PCA benchmark analysis using the ADVANTG3.0.1/MCNP6.1.1b codes

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6. Summary and conclusions
1. PCA benchmark definition

- Pool Critical Assembly Pressure Vessel (PCA) benchmark
  - A well known benchmark from the SINBAD database
  - Based on the PCA facility experiments at the ORNL
  - A small pool-type highly enriched experimental reactor
  - Measured and calculated (DORT) equivalent fission fluxes
  - Validation of transport theory codes and XS libraries
  - Prediction of the in-vessel neutron flux gradients

- Scope of the PCA benchmark
  - Validation of the methodology to predict the reaction rates in ex-core region
  - Qualification of the pressure vessel fluence calculation methodology
  - Simulation of the neutron flux gradient inside carbon steel (RPV)
  - RPV surveillance programs of existing USA NPPs (RPV damage)
  - Measured RR inside RPV (A4, A5, A6) and water gap in-front (A3, A2)
  - Well defined neutron source, materials, and simple geometry
  - DORT libraries in the PCA benchmark: BUGLE-93, SAILOR-95, BUGLE-96
  - Computational requirements by the U.S. NRC Regulatory Guide 1.190
2. PCA benchmark description

PCA benchmark “12/13” configuration

- PCA core with components mock up the core-to-cavity region in PWRs
- Al plate, Thermal shield (TS), pressure vessel simulator (PVS), void box (VB)
- Water gap between Al plate and TS: 12 cm
- Water gap between TS and RPVS: 13 cm
- PCA facility is immersed in a large pool of water (coolant and moderator)
- PCA core has 25 material test reactor (MTR) plate-type elements (e=93%)
2. PCA benchmark description

PCA benchmark “12/13” configuration

Cross sectional view through the control element

Boron carbide
(1.6 g/cc)

Lead
(11.34 g/cc)

Al-U alloy
(fuel plate)

PCA standard MTR fuel element (water included)

PCA control rod (water included)
2. PCA benchmark description

☐ PCA benchmark “12/13” configuration

Fig. 1.2 Horizontal cross section of the PCA pressure vessel benchmark facility 12/13 configuration (dimensions are in cm)
2. PCA benchmark description

- PCA benchmark “12/13” configuration

Fig. 1.3 Vertical cross section of the PCA pressure vessel benchmark facility (dimensions are in cm)
2. PCA benchmark description

- Experimental measurements: A1 – A7

Table 1.6 Experimental results for fission chamber and radiometric measurements of equivalent fission fluxes

<table>
<thead>
<tr>
<th>Location</th>
<th>Distance* (cm)</th>
<th>Equivalent fission fluxes** [per 1 PCA core fission neutron per second (cm(^{-2})) ]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( ^{237}\text{Np} )</td>
<td>( ^{238}\text{U} )</td>
</tr>
<tr>
<td>A1</td>
<td>12.0</td>
<td>6.64 E-6 ± 6.2%</td>
</tr>
<tr>
<td>A2</td>
<td>23.8</td>
<td>-</td>
</tr>
<tr>
<td>A3</td>
<td>29.7</td>
<td>2.27 E-7 ± 6.3%</td>
</tr>
<tr>
<td>A4</td>
<td>39.5</td>
<td>9.27 E-8 ± 5.5%</td>
</tr>
<tr>
<td>A5</td>
<td>44.7</td>
<td>5.18 E-8 ± 5.7%</td>
</tr>
<tr>
<td>A6</td>
<td>50.1</td>
<td>2.70 E-8 ± 5.8%</td>
</tr>
<tr>
<td>A7</td>
<td>59.1</td>
<td>7.25 E-9 ± 9.2%</td>
</tr>
</tbody>
</table>

Reaction cross sections, averaged over \( ^{235}\text{U} \) fission spectrum *** (mb)

|          | 1312 ± 50 | 305 ± 9 | 733 ± 38 | 189 ± 8 | 109 ± 6 | 0.705 ± 0.040 |

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* Distance to core face of the aluminum window.

Equivalent fission fluxes at detector locations:

\[
\phi_{eq} = \frac{\text{reaction rates}}{\sigma_i} = \frac{\int \sigma_i(E)\phi(E)dE}{\int \sigma_i(E)\phi(E)dE} = \frac{\int \phi(E)dE}{\int \phi(E)dE}
\]
2. PCA benchmark description

- **Reactions of interest (shielding calculations)**
  - \( ^{237}\text{Np}(n,f)^{137}\text{Cs}, ^{238}\text{U}(n,f)^{137}\text{Cs}, ^{103}\text{Rh}(n,n')^{130\text{m}}\text{Rh}, ^{115}\text{In}(n,n')^{115\text{m}}\text{In}, ^{58}\text{Ni}(n,p)^{58}\text{Co}, ^{27}\text{Al}(n,\alpha)^{24}\text{Na} \)
  - Results are given per unit PCA core neutron source (normalized)
  - Calculated-to-measured (C/M) ratios of equivalent \( ^{235}\text{U} \) fission fluxes
  - Measurements in core midplane (z=0 and y=0) at locations A1 to A7
  - Experimental access tubes: steel in PV and Plexiglas in water locations
  - Minimization of the perturbations of the neutron field
  - DORT reaction rates (/atom/s) are given for dosimeters A1-A8

- **Critical configuration (eigenvalue calculations)**
  - Fully inserted control rod reaches bottom of the fuel
  - Withdrawn length is measured from the bottom of the fuel
  - Safety rods (S1, S2 and S3) critical positions: 48.26 cm
  - Regulating rod (RR) position: 38.43 cm
  - Total critical mass of \( ^{235}\text{U} \): 3336.01 g
3. ADVANTG3.0.1/ MCNP6.1.1B codes

- **ADVANTG3.0.1 code (ORNL)**
  - Automated mesh-based tool for generating VR parameters for MCNP code
  - Approximate 3-D multigroup SN forward/adjoint transport solutions
  - Denovo SN solver developed at ORNL with CADIS/FW-CADIS formalism
  - VR parameters: space-energy weight-windows (WW) and biased source distributions (SB) cards for the MCNP input

- **MCNP6.1.1b code (LLNL)**
  - General-purpose Monte Carlo N-Particle code with arbitrary 3D geometry
  - Neutron, photon, electron, or coupled n/p/e transport
  - XS libraries: continuous, discrete, multigroup, S(a,b) law, dosimetry, ...
  - Powerful general source, rich collection of VR techniques, flexible tallies
  - Pointwise XS data with MAKXSF for XS libraries with Doppler broadening
3. ADVANTG3.0.1/ MCNP6.1.1B codes

Hybrid shielding

\[ q^s(\vec{r}, E) = \sigma_d(\vec{r}, E) \quad \text{Adjoint source} \]

\[ \hat{q}(\vec{r}, E) = \frac{1}{R} q(\vec{r}, E) \phi^s(\vec{r}, E) \quad \text{Biased source} \]

\[ \bar{w}(\vec{r}, E) = \frac{R}{\phi^s(\vec{r}, E)} \quad \text{Target weight} \]

\[ w_0(\vec{r}, E) = \frac{q(\vec{r}, E)}{\hat{q}(\vec{r}, E)} = \frac{R}{\phi^s(\vec{r}, E)} \quad \text{Initial weight} \]

\[ q^s(\vec{r}, E) = \frac{\sigma_d(\vec{r}, E)}{\int \sigma_d(\vec{r}, E) \phi(\vec{r}, E)} \quad \text{Weighted adjoint source} \]

point detector = adjoint source

MCNP model of the 1/4 cask

ADVANTG SN mesh for VR parameters

Adjoint function (1.8-2.4) MeV
4. PCA response functions

Cross sections from the IAEA NDS service

- ENDF/B retrieval service (www-nds.iaea.org)
- IRDF-2002 and IRDFF-2014 dosimetry libraries

Evaluating Nuclear Data File (ENDF)
Database Version of 2017-06-01

Selection of XS library and reaction type

IRDFF-1.05 library
Al-27(n,a)Na-24

XS reaction plotting and extracting for MCNP

Cross sections with reconstructed resonances and applied Doppler broadening at the temperature 293 K

Output Data

XS reaction data in the ENDF-6 format
4. PCA response functions

- Cross sections from the IAEA NDS service
  - IRDFF-2014 and IRDF-2002 dosimetry library
  - Neutron excitation \((n,n')\) of the first isomeric state \(\text{Rh}\) (56.12 min) and \(\text{In}\) (4.486 h)
  - Metastable isomers \(^{103}\text{Rh}\) and \(^{115}\text{In}\) with reactions \(\text{MF/MT} = 3/51\)

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5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- MCNP6.1.1b eigenvalue results:

  \[
  \text{keff} = (0.99924 \pm 0.00100)
  \]

- kcode 2000 1.0 50 350 1e4
- ksrc 20.22 31.46 0 $ starting point

- keff neutron flux in z=0 cm plane
- keff neutron flux RE in z=0 cm plane
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- **ADVANTG3.0.1 parameters:**
  - FW-CADIS method for one reaction on all detectors (A1-A8)
  - S4/P1, SC spatial differencing, eps=1e-3, 1.6e6 mesh cells
  - ANISN-format coupled n-g multigroup library BPLUS (updated BUGLE-96)
  - BUGLE-96 library: LWR shielding, PV dosimetry, VITAMIN-B6 collapsing
  - 5 weighting spectra of 1-D model of a reactor cavity and bioshield
  - BPLUS library: 47n/20g, 393 isotopes, ENDF/B-VII.0 evaluation
  - Mixed 11 pure materials into 26857 macro materials
  - Memory requirements (GB): 6-9 FW Denovo, 10-14 ADJ Denovo

- **MCNP6.1.1b parameters:**
  - Continuous XS for neutron transport with Doppler correction and S(a,b) law
  - MCNP6.1.1b with distributed (PVM) calculation on Quad Core CPU
  - Using point detectors inside small void spheres at centers of A1-A8
  - Mesh tally for capturing the global MC neutron transport
  - card “ctme 720” $ cumulative time in min
  - About 2e6 neutron histories per MC simulation
  - Point detectors have RE on average 1-2 %
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

ADVANTG3.0.1 FW-CADIS results for $^{27}$Al(n,a)$^{24}$Ni
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- MCNP6.1.1b results for all reactions

**MC neutron flux solution for Al-27(n,a)Ni-24 in z=0 cm plane**

**MC neutron flux RE on 1 sigma level for Al-27(n,a)Ni-24 in z=0 cm plane**

**Equivalent fission fluxes C/M ratios**

(“-” experimental result not provided in the PCA benchmark)

<table>
<thead>
<tr>
<th>Location</th>
<th>$^{237}$Np(n,f)</th>
<th>$^{238}$U(n,f)</th>
<th>$^{27}$Al(n,a)</th>
<th>$^{58}$Ni(n,p)</th>
<th>$^{115}$In(n,n')</th>
<th>$^{103}$Rh(n,n')</th>
<th>MCNP Avg ± sig</th>
<th>DORT Avg ± sig</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>0.862</td>
<td>-</td>
<td>0.801</td>
<td>0.887</td>
<td>0.902</td>
<td>0.945</td>
<td>0.88 ± 0.02</td>
<td>0.91 ± 0.02</td>
</tr>
<tr>
<td>A2</td>
<td>-</td>
<td>-</td>
<td>0.852</td>
<td>0.938</td>
<td>0.986</td>
<td>-</td>
<td>0.93 ± 0.04</td>
<td>0.92 ± 0.01</td>
</tr>
<tr>
<td>A3</td>
<td>0.908</td>
<td>-</td>
<td>0.765</td>
<td>0.835</td>
<td>0.877</td>
<td>-</td>
<td>0.85 ± 0.03</td>
<td>0.96 ± 0.02</td>
</tr>
<tr>
<td>A4</td>
<td>0.869</td>
<td>0.882</td>
<td>0.874</td>
<td>0.898</td>
<td>0.935</td>
<td>0.905</td>
<td>0.90 ± 0.01</td>
<td>0.94 ± 0.03</td>
</tr>
<tr>
<td>A5</td>
<td>0.914</td>
<td>0.880</td>
<td>0.929</td>
<td>0.919</td>
<td>0.935</td>
<td>0.877</td>
<td>0.91 ± 0.01</td>
<td>0.92 ± 0.03</td>
</tr>
<tr>
<td>A6</td>
<td>0.878</td>
<td>0.884</td>
<td>0.968</td>
<td>0.957</td>
<td>0.969</td>
<td>0.881</td>
<td>0.92 ± 0.02</td>
<td>0.91 ± 0.04</td>
</tr>
<tr>
<td>A7</td>
<td>0.939</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.94 ± 0.00</td>
<td>0.89 ± 0.00</td>
</tr>
<tr>
<td>A8</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

[Lower quality results since ADVANTG was used with default eps=1e-3]
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- Isotopes of Fe and self-shielding
  - Neutron spectrum “softening” inside the RPV simulator
  - Neutrons > 1 MeV are shifted to resonance region of Fe => self-shielding!
  - Important reaction becomes inelastic neutron scattering (n,n')

\[
\sigma_{t,l}(E) = \frac{N\pi\mathcal{K}^2 g\Gamma_n}{(E - E_0)^2 + 1/4\Gamma^2} \left( \Gamma - 2\Gamma\sin^2 \delta_l + 2(E - E_0)\sin 2\delta_l \right) + 4N\pi\mathcal{K}^2(2l + 1)\sin^2 \delta_l
\]

Hard-sphere nuclear model

\[
\tan \delta_l = \frac{J_l(R/\mathcal{K})}{N_l(R/\mathcal{K})}
\]

\[
\begin{align*}
\delta_0 &= R/\mathcal{K} & \text{(LWR)} \\
\delta_l &= \delta_0 - \tan^{-1}(R/\mathcal{K}) & \text{(FBR)}
\end{align*}
\]

\[
\sigma_{t,0}(E) = \sigma_0 \sqrt{\frac{E_0}{E}} \frac{\Gamma^2}{4(E - E_0)^2 + \Gamma^2} \left[ 1 + \frac{4(E - E_0)R}{\Gamma}\frac{R}{\mathcal{K}} \right] + \sigma_{pot}
\]

- Total cross section (MT=1) of iron isotopes
- Inelastic scattering (MT=3) of iron isotopes
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- MCNP FOM factors for all reactions

  - Computational model metric addressing memory and CPU time
  - Figure-of-merit (FOM) factor: CPU time necessary to reach a given level $RE$
  - $FOM = 1/(RE^2 \times T)$, where $RE$ is MC rel.error and $T$ is CPU time in min

FOM factors for different detector locations

$FOM$ factor vs Detector position (cm)
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- ADVANTG3.0.1 CADIS optimization of A3 detector

- Integrated adjoint flux in z=0 cm

- MC neutron flux solution for Al-27(n,a)Ni-24 in z=0 cm plane

- MC neutron flux RE on 1 sigma level for Al-27(n,a)Ni-24 in z=0 cm plane
5. PCA results using ADVANTG3.0.1/ MCNP6.1.1b

- ADVANTG3.0.1 FW-CADIS global flux solution

- Integrated forward and adjoint flux in z=0 cm

- Local SN mesh refinement?

- More histories needed!

- Average RE \( \approx 30\% \)

- MC neutron flux global solution in z=0 cm plane

- MC neutron flux RE in z=0 cm plane
6. Summary and conclusions

- Hybrid shielding:
  - FW-CADIS for distributed detectors and global flux solution
  - CADIS for local answers, would require 6 reactions x 8 locations = 48 runs!
  - SN based VR technique removes burden of manual VR preparation
  - Computational trade-off between SN and MC simulations

- PCA benchmark:
  - Good agreement between calculated (C) and measured (M) results
  - Obtained results in accordance with the Regulatory Guide 1.190
  - Sensitivity of BPLUS shielding library on the iron XS (self-shielding)
  - Differences due to XS libraries, weighting spectrum, core modeling,…
  - More neutron groups are preferred due to spectral effects

- Commercial hybrid shielding codes today:
  - SCALE6.2 (CADIS/FW-CADIS in MAVRIC)
  - ADVANTG3.0.1 + MCNP5v1.6 (or MCNP6.1.1b)
  - A³MCNP (TORT + MCNP5v1.6)
  - ATTILA + MCNP6.1.1B
References: