

Feedback from RPSD-2018

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National Nuclear Data Center

BROOKHAVEN
NATIONAL LABORATORY





RPSD 2018

August 26-31, 2018 | Santa Fe, NM
20th Topical Meeting of the Radiation Protection and Shielding Division

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**Very useful: met class of users rarely interact with —
the shielding community!**

**and thank you Wim for
making me go**

Things I took note of

- **SINBAD**
- **The many users of our electro- and photo-atomic libraries**
- **EPICS problems**
- **Fe problems**
- **Other data problems**

SINBAD

- Introduction to SINBAD— Tutorial (I. Kodeli) #25448
- The Future of SINBAD: Learning from the Best Practices of ICSBEP (J.D. Bess, T. Ivanova) #24622
- New WPEC SG-47 “Use of Shielding Integral Benchmark Archive and Database for Nuclear Data Validation” approved
 - 1st target of investigation: LLNL Pulsed Spheres

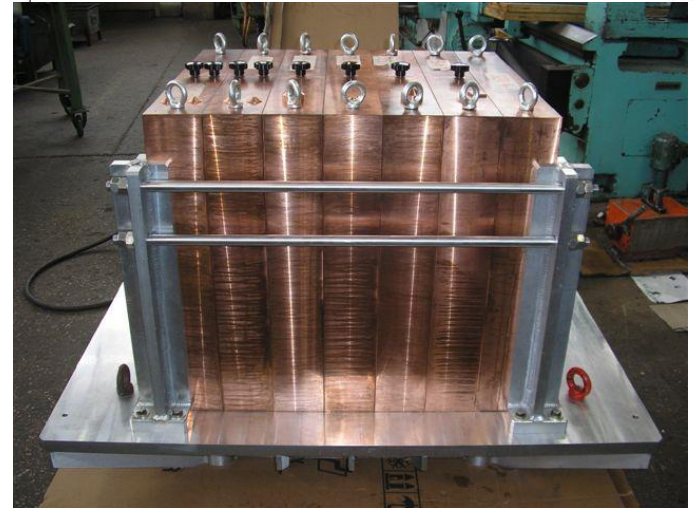
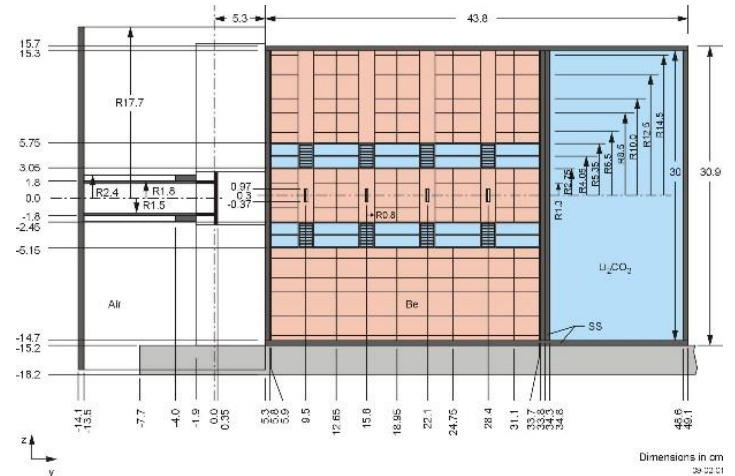


Fig. 2. New SINBAD benchmark compilations (top FNG-HCPB, below FNG-Cu).

I. Kodeli, ANS RPSD 2018–20th Topical Meeting of the Radiation Protection & Shielding Division of ANS, Santa Fe, NM, August 26–31, 2018, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2018)

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The many users of ENDF/B-VIII.0 electro-, photo-atomic data

- **GEANT4**
(POC for e⁻, γ transport:
Maria Grazia Pia, INFN Genova)
- **PHITS**
(<https://phits.jaea.go.jp>)
(POC: T. Furuta, JAEA)
- **FLUKA** (fluka.org)
- **MCNP**
- **PENELOPE**
(POC: F. Salvat, U. Barcelona)
 - Integrated into **penORNL**
- **EGS**, obsolete but forked into
 - **EGSnrc** (<https://nrc-cnrc.github.io/EGSnrc>)
 - **EGS5** integrated into PHITS
- **ITS** (POC: Brian Franke, SNL)
- **SCEPTRE**
(POC: Clif Drumm, SNL)
- **CEPXS** (SNL)
- Method development codes:
 - **FRENSIE** (U. Wisconsin),
 - **P++** (RPI)

Talks that discussed validation (mostly of codes, but data included)

- **Electron Transport Algorithms in the Integrated Tiger Series (ITS) Codes** (B.B. Franke & R.P. Kensek) # 25576
- **Preliminary Performance Evaluation of P++ Single Event Proton Scattering Algorithms on GPUs** (K. Zieb, G. Xu) #25688
- **Energy Deposition Validation Results for the Evaluated Electron Data Library in FRENSE** (L. Kersting, D. Henderson, A. Robinson, E. Moll) #25357
- **First Assessment of the New Atomic Data in ENDF/B-VIII** (M. Grazia Pia)

We need options for validating electro- or photo- atomic data

- Shielding benchmarks?
- **Lockwood energy deposition experiment**
- Hanson angular scattering
- Tabata charge deposition
- ...

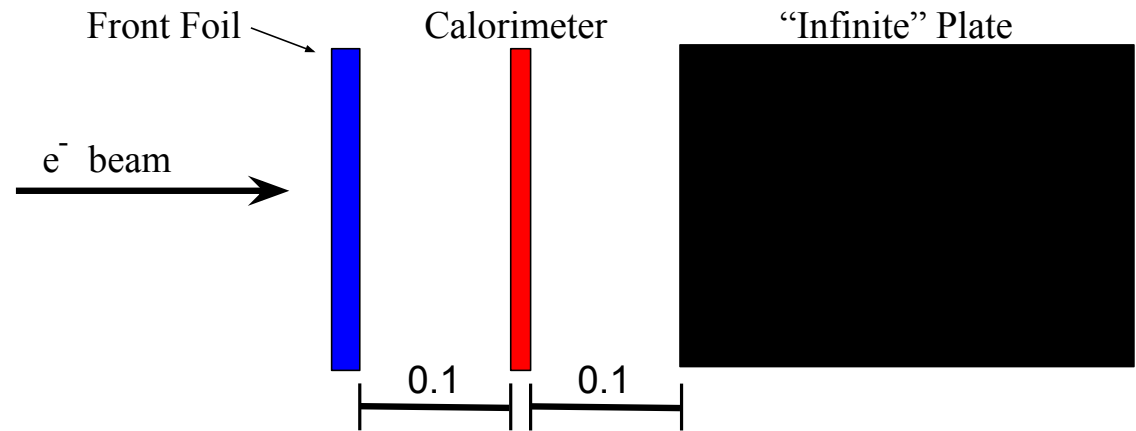


Fig. 2. The experimental setup of the Lockwood experiment consisting of a front foil, calorimeter foil, and “infinite” plate all of the same material and contained in vacuum.

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Maria Grazia Pia (INFN) presented a thorough and critical review of the new atomic transport data in ENDF/B-VIII.0

- GEANT4 Physics Developments and Validation page (<https://www.ge.infn.it/geant4/index.html>)
- This talk's content from <https://www.ge.infn.it/geant4/talks/rpsd2018/datalib.pdf> and posted in indico
- IEEE Trans. Nucl. Sci. (<https://doi.org/10.1109/TNS.2018.2849328>).
- Other papers concerning EADL/EEDL/EPDL validation published by her research group are listed in <https://www.ge.infn.it/geant4/papers/index.html>



Maria Grazia Pia

She couldn't make it to CSEWG, but is very interested in collaborating with us

Formatting problems with EPICS

Content

Different content for different data formats

Not trivial to retrieve what contains what

Physics Data	EADL	EADL91		EPICS2014		EPICS2017	
		ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Number of electrons		yes	yes	yes	yes	yes	yes
Binding energy		yes	yes	yes	yes	yes	yes
Kinetic energy		yes	-	yes	-	yes	-
Average radius		yes	-	yes	-	yes	-
Radiative level width		yes	-	yes	-	yes	-
Non-radiative level width		yes	-	yes	-	yes	-
Average energy to the residual atom per initial vacancy		yes	-	yes	-	yes	-
Average energy of particles per initial vacancy		yes	-	yes	-	yes	-
Average number of particles per initial vacancy		yes	-	yes	-	yes	-
Radiative transition probability and emitted particle energy		yes	yes	yes	yes	yes	yes
Non-radiative transition probability and emitted particle energy		yes	yes	yes	yes	yes	yes

Physics Data	EPDL	EPDL97		EPICS2014		EPICS2017	
		ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total photon cross section		-	-	-	-	-	yes
Coherent scattering: integrated cross section		yes	yes	yes	yes	yes	yes
Coherent scattering: average energy of the scattered photon		yes	-	yes	-	yes	-
Coherent scattering: form factor		yes	yes	yes	yes	yes	yes
Coherent scattering: imaginary anomalous scattering factor		yes	yes	yes	yes	yes	yes
Coherent scattering: real anomalous scattering factor		yes	yes	yes	yes	yes	yes
Incoherent scattering: integrated cross section		yes	yes	yes	yes	yes	yes
Incoherent scattering: scattering function		yes	yes	yes	yes	yes	yes
Incoherent scattering: average energy of the secondary particles		yes	-	yes	-	yes	-
Photoelectric: integrated cross section		yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom		yes	-	yes	-	-	-
Photoelectric: average energy of secondary particles		yes	-	yes	-	-	-
Photoelectric: cross section by subshell		yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom by subshell		yes	-	yes	-	yes	-
Photoelectric: average energy of secondary particles by subshell		yes	-	yes	-	yes	-
Pair production: integrated cross section		yes	yes	yes	yes	yes	yes
Pair production: average energy of secondary particles		yes	-	yes	-	yes	-
Triplet production: integrated cross section		yes	yes	yes	yes	yes	yes
Triplet production: average energy of secondary particles		yes	-	yes	-	yes	-
Pair and triplet production: integrated cross section		-	yes	-	yes	-	yes

Physics Data	EEDL	EEDL91		EPICS2014		EPICS2017	
		ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total electron cross section		-	-	-	-	-	yes
Large angle elastic scattering: integrated cross section		yes	yes	yes	yes	yes	yes
Large angle elastic scattering: average energy to the residual atom		yes	-	yes	-	yes	-
Large angle elastic scattering: average energy of the scattered electron		yes	-	yes	-	yes	-
Large angle elastic scattering: angular distributions		yes	yes	yes	yes	yes	yes
Elastic scattering: integrated cross section		yes	-	yes	-	yes	yes
Ionisation: integrated cross section		-	-	-	-	yes	yes
Ionisation cross section by subshell		yes	yes	yes	yes	yes	yes
Ionisation: average energy of secondary particles by subshell		yes	-	yes	-	yes	-
Ionisation: spectra of the recoil electron by subshell		yes	yes	yes	yes	yes	yes
Bremsstrahlung: integrated cross section		yes	yes	yes	yes	yes	yes
Bremsstrahlung: energy spectra of the secondary photon		yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary photon		yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary electron		yes	-	yes	-	yes	-
Excitation: integrated cross section		yes	yes	yes	yes	yes	yes
Excitation: average energy to the residual atom		yes	yes	yes	yes	yes	yes

Version control issues with EPICS

Example: Carbon
(screenshots on 18/6/2018)

EPICS2017

Electron Photon Interaction Cross Sections (2017)

The Official ENDF/B-VIII Electron and Photon Data

(<http://www.nndc.bnl.gov/endl/epics/>)

Updated!

ENDF/B-VIII.0 Download ENDF/B-VIII.0

Not updated!

Atomic Relaxation Reaction Sublibrary
[2.7 Mb zipfile] [Release Notes] [Changelog]
[Material List]
Download checksums:
MD5: e04d50098cb2a7e4fe404ec407161cc
SHA1: 486a89705cb45720feb6c3a4ab126be3444846a3
cksum: 1302098210

(<http://www.nndc.bnl.gov/endl/b8.0>)

International Atomic Energy Agency
Nuclear Data Services
Provided by the Nuclear Data Section

Not updated!

EPICS2017

Electron and Photon
Interaction Cross Sections

(<https://www-nds.iaea.org/epics/>)

6000.00000	11.9078164	0	0
1.00000000	0.0	0	0
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	276.740000	5.61488D-4
4.00000000	0.0	276.740000	.001120600
2.00000000	2.00000000	254.820000	.413609000
2.00000000	3.00000000	260.150000	.136190000
2.00000000	4.00000000	260.150000	.271099000
3.00000000	3.00000000	265.480000	.004207480
3.00000000	4.00000000	265.480000	.110012000
4.00000000	4.00000000	265.480000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

6000.00000	11.9078164	0	0
1.00000000	0.0	0	0
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	282.020000	5.61488D-4
4.00000000	0.0	282.030000	.001120600
2.00000000	2.00000000	255.890000	.413609000
2.00000000	3.00000000	264.460000	.136190000
2.00000000	4.00000000	264.470000	.271099000
3.00000000	3.00000000	273.030000	.004207480
3.00000000	4.00000000	273.040000	.110012000
4.00000000	4.00000000	273.050000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

6000.00000	11.9078164	0	0
1.00000000	0.0	0	0
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	282.020000	5.61488D-4
4.00000000	0.0	282.030000	.001120600
2.00000000	2.00000000	255.890000	.413609000
2.00000000	3.00000000	264.460000	.136190000
2.00000000	4.00000000	264.470000	.271099000
3.00000000	3.00000000	273.030000	.004207480
3.00000000	4.00000000	273.040000	.110012000
4.00000000	4.00000000	273.050000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

- Red sent final version in April, well after ENDF/B-VIII.0 released.
- Final version fixes consistency problems with binding energies

- Not reflected in ENDF/B-VIII.0 release tarballs nor IAEA page, only EPICS page and ENDF/B-VIII.0 Errata page
- We look like idiots and I'm p*ssed
- More importantly, users are VERY confused

First validation test

Electron ionisation cross sections

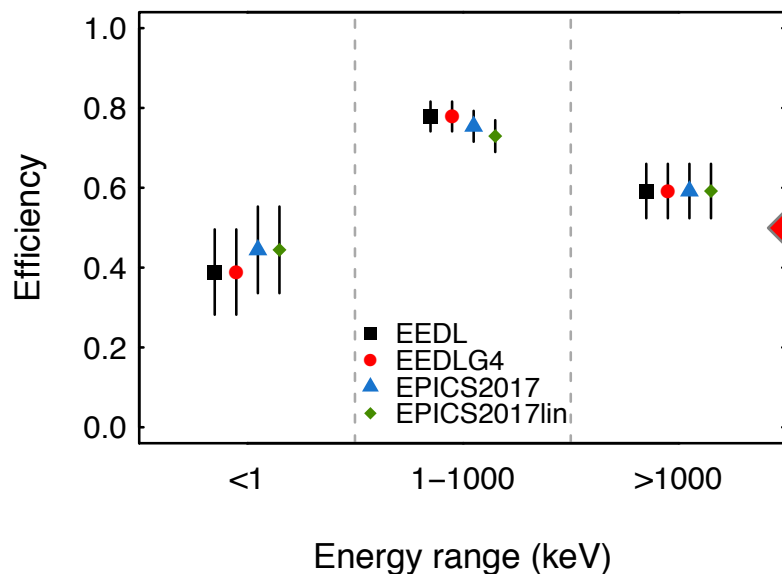
~ 2800 K shell cross section measurements

Goodness-of-fit tests

- χ^2
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

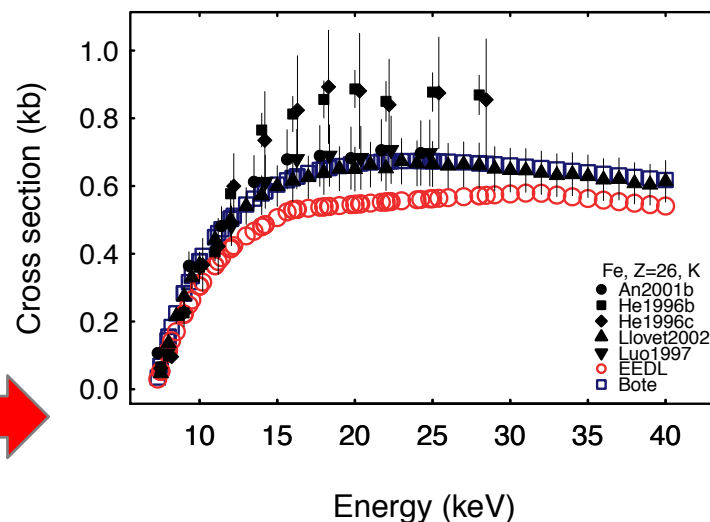
0.01 significance level

efficiency = fraction of test cases
where H_0 is not rejected



Slightly different results with EPICS2017 w.r.t. EEDL91, however the difference in compatibility with experiment is **not statistically significant**

...but interpolation issues due to the coarse granularity of tabulations!



Summary of shortcomings

- **Documentation:**

- Unclear what was improved in this release (Red's documentation "incomplete")
- What is documented is not what is in files
- ENDF documentation that clarified formats used by author only generally available after release

- **Version control:**

- Library content is format dependent (ENDL vs. ENDF/GNDS)
- Version screwups due to blowing past deadline

- **Verification rushed:**

- Binding energy error could have been caught with time (EADL unchecked), eliminating post-release errata

- **Validation issues:**

- Precision choices made by author impact validation
- No apparent validation done by author and we had no contacts that could perform validation
- Validation by Grazia Pia's groups found issues

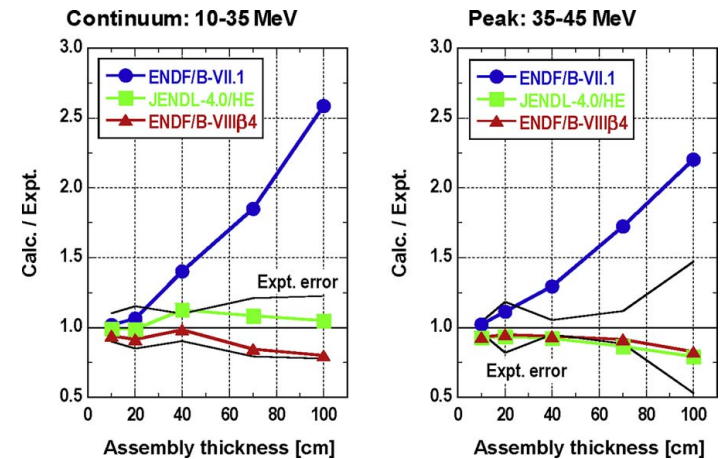
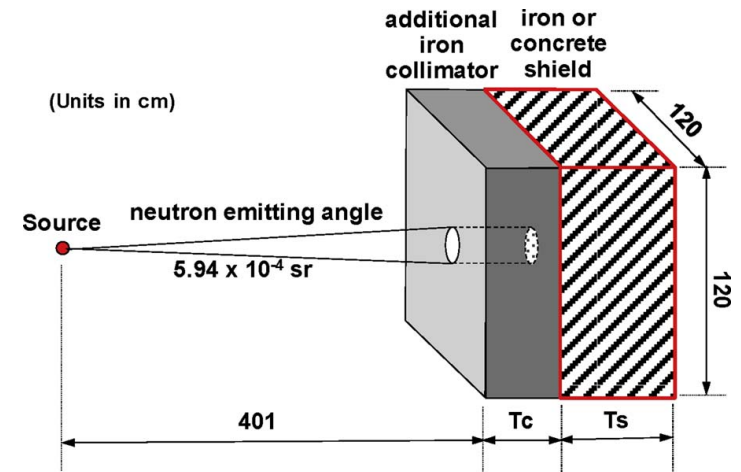
**In lieu of the many users of these libraries,
we need help so we don't repeat this mess-up**

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We heard earlier about Fe problems, here is a small recap

- Elastic scattering angular distribution covariances are incomplete
 - *General statement: we need covariances for more than just P1*
- Elastic vs. inelastic shielding issues from IPPE shielding experiments
- TIARA: poor performance in high energy (> 60 MeV) shielding experiments from JAEA.
Contact: Chikara Konno



Kwon, Ohta, Ochiai, Fusion Engineering & Design, in press (2018).

Other reported problems (some are previously known issues)

- **Dosimetry reactions that need fixing**

- $^{103}\text{Rh}(n,n')^{103\text{m}}\text{Rh}$ incorrect (noted in 2 talks, #25409 and #25428)
- $^{115}\text{In}(n,n')^{115\text{m}}\text{In}$ incorrect [Tracker #1122]
- $^{90}\text{Zr}(n,2n)$, $^{127}\text{I}(n,2n)$ (noted in #25362)

- **Missing gammas**

- Discretas don't match known gammas/levels
- Continuum energy balance issues
- Especially capture gammas (including primary)

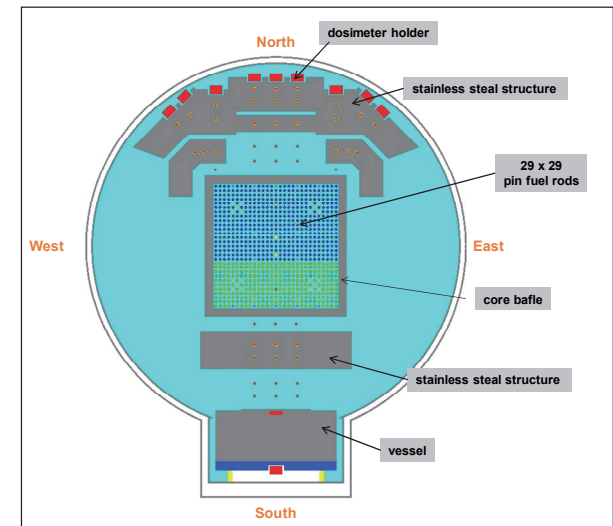


Fig. 1. FLUOLE-2 device.

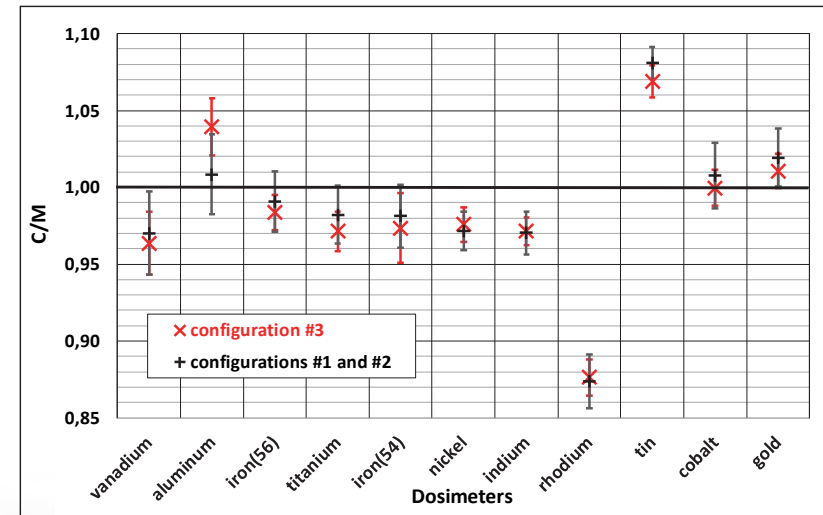


Fig. 7. Comparison of C/M results for in-core dosimeters.

S. Bourganel, N. Thiollay, P. Mosca, RPSD-2018 contribution #25409