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Non-Fertile Fuel Benchmark: Sensitivity of the Calculational Results Against the Basic Cross Section Libraries

by

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Motivation for this work

- **U-free** fuel, consisting of a mixture of **Pu**, Er, Zr and Al in form of oxides.

- Void ==> Neutron spectrum hardening.
  Problem: Zr-resonances
  (in the fuel and in the cladding).
  Additionally: Er-resonances
  (in the fuel).

- **Large deviations** of the **computed void coefficients**.

- Validation necessary.

Available Results for RG-1, RG-3, WG-1:

- k_∞,
- **Fluxes,**
- **Reaction rates:**
  - Fission, "absorption" (absorption - (n,2n)), production rates
  - for the nuclides,
  - for fuel, cladding, coolant, and the cell,
  - given in 6 energy groups (with boundaries at 14.9 MeV, 821 keV, 9.1 keV, 4 eV, 1.3 eV, 407 meV, 0.0), and
  - normalised such that the macroscopic "absorption" rate is unity.
- **Void coefficients for 10%, 50%, 95%, and 99.9% void.**
- **Temperature coefficients of the fuel** from 600 to 900 degree C.

Methods and Data

- Methods

  Heterogeneous calculations (in 3 regions) with **MICROX-2/ONEDANT (M/O)**.

- Data

  – Specific data libraries for the cell code MICROX-2 were generated based on the **JEF-1.1, JEF-2.2, ENDF/B-VI (Rev. 4)**, and **JENDL-3.2** evaluations, using **NJOY94.10/MICROR**.

  – The **"Reference" Analysis** is based on a mixed library, which combines **ENDF/B-IV data for natural zirconium** with **JEF-1.1 data** for the remaining nuclides (===> **as in BOXER**).

(Cell) Calculations with MICROX-2

- Fission spectrum: Linear combination of data for the single actinides.
- **Dancoff factors:** pre-calculated **analytically** (Segev's method) for the square lattice.
- **Above 7.1 keV: Bondarenko formalism:**
  - semi-log,
  - $\sigma_0 = 10^{10}$, 1000, 100, 50, 20, 10, 5, 1 barns, for all nuclides except ^{16}O,
  - in 60 fine groups:
    - $\Delta U = 0.1$ for E > 111.1 keV (groups 1-50),
    - $\Delta U = 0.25$ for E < 111.1 keV (groups 51-60),
  - weighting function: **EPRI cell LWR** (IWT=5), irrespective of the voided situation.
- **Resonance calculation in 2 zones**, performed
  - in the energy range **7.1 keV - 2.4 eV**,
  - using $\sim$ 10000 energy points equally spaced in lethargy,
  - **clad and moderator are smeared.**
- **Below 2.4 eV**: Thermal treatment **in 101 fine energy "points"**.

(Discrete-Ordinates) Transport Calculations with ONEDANT

- based on the original benchmark-models (non-buckled **three-region cells with white reflection conditions on the outer boundaries**),

- therefore using (**"uncollapsed"**) $\mathbf{P_0}$-$\mathbf{P_2}$ broad-group cross sections from MICROX-2, (diagonal transport correction with the correct Legendre moment dependence of the total cross section),

- S_8 approximation,

- **20 fine meshes** in each of both fuel and water regions, and 2 meshes in the cladding.

Multiplication Factor k_∞ at BOL

Cell Type	M/O "ref." anal.	PSI BOXER	M/O JEF-1.1	M/O JEF-2.2	CEA JEF-2.2	M/O ENDF/B-VI (Rev. 4)	M/O JENDL-3.2	JAERI JENDL-3.2
RG-1	1.456	1.462	1.458	**1.452**	**1.451**	1.446	1.445	1.450
WG-1	1.622	1.627	1.625	**1.617**	**1.616**	1.617	1.618	1.623
RG-3	**1.100**	**1.107**	1.103	**1.098**	**1.100**	1.104	**1.100**	**1.109**

- The agreement of both calculations based on the JEF-2.2 library is **good**.
- The k_∞s from the "reference" analysis are systematically smaller than the PSI values based on the BOXER code (maximum **~700 pcm for RG-3**), and
- a similar, but more enhanced trend, is shown by comparing the results from the calculations based on the JENDL-3.2 library.
- **The maximum k_∞ spread** as originating from calculations **based on the same data library** is **~900 pcm**.

k_∞ Variation at BOL, Using the Same Method (M/O) but Different Data Libraries (with Respect to the "Reference" Analysis)

Δk_∞ (pcm)[1]				
Cell Type	JEF-1.1	JEF-2.2	ENDF/B-VI (Rev. 4)	JENDL-3.2
RG-1	249	-345	-938	-1047
WG-1	274	-515	-518	-405
RG-3	343	-154	475	89

[1] Δk_∞=0 for the "reference" analysis

- The resulting k_∞ spreads are **~600 pcm for RG-3, ~800 pcm for WG-1, and ~1300 pcm for RG-1** respectively.
- The maximum spread achieved is therefore **~1300 pcm**, diminishing to **~700 pcm** if the results from the "reference" analysis as well as those obtained using the JEF-1.1 library are excluded from the comparison.
- **It therefore appears that the uncertainties due to data and methods are similar, corresponding to the 1% spread in k_∞ values at BOL reported earlier.**

Void Coefficients at BOL

Cell Type	VF (%)	"ref." anal.	PSI BOXER	M/O JEF-1.1	M/O JEF-2.2	CEA JEF-2.2	M/O ENDF/B-VI (Rev. 4)	M/O JENDL-3.2	JAERI JENDL-3.2
RG-1	**10**	**-86.8**	**-87.4**	**-85.5**	**-84.1**	**-86.5**	**-85.1**	**-86.9**	**-85.9**
	50	-102.4	-105.0	-100.7	-97.6	-102.1	-97.6	-101.0	-101.2
	95	-6.8	-17.6	0.9	14.0	12.2	22.8	5.7	1.0
	99.9	1.0	-5.8	17.5	40.1	38.5	47.3	25.4	14.0
WG-1	10	-52.0	-52.8	-50.9	-49.3	-50.9	-43.8	-44.8	-49.1
	50	-68.6	-70.9	-66.6	-63.9	-66.7	-63.2	-66.0	-65.1
	95	-50.7	-59.0	-45.8	-31.1	-33.0	-29.8	-40.1	-43.4
	99.9	-52.5	-53.9	-38.1	-15.3	-16.9	-20.4	-29.6	-40.0
RG-3	10	-135.0	-137.0	-132.9	-131.0	-134.3	-112.4	**-115.4**	**-129.3**
	50	-120.7	-126.2	-117.3	**-113.4**	**-119.3**	-106.0	-111.9	-112.9
	95	**59.1**	**42.6**	66.7	85.0	81.4	109.2	90.3	97.2
	99.9	86.1	80.9	102.6	132.3	130.5	146.0	**127.4**	**137.8**

- **For the cells without erbium, the void coefficients agree fairly well for not too high void fractions <50%.**
- The new results with the JEF-2.2 library are slightly more positive (less negative) than the CEA values (**max. 5.9 pcm/% void**).
- Those from the "reference" analysis agree sufficiently well with the other BOXER values, except for the cells with 95% void, the "reference" analysis giving systematically more positive (less negative) values (**max. 16.5 pcm/% void**).
- Larger deviations of the new JENDL-3.2 results from the JAERI values. varying from **14 to -10 pcm/% void**.

Variation of the Void Coefficients at BOL, Using the Same Method (M/O) but Different Data Libraries (with respect to the "Reference" Analysis)

ΔC_V^{VF} (pcm/% Void)[1]					
Cell Type	**VF (%)**	**JEF-1.1**	**JEF-2.2**	**ENDF/B-VI (Rev. 4)**	**JENDL-3.2**
RG-1	10	1.3	2.7	1.7	-0.1
	50	1.7	4.8	4.8	1.4
	95	7.7	20.9	29.6	12.5
	99.9	16.5	39.1	46.3	24.4
WG-1	10	1.1	2.7	**8.2**	7.2
	50	2.0	4.7	5.4	2.6
	95	5.0	19.7	21.0	10.7
	99.9	14.4	37.3	32.2	23.0
RG-3	10	2.1	4.0	**22.6**	19.6
	50	3.4	7.3	14.7	8.7
	95	7.5	25.9	50.0	31.1
	99.9	16.6	46.2	**59.9**	41.3

[1] ΔC_V^{VF}=0 for the "reference" analysis

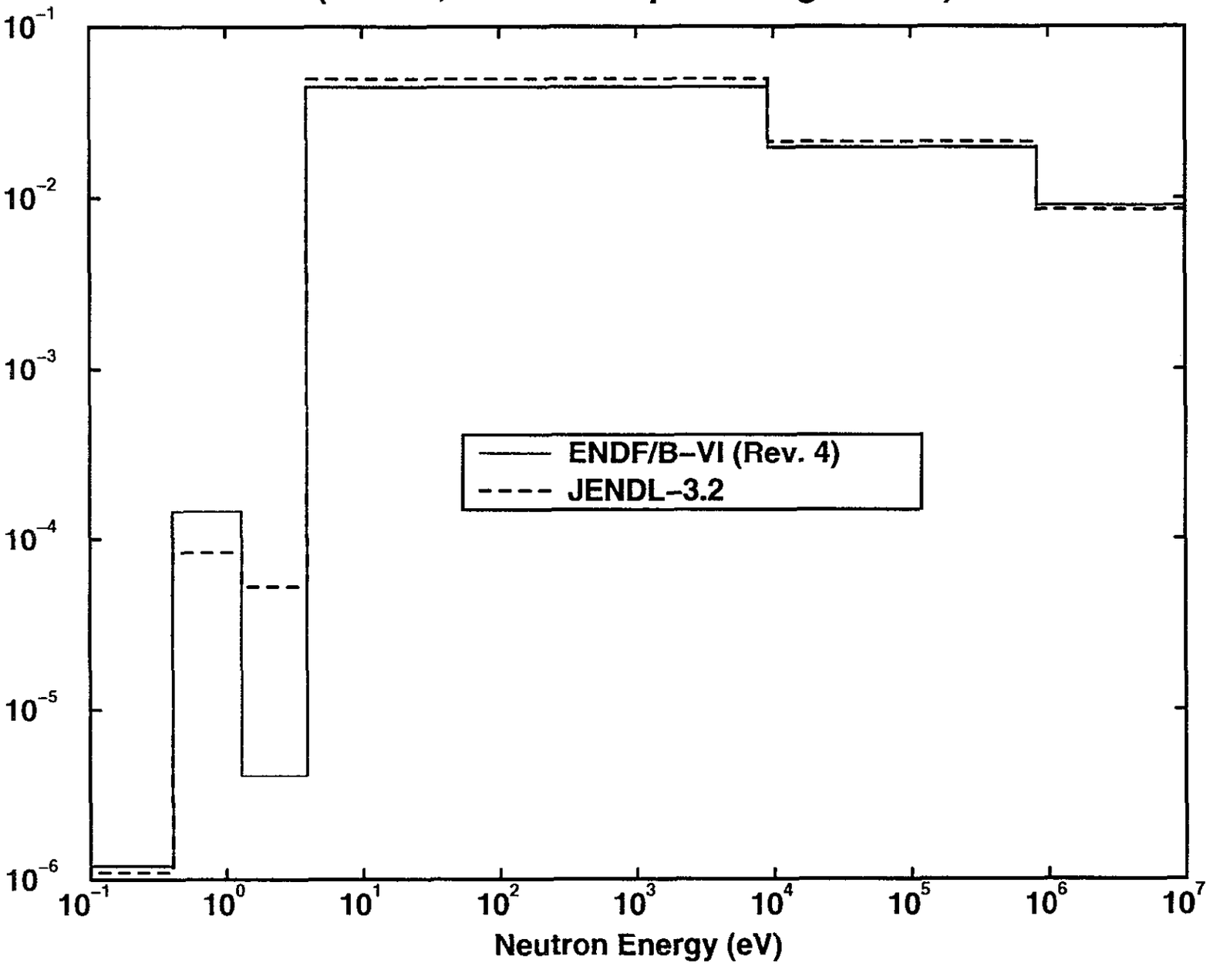
- Except for RG-3, **data effects are relatively small for cells with void fractions upto 50% (<9 pcm/% void)**.
- For RG-3, the larger spread (**22.6 pcm/% void**) is dominated by effects due to data (erbium).
- **The data sensitivity increases and dominates when the void fraction is increased from 50% to 99.9% (maximum spread is 59.9 pcm/% void for RG-3).**

Contributions (α_is) to the Void Coefficient (α) at BOL (RG-3, Void Fraction 99.9 %)

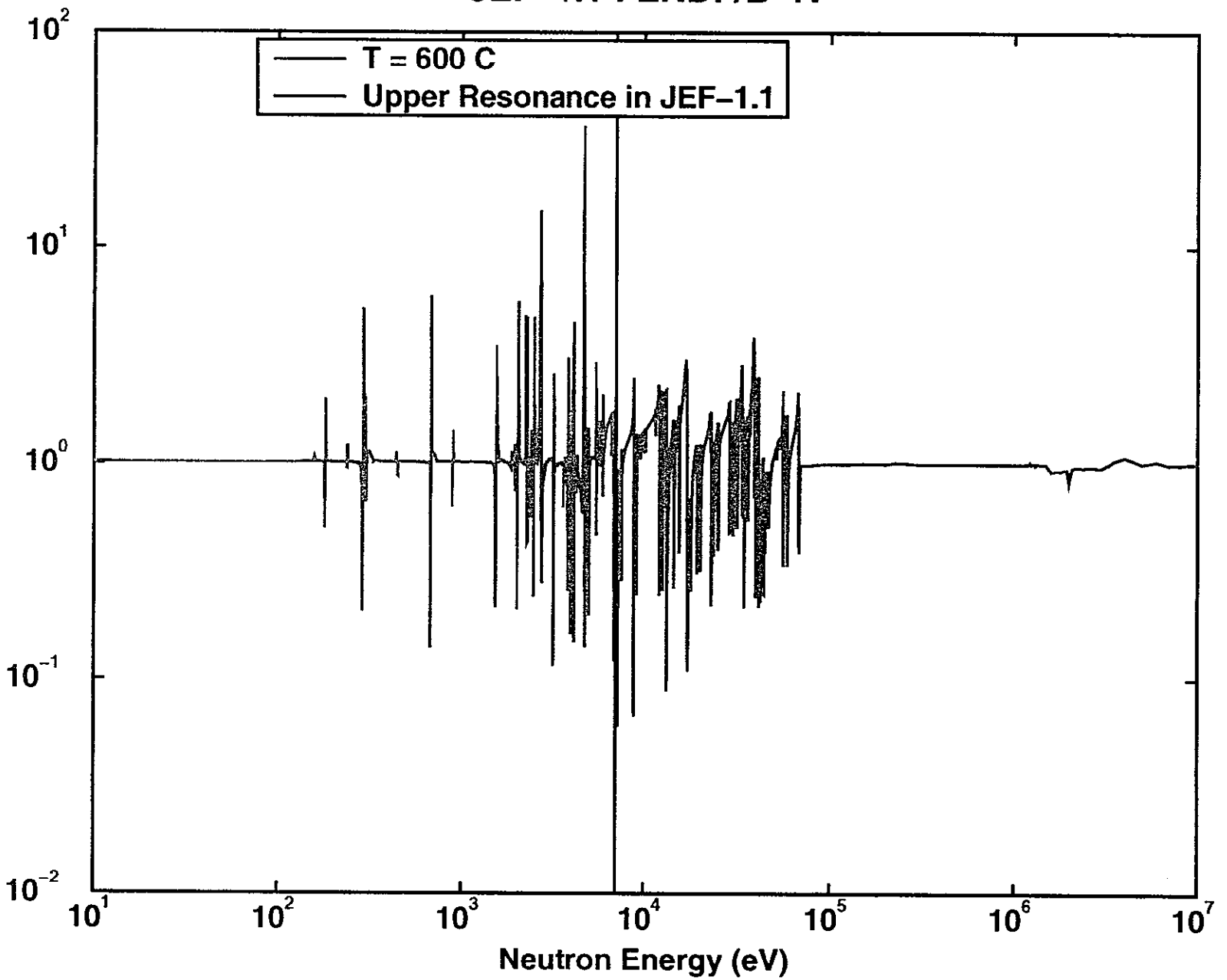
α_i (pcm/% void)												$C_V^{99.9}$
Region	Fuel									Cladding	Moderator	Cell
Nuclide (or Region)	^{16}O	^{166}Er	^{167}Er	Zr	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	Fuel Total	Cladding Total	Moderator Total	Cell Total
"reference" analysis	-2.9	-19.8	97.5	**-123.5**	-4.2	137.0	17.7	14.8	116.6	**-45.1**	14.5	**86.1**
JEF-1.1	-2.8	-20.3	98.0	**-113.1**	-5.3	138.5	18.2	15.0	128.1	**-40.3**	14.8	**102.6**
JEF-2.2	-3.5	-20.8	100.9	**-99.6**	**-2.3**	**143.4**	18.8	15.6	152.6	**-36.1**	15.8	**132.3**
ENDF/B-VI (Rev. 4)	-3.6	**-30.2**	**122.9**	-109.0	-5.0	**154.3**	22.7	18.2	170.2	-40.2	16.1	**146.0**
JENDL-3.2	-2.6	-29.4	122.4	**-114.1**	-4.1	**143.5**	22.5	15.9	154.1	**-41.5**	14.8	**127.4**

[1] $\Delta\alpha_i$=0 for the "reference" analysis

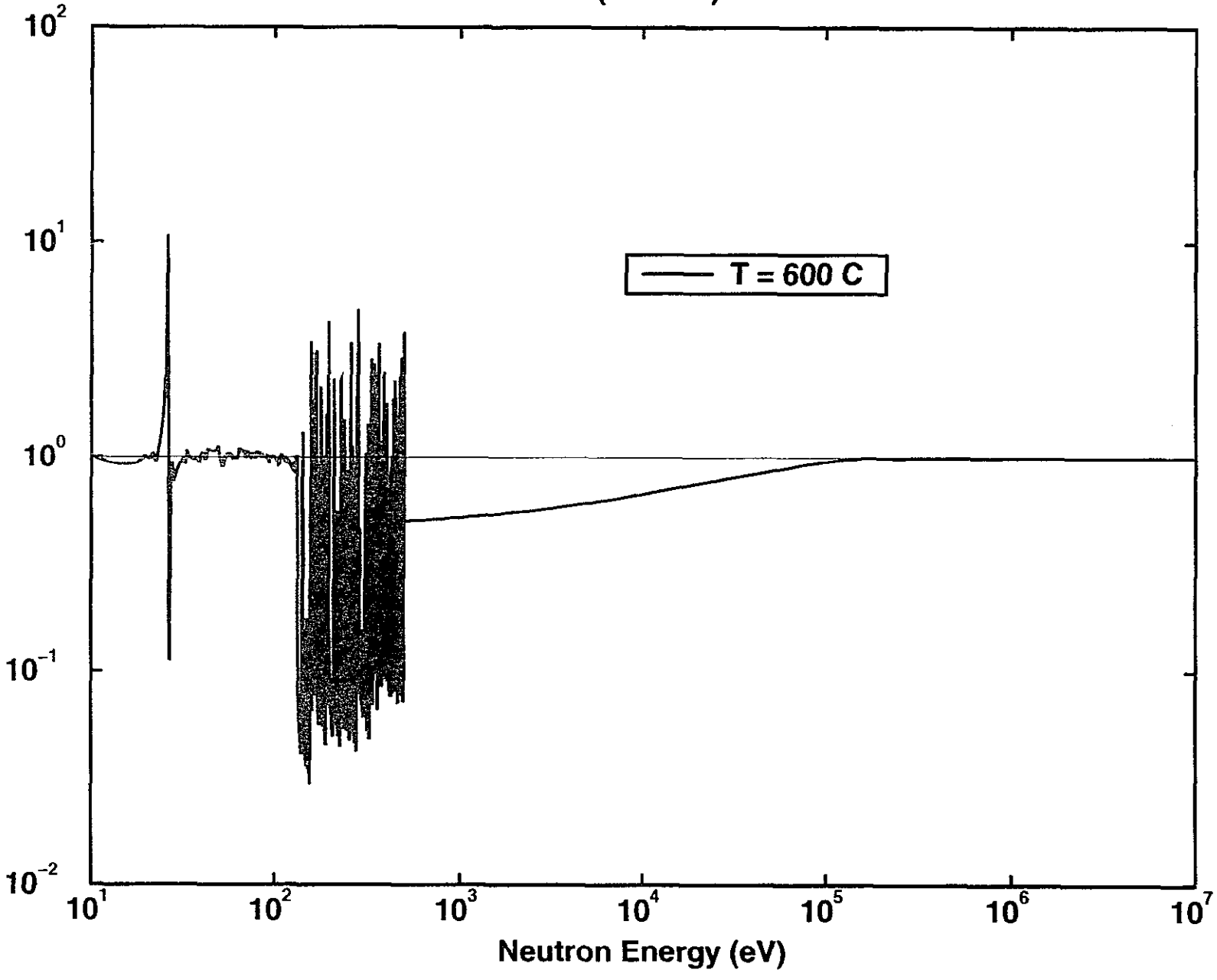
- Two positive contributions (fuel, moderator), one negative contribution (cladding).
- **"Reference" Analysis ==> JEF-1.1**: α **more positive** (zirconium data).
- **JEF-1.1 ==> JEF-2.2**: α **more positive** (zirconium and plutonium data + spectral effects).
- **JEF-2.2 ==> ENDF/B-VI (Rev. 4)**: α **more positive** (erbium and ^{240}Pu data + spectral effects).
- **ENDF/B-VI (Rev. 4) ==> JENDL-3.2**: α **less positive** (zirconium and ^{240}Pu data).


Total "Absorption" Rates of Pu240 for RG–3 (99.9% Void)
(=0.169, due to compensating effects)
ENDF/B–VI (Rev. 4)
JENDL–3.2
Neutron Energy (eV)

Ratio of Total Cross Sections for Zirconium
JEF–1.1 : ENDF/B–IV



Ratio of Total Cross Sections for Er167
ENDF/B–VI (Rev. 4) : JEF–1.1



Conclusions (Methods)

- Well **thermalised** cells with void fractions upto 50%: **Upper energy boundary for thermal range: ~2 eV recommended.**

- **Fast spectrum** cells with large void fractions >90%: **Appropriate shielding of cross sections of zirconium in the cladding required.**

Conclusions (Methods and Data)

- k_∞ (at BOL):

  Methods∼data uncertainties (∼1%).

- Void Coefficients (at BOL):
  - For not too high void fractions $\leq$**50%**:
    - Cells without erbium: Methods∼data uncertainties. **Void coefficients predicted with sufficient consistency**.
    - Cells with erbium: Uncertainties increase if the void fraction is increased (===> data for erbium).
  - For high void fractions >**50%**:

    Each cell type: Uncertainties increase if the void fraction is increased (===> **data for zirconium, erbium, and plutonium**). Large uncertainties (**data**) for void fractions $\geq$**90%**.

Recommendation

- Assign a high priority to the reduction of the uncertainty of these data (JEFF-3 ?)

- ===> Further step in clarifying the neutronics of advanced fuel cycles based upon such innovative fuels.