OECD/NEA WPEC SG45

WPEC SG45 Progress Report

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May 15, 2020

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

May 15, 2020

Paris (France) – Santa Fe, NM (USA)

- Contributed input files
- SG45 documents
- SG45 input files

Contributed input files

The OECD/NEA SG45 gitlab site has received 3 contributions

- IAEA Nuclear Data Section : MCNP input decks
  - Skip Kahler suite and internally produced files
- NRG (Steven Van der Marck) : MCNP input decks
  - ICSBEP appendices and internally produced files
- JAEA : MVP input decks

LANL inputs not submitted yet (pending approval and QA archival)

- The main sources of these inputs are already on the OECD/NEA SG45 gitlab site
  - Skip Kahler and Russ Mosteller suite, which was produced at LANL
- Different suites maintained at LANL :
  - The WHISPER suite (based on the Kahler 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

SG45 documents

SG45 input file QA document:

- 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
- A draft document is/will be made available
  - See https://git.oecd-nea.org/science/wpec/sg45/documents

Material balance tables for input file verification

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

SG45 documents

Calculation result 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

```
# 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 } } } }
```

```
[ { "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" } } } ]
```

SG45 input files for MCNP

The following general roadmap is proposed to produce a first set

1. Make the repository for MCNP input files
2. Add a first set of cases from the LANL Whisper suite already under LANL QA
   - For example : ~100 Pu and/or HEU cases
   - Using the proper naming convention, archiving current LANL QA review documentation
   - Produce the material balance tables from the ICSBEP benchmark specifications
3. Verify the set against the material balance tables, review and correct discrepancies
4. Transform the set to be in line with the VaNDaL input requirements
   - Clean the files and add header information and standardised title
   - Replace material specifications using the verified material balance tables
   - Replace kcode card with the accepted VaNDaL default
5. Verify the generated input files using the appropriate policies against the originals
   - LANL Nuclear Criticality Safety division policies will be used
6. Verify and update the volume information in the material balance tables

SG45 input files for MCNP

Template MCNP file

```
pu-met-fast-001-000-rev4
1    1 4.029014e-2  -1    imp:n=1
2    0               1    imp:n=0

1    so  6.39157

mode n
totnu
kcode
ksrc 0. 0. 0.
c material 1: Plutonium
m1    94239 3.7047e-2
      94240 1.7512e-3
      94241 1.1674e-4
      31000 1.3752e-3
```

Generated MCNP file

```
pu-met-fast-001-000-rev4
c policy : defaultAbundanceFile
c policy : defaultCalculationPrecision
c policy : userCalculateEffectiveDelayedNeutronFraction
1    1 4.029014e-2  -1    imp:n=1
2    0               1    imp:n=0

1    so  6.39157

mode n
totnu
kcode 10000 1. 100 600
kopts kinetics=yes
ksrc 0. 0. 0.
c material 1: Plutonium
m1
      94239 0.037047
      94240 0.0017512
      31069 0.000826605216
      31071 0.000548594784
```