiving the input files

Digital archive & repository

- Input files, material balance files and associated review documentation are to be included in the GIT repository for the code it relates to

- Repository for each individual calculation code

- Same structure for each code
  - First directory
    - Benchmark type designator: heu-met-fast
  - Subdirectory
    - Full benchmark name: heu-met-fast-001
      - Review documentation
        - Rev0: all files pertaining to the review procedure for the revision 0 files
        - Rev1: all files pertaining to the review procedure for the revision 1 files
        - …
      - pu-met-fast-001-001-simple-rev3.mcnp
      - pu-met-fast-001-001-simple-rev4.mcnp

Verification & validation summary

- Still in progress
  - Discussions are needed

- Proposal
  - Report containing
    - Calculation route and tools used (version numbers…)
    - Overview of ICSBEP classification
    - List of experimental and calculation results with the differences between them
    - Whenever available, comparison with other codes calculations that are normally used as references
    - Analysis of differences between experimental and calculation results
    - Deviations from benchmark specifications

Thanks for your attention!