

**JEF/DOC-596**

**Inter-code comparisons for highly enriched  
Uranium Fluorine benchmarks**

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## ABSTRACT

An inter-code comparison exercise for nitrate plutonium solutions is underway aimed at resolving important discrepancies observed for JEF2.2 criticality benchmark studies<sup>1</sup>. It has been decided that it would be useful to extend the exercise to encompass other type of system, so that a co-ordinated view of the accuracy achievable with JEF2.2-based libraries can be achieved over a broader range of library applications.

The next stage of the exercise reported here considers high-enriched uranium fluoride solutions ( $\text{UO}_2\text{F}_2$ ) with the experimental descriptions having been taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook<sup>2</sup>. This report describes the new benchmarks and summarises the results for contributions received to date. Further analysis of these results will be performed later in an updated version of this document.

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<sup>1</sup> A Nouri and N Smith : Inter-code Comparison for Uranium and Plutonium Homogeneous Solutions using JEF2.2 (JEF/DOC-545)

<sup>2</sup> International Handbook of Evaluated Criticality Safety Benchmark Experiments (NEA/NSC/DOC(95)03)

## I - EXPERIMENTAL BENCHMARKS AND CALCULATION RESULTS

Three experiments involving uranium oxyfluoride ( $\text{UO}_2\text{F}_2$ ) solutions have been studied for this inter-code comparison exercise. All three are recently evaluated benchmark descriptions from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook and are part of a programme of experiments performed at Oak Ridge National Laboratory in the 1950s.

In total six experimental configurations have been selected from the three evaluations and all comprise spherical vessels of solution surrounded by a water reflector. The six experiments have been selected to give a wide range of uranium concentrations (ranging from 20 g/l up to almost 700 g/l). In each case the uranium is high-enriched ( $\sim 93\%$  U235).

These benchmarks have been calculated using JEF2.2-based libraries with the UK criticality Monte Carlo code MONK (13193 groups) and the French criticality system of codes APOLLO-1 + MORET-3 (99 groups + self-shielding). To date this report simply includes the calculated k-effective values for the experimental configurations, the infinite media of each type of solution and the approximately-critical bare spheres of solution.

The following provisional conclusions can be drawn from the results to date:

- Very good agreement is observed between the two codes for the infinite multiplication factors (within the statistical uncertainty)
- Generally satisfactory agreement is observed for the bare and reflected systems (maximum discrepancy 690 pcm) with the generally lower APOLLO-1 + MORET-3 results being attributed to the anisotropy treatment in MORET (limited to  $P_1$  approximation). Improvements to this treatment are being investigated.

## II - SPECIFICATIONS

Case No.	1	2	3	4	5	6
Reference <sup>3</sup>	009-C01	009-C02	009-C03	009-C04	011-C01	012-C01
C(U) g/l atm/b-cm	696.42	543.05	348.84	213.19	53.02	20.50
<sup>234</sup> U atm/b-cm	1.7561E-05	1.3694E-05	8.7965E-06	5.3760E-06	1.3369E-06	5.5393E-07
<sup>235</sup> U atm/b-cm	1.6626E-03	1.2965E-03	8.3281E-04	5.0898E-04	1.2657E-04	5.2444E-05
<sup>236</sup> U atm/b-cm	8.8837E-06	6.9272E-06	4.4499E-06	2.7195E-06	6.7629E-07	2.8022E-07
<sup>238</sup> U atm/b-cm	9.4079E-05	7.3359E-05	4.7124E-05	2.8800E-05	7.1620E-06	2.9675E-06
Fluorine atm/b-cm	3.5663E-03	2.7809E-03	1.7864E-03	1.0917E-03	2.7149E-04	1.1249E-04
Oxygen atm/b-cm	3.3360E-02	3.3396E-02	3.3467E-02	3.3278E-02	3.3396E-02	3.3473E-02
H atm/b-cm	5.9587E-02	6.1229E-02	6.3362E-02	6.4373E-02	6.6248E-02	6.6722E-02
Exp. radius (Solution) - cm	11.5177	11.4695	11.5177	11.8442	15.9572	27.9244
Exp. radius (Vessel) -cm	11.6764	11.6282	11.6764	12.0029	16.0842	28.1244
Exp. radius (Reflector) - cm	35.0	35.0	35.0	35.0	35.0	43.1244
Bare radius (Calculated) -cm	15.1637	15.0758	15.0805	15.5223	19.7487	32.8366

<sup>3</sup> Experiment from ICSBEP Handbook. 009-C01 is Case 1 from experiment HEU-SOL-THERM-009.

**ALUMINIUM ATOM DENSITIES (VESSEL WALL)**

	Atom density atm/b-cm
Al	5.9699E-02
Si	5.5202E-04
Cu	5.1364E-04
Zn	2.4958E-05
Mn	1.4853E-05

**WATER ATOM DENSITIES (REFLECTOR)**

Element	Atom density atm/b-cm
H	6.6659E-02
O	3.3329E-02

The submission specification format is the same as used for the plutonium solution exercise (reference 1).

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### III) RESULTS

#### Neutron balance in infinite media

Case #	1	2	3	4	5	6
slowing-down current	0.66	0.72	0.81	0.87	0.96	0.98
U234 A	0.0074	0.0064	0.0049	0.0037	0.0019	0.0012
U234 P	0.0006	0.0005	0.0003	0.0002	-	-
U235 A	0.9584	0.9560	0.9474	0.9288	0.7878	0.6091
U235 P	1.8519	1.8700	1.8867	1.8768	1.6245	1.2612
U236 A	0.0017	0.0014	0.0010	0.0007	0.0002	-
U236 P	0.0002	0.0001	-	-	-	-
U238 A	0.0123	0.0107	0.0078	0.0053	0.0016	0.0007
U238 P	0.0008	0.0006	0.0004	0.0002	-	-
H <sub>2</sub> O A	0.0192	0.0248	0.0384	0.0613	0.2084	0.3888
O A	0.0004	0.0003	0.0002	0.0001	-	-
F A	0.0007	0.0006	0.0004	0.0002	-	-

#### Infinite multiplication factors

Case #	1	2	3	4	5	6
slowing-down current	0.66	0.72	0.81	0.87	0.96	0.98
MONK-7 13193 g	1.8530	1.8706	1.8868	1.8761	1.6230	1.2598
APOLLO-1 99 g	1.8534	1.8711	1.8875	1.8773	1.6247	1.2613

A very good agreements between the two codes is found. The maximum discrepancy is about 120 pcm which is statistically insignificant.

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### Multiplication factors for bare spheres systems

The following table shows the calculated  $k_{\text{eff}}$  for the bare spheres systems and the proportion of leakage. The agreement between the two codes is generally satisfactory; the discrepancy ranges from -440 pcm to +290 pcm. APOLLO-1 + MORET-3 generally leads to lower values of  $k_{\text{eff}}$ . A recent study<sup>4</sup> shows that the anisotropy treatment in MORET (limited to the  $P_1$  approximation) tends to underpredict  $k_{\text{eff}}$ . The improvement of this model is discussed in reference 4.

Case #	1	2	3	4	5	6
slowing-down current	0.36	0.40	0.45	0.50	0.66	0.83
MONK-7 12630 g	1.0001 45.9%	0.9992 46.4%	1.0014 46.7%	1.0041 46.3%	1.0234 36.9%	1.0194 19.0%
APOLLO-1 + MORET 99 g	0.9974 46.0 %	0.9948 46.5 %	0.9994 46.5%	1.0028 46.4%	1.0201 37.0 %	1.0224 18.9 %

### Multiplication factors for reflected spheres

The multiplication factors and the proportions of leakage calculated for the experimental configurations are shown in the following table. The agreement between the two codes is again quite good. The discrepancy ranges from -40 pcm to -690 pcm. Again, APOLLO-1 and MORET-3 tends to underpredict the  $k_{\text{eff}}$ . The observation made in the previous subsection concerning the anisotropy treatment in MORET is also valid here.

Case #	1	2	3	4	5	6
slowing-down current	0.83	0.85	0.89	0.92	0.95	0.96
MONK-7 12630 g	1.0070 2.9 %	1.0068 2.9 %	1.0039 2.9 %	0.9974 2.9 %	1.0028 3.8 %	1.0007 3.1 %
APOLLO-1 + MORET 99 g	1.0001 2.7 %	1.0010 2.7 %	0.9983 2.7 %	0.9905 2.7 %	1.0022 3.6 %	1.0003 3.0 %

<sup>4</sup> A. Nouri, A. Le Cocq, P. Reuss and E. Lejeune : « Anisotropy Treatment in Criticality Multigroup Monte-Carlo Codes », accepted for presentation in PHYSOR'96, Mito, Sept 96 (JAPAN)