OECD/NEA WPEC SG45

Progress review

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- Contributed input files
- Input file comparison
- Input file QA document
- General calculation results
- Material balance tables

Contributed input files

The OECD/NEA SG45 gitlab site has received 3 contributions

- IAEA Nuclear Data Section : MCNP input decks
- NRG (Steven Van der Marck) : MCNP input decks
- JAEA : MVP input decks

IAEA NDS : MCNP

- Main source : the Skip Kahler suite
- Additional sources :
  - ICSBEP CD or pdf files, this includes revisions: e.g. pu-met-fast-001 revision 4 (J. Favorite)
  - Inputs produced internally at the IAEA
- The nice thing about it :
  - Reference experimental data files associated to each input file that could be mined
  - Tallies for spectra and additional measurements
  - There’s 2828 total cases available

Contributed input files

NRG : MCNP

- Main source : ICSBEP appendices
- Additional sources :
  - Inputs produced internally at NRG
- The nice thing about it :
  - We can use these to complement the Kahler Suite
  - Not only keff benchmarks! There's some beff, Rossi-a and IRPhE benchmarks.

JAEA : MVP

- Main source : ICSBEP modelling by different authors over several years
- The nice thing about it :
  - It's not MCNP
- The downside:
  - It's not MCNP, I don't know how to parse MVP input files to easily get information out of them

Contributed input files

Additional contributions that have not been submitted yet

- LANL inputs (pending approval and QA archival – see my last presentation)
- LLNL inputs?
- ORNL inputs?

LANL inputs : MCNP and a few other codes

- Main source : the Skip Kahler and Russ Mosteller suite, which was produced at LANL
- Other sources :
  - The WHISPER suite (this one is undergoing QA since 2017)
  - The NCS suite (mainly the WHISPER suite, differences in uranium cases)
  - The XCP-5 Nuclear Data Team adds some PARTISN and SENSMG inputs
  - The Steven Van der Marck suite
- The nice thing about it :
  - The main sources of these sets are already on the OECD/NEA SG45 gitlab site

Input file comparison

DOE NCSP collaboration led by IRSN to compare results of transport codes and nuclear data for critical benchmarks

- IRSN: MORET with JEFF-3.3, ENDF/B-VII.1, -VIII.0 data
- LANL: MCNP6 with ENDF/B-VII.1 data
- LLNL: COG with ENDF/V-VII.1, -VIII.0, JEFF-3.3 data
- ORNL: SCALE with ENDF/B-VII.1 data

Impact at LANL for Pu and HEU:

- Reviewed 18 HEU Experiments & 10 Pu experiments where results appear inconsistent with other codes
- Report will be available : https://git.oecd-nea.org/science/wpec/sg45/documents

Input file comparison – LANL overview

70 cases reviewed, 33 input files revised

- 2 experiments updated to match revision in Handbook
  - PU-MET-FAST-001 → in 100 pcm Δ
  - HEU-MET-FAST-051 (10 cases) → in Δ 12 - 369 pcm
- 15 experiments used the wrong experimental keff and/or uncertainty
- 13 cases revised for material changes, < 50 pcm except:
  - PU-MET-FAST-003 → Δ 267pcm due to typo in the number density for 240Pu
  - PU-SOL-THERM-001 → 85 pcm Δ due to change in N abundances of plutonium nitrate solution
- 3 experiments (9 cases) revised for material changes & geometry errors:
  - HEU-COMP-INT-003-006 → Δ 84 pcm
  - HEU-MET-FAST-007-035 → Δ 737 pcm
  - PU-MET-FAST-045 → 7 cases all resulting in > 500 pcm Δ

Generally, geometry changes result in greater change than material changes

Input file comparison – LANL overview

Removed HEU-MET-FAST-077

- Feedback from LLNL
- Nimbus experiments not accepted into Handbook had already been added to LANL collection

Challenges that were identified

- Naming conventions
  - Simple vs. detailed model
  - Materials impurities vs. no impurities
- Revision, revision, and did I mention revision?
- Various specifications for natural abundances
- Setting up review & revision infrastructure

Input file QA document

Before we start producing input files under the SG45 VaNDaL banner, we need a QA document

Work on this aspect has included the following:

- Review of QA procedures from organisations that have put in place such a procedure
- Drafting a proposal for SG45 VaNDaL QA document
  - Formalising input for SG45 VaNDaL input file creation for all codes
  - Reusing review procedures that are already in place at different organisations
  - Take into account lessons learned from the intercomparison
- See presentation from Nicolas Leclaire (IRSN) for a more detailed overview

A draft document is/will be made available

- See https://git.oecd-nea.org/science/wpec/sg45/documents

General calculation results


```
[ { "type" : "effectiveMultiplicationFactor",
    "data" : { "values" : [ 1.0000 ],
               "uncertainties" : [ 0.0001 ] } },
  { "type" : "sensitivityProfile",
    "response" : "effectiveMultiplicationFactor",
    "parameter" : "crossSection",
    "particleId" : "neutron",
    "nuclide" : "U235",
    "reaction" : "fission",
    "material" : "total",
    "data" : { "values" : [ -1.7129e-17, 1.4106e-09 ],
               "uncertainties" : [ 0.0034, 0.0033 ],
               "structure" : [ { "name" : "energy-in",
                                 "type" : "histogram",
                                 "limits" : [ 1e-11, 10.0, 20.0 ],
                                 "unit" : "MeV"} ],
               "units" : { "value" : "%/%", "uncertainty" : "relative" } } } ]
```

General calculation results

Recent work on this format:

- The use of standardised nuclide identifiers and reactions for generic use
- LANL has developed a few applications involving sensitivity analysis using this format

The proposed calculation exchange format has been formalised

- Description document : LA-UR-19-32580 report
- Standardised schema for validation is available (https://json-schema.org)
- See https://git.oecd-nea.org/science/wpec/sg45/documents
  - LaTeX source of the report will be added later because … COVID19

More information : see previous WPEC SG45 meetings

Material balance tables

```
# example for pu-sol-therm-002-001-rev1
{ "materials" :
  { "Solution 1" : { "name": "Solution 1",
                     "nuclides": [ "H", "N", "O", "Fe", "Pu239", "Pu240" ],
                     "sab": [ "H-H2O" ],
                     "volume": 15120,
                     "totalAtomDensity": 0.100744779,
                     "atomDensity": { "H": 6.3772E-02, "N": 1.3452E-03, "O": 3.5500E-02,
                                      "Fe": 2.0380E-06, "Pu239": 1.2164E-04,
                                      "Pu240": 3.9010E-06 } } },
    "347 Stainless Steel" : { "name": "347 Stainless Steel",
                              "nuclides": [ "Fe", "Cr", "Ni" ],
                              "totalAtomDensity": 8.69144E-02,
                              "atomDensity": { "Fe": 6.0386E-02, "Cr": 1.6678E-02,
                                               "Ni": 9.8504E-03 } },
    "Water at 27C" : { "name": "Water at 27C",
                       "nuclides": [ "H", "O" ],
                       "sab": [ "H-H2O" ],
                       "totalAtomDensity": 9.9933E-02,
                       "atomDensity": { "H": 6.6622E-02, "O": 3.3311E-02 } } } }
```

Material balance tables

These tables can store information extracted from input and output

- To be used as part of comparing the input files from different codes
- To be used as a reference for verification of new input files

Recent work on these tables:

- The use of standardised nuclide identifiers for generic use
- The addition of a thermal scattering field to indicate which thermal scattering laws should be applied to each material
- LANL is producing some tables from the ICSBEP benchmark specifications

These material tables will be formalised

- Description document is being drafted
- Standardised schema for validation will be made available (https://json-schema.org)