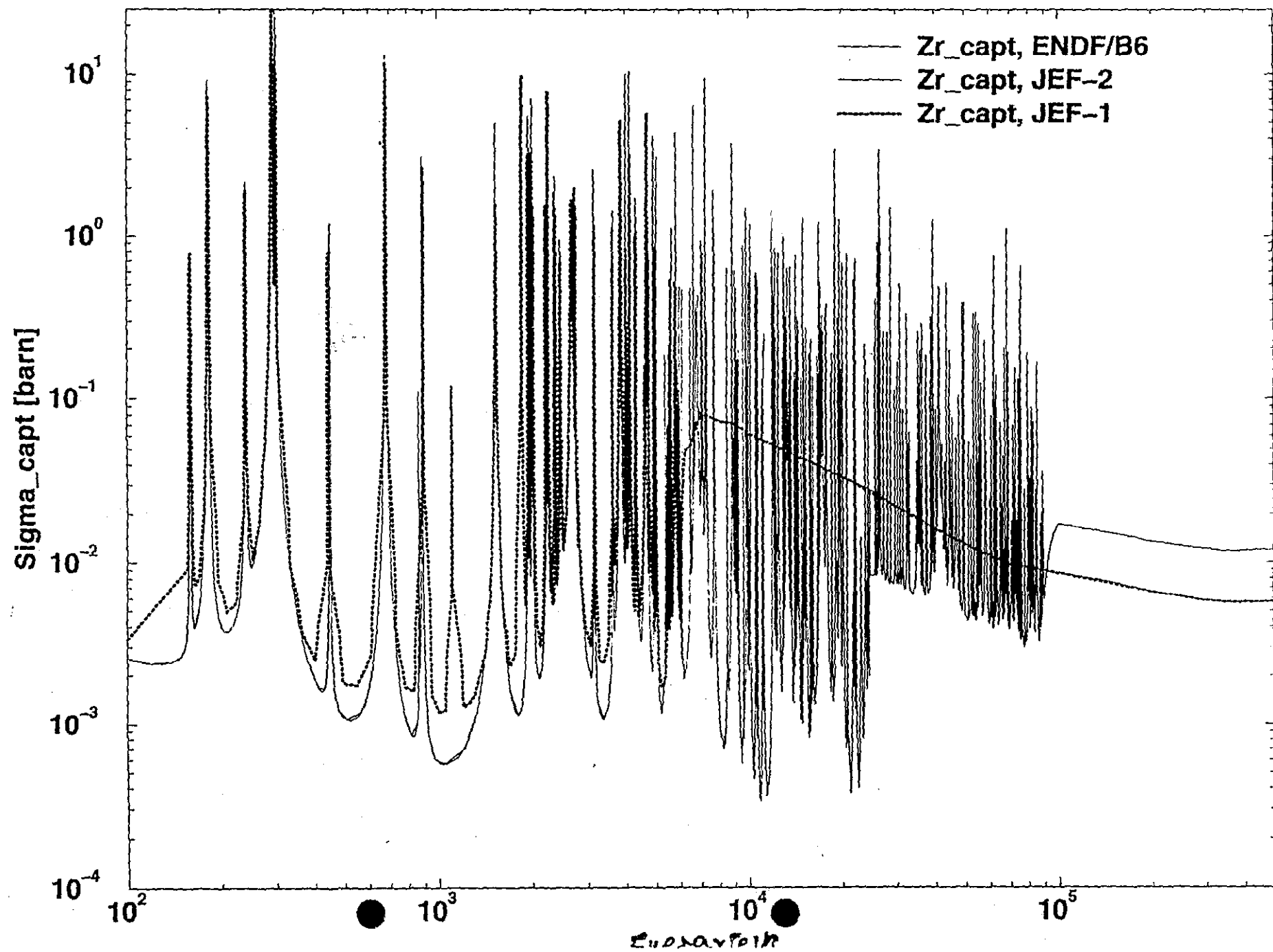


Impact of Zirconium Data on the Physics of U-Free Cells

by

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Comparison of Zr Absorption Cross Sections from Different Libraries



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Available Results

- for RG1, RG3, WG1,
- at BOL and EOL,
- using data from the JEF-1.1, JEF-2.2, and ENDF/B-VI (Rev. 4) evaluations^{1,2},
- Zr data from Zr-nat,
- Zr data from the Zr-isotopes.

¹ Additionally, Zr data from the ENDF/B-IV evaluation, because BOXER is using this data.

² Data from the JENDL-3.2 library is in preparation (water and erbium are not available on the data basis).

Computed:

- k_{∞}
- Fluxes,
- reaction rates
 - fission, "absorption - (n,2n)", and production,
 - in 6 energy groups
(with boundaries at 14.9 MeV, 821 keV, 9.1 keV, 4 eV, 1.3 eV, 407 meV, 0.0),
 - normalised to a total absorption of unity,
 - for the single nuclides,
 - for fuel, clad, coolant, and the cell.
- Void coefficients for 10%, 50%, 95%, and 99.9% void.
- Temperature coefficient of the fuel from 600 to 900 degree C.

Methods and Data

- Methods

- Homogeneous reference calculations with **MICROX-2/ONEDANT**,
 - * using cell averaged cross sections,
 - * in which **different data libraries** are used with variable upper energy boundaries for the thermal range.
- Heterogeneous calculations with **MICROX-2/ONEDANT**,
 - * using region averaged cross sections,
 - * in which **different data libraries** are used with a different number of energy groups.

Methods and Data (Continued)

- Methods

- – Heterogeneous calculations with **MICROX-2/ONEDANT**, in which the **BOXER** methodology is simulated:
 - * Zr cross sections in the clad are the same as in the fuel,
 - * the resonance calculation is performed starting from 900 eV.

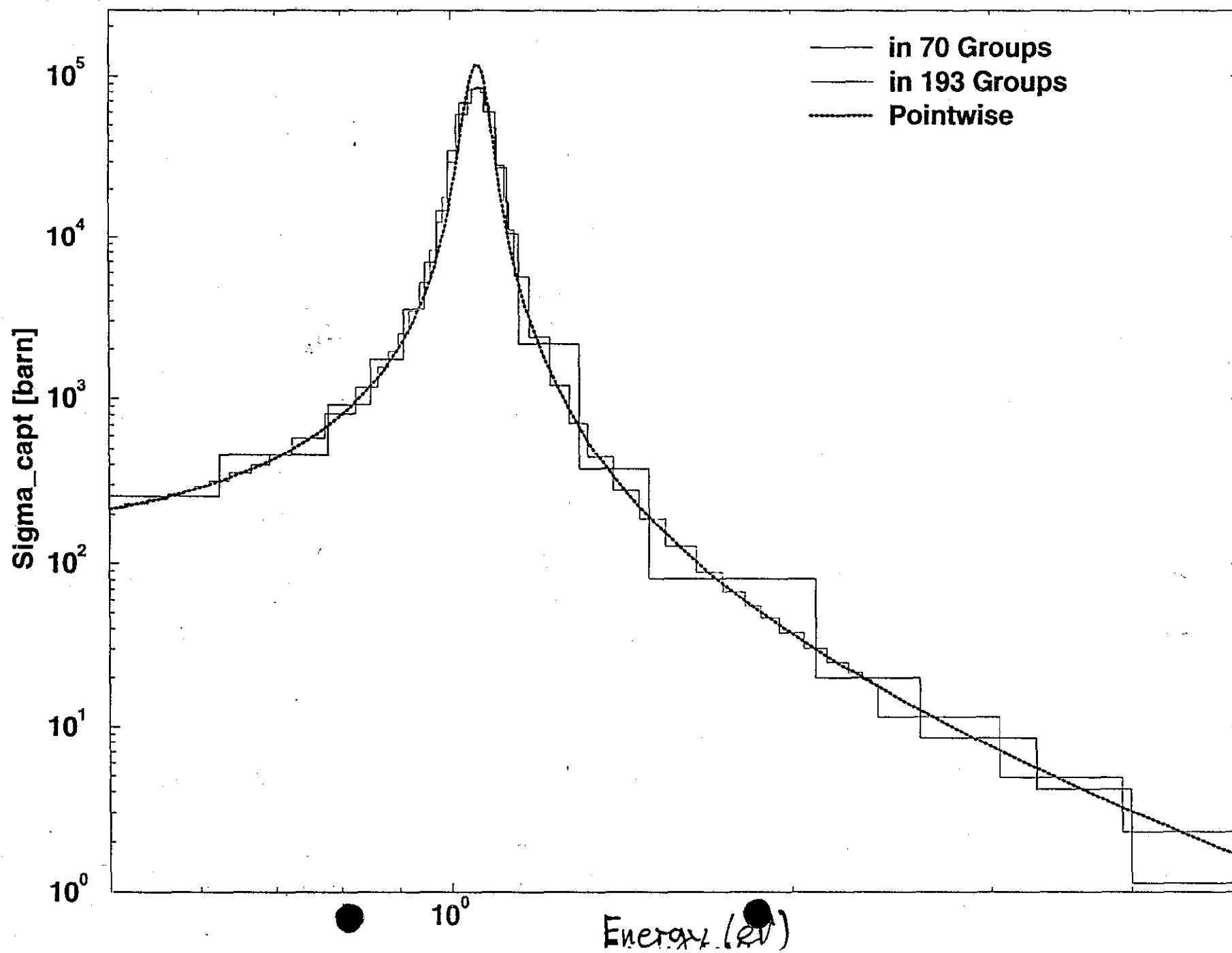
- Data

Specific data libraries for the cell code **MICROX-2** were generated using **NJOY94.10/MICROR**.

MICROX-2 (Reference) Calculations

- 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 ($\Delta U = 0.1$),
 - 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 ~ 10000 energy points equally spaced in lethargy,
 - clad and moderator are smeared,
 - UR range is not shielded.
- **Below 2.4 eV: Thermal treatment in 101 fine energy "points"**.

Comparison of Pu-240 Capture Cross Sections



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Results (10% Void)

Δk_{∞} against results with pure JEF-1.1 data		
pcm	JEF-2.2	ENDF/B-VI (Rev. 4)
RG3 (0 % void)	-497	+132
WG1 (0 % void)	-789	-792

Δk_{∞} against results with pure JEF-1.1 data		
pcm	JEF-2.2	ENDF/B-VI (Rev. 4)
RG3 (10 % void)	-469	+357
WG1 (10 % void)	-759	-673

Variation of the void coefficient		
pcm/% void	JEF-2.2	ENDF/B-VI (Rev. 4)
RG3	+2	+20
WG1	+2	+7

Results (95% Void)

Δk_{∞} against results with pure JEF-1.1 Data				
pcm	JEF-1.1 (Zr-Isos)	JEF-2.2	JEF-2.2 (Zr-Isos)	ENDF/B-VI (Rev. 4)
RG3 (0 % void)	-288	-497	-669	+132
WG1 (0 % void)	-294	-789	-916	-792

Δk_{∞} against results with pure JEF-1.1 Data				
pcm	JEF-1.1 (Zr-Isos)	JEF-2.2	JEF-2.2 (Zr-Isos)	ENDF/B-VI (Rev. 4)
RG3 (95 % void)	-312	+1611	+793	+4676
WG1 (95 % void)	-638	+1335	+542	+1753

Variation of the void coefficient				
pcm/% void	JEF-1.1 (Zr-Isos)	JEF-2.2	JEF-2.2 (Zr-Isos)	ENDF/B-VI (Rev. 4)
RG3	-0	+21	+14	+43
WG1	-2	+14	+9	+16

$$\alpha_i = \frac{\frac{1}{P_2} \cdot \left(\frac{\Delta P_i}{k_1} - \Delta A_i \right)}{\Delta x}$$

and

$$C_x = \frac{\Delta \rho}{\Delta x} = \sum_i \alpha_i$$

with:

C_x : Differential Reactivity Change

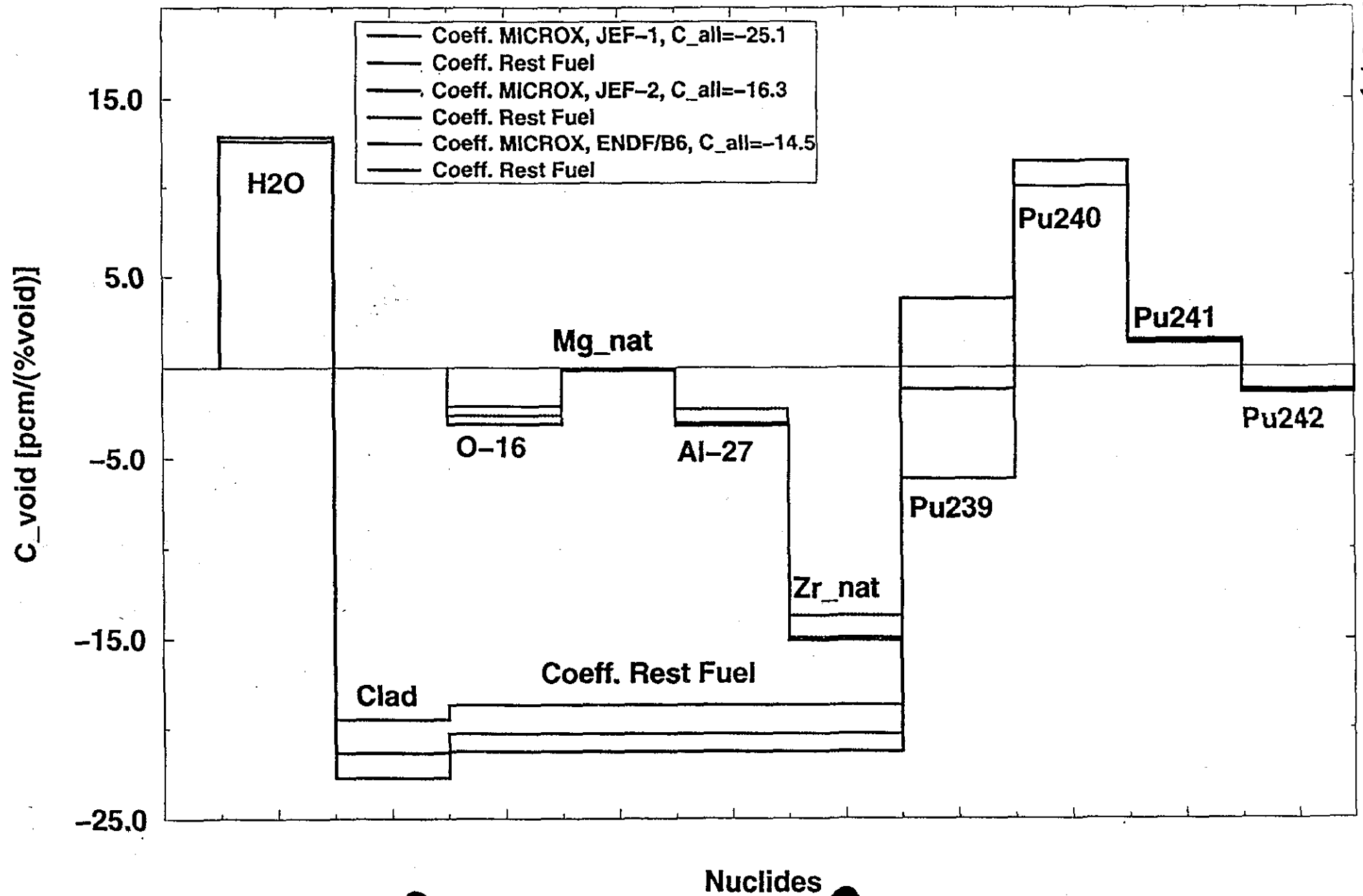
α_i : Contribution of Nuclide i

P : Production Rates

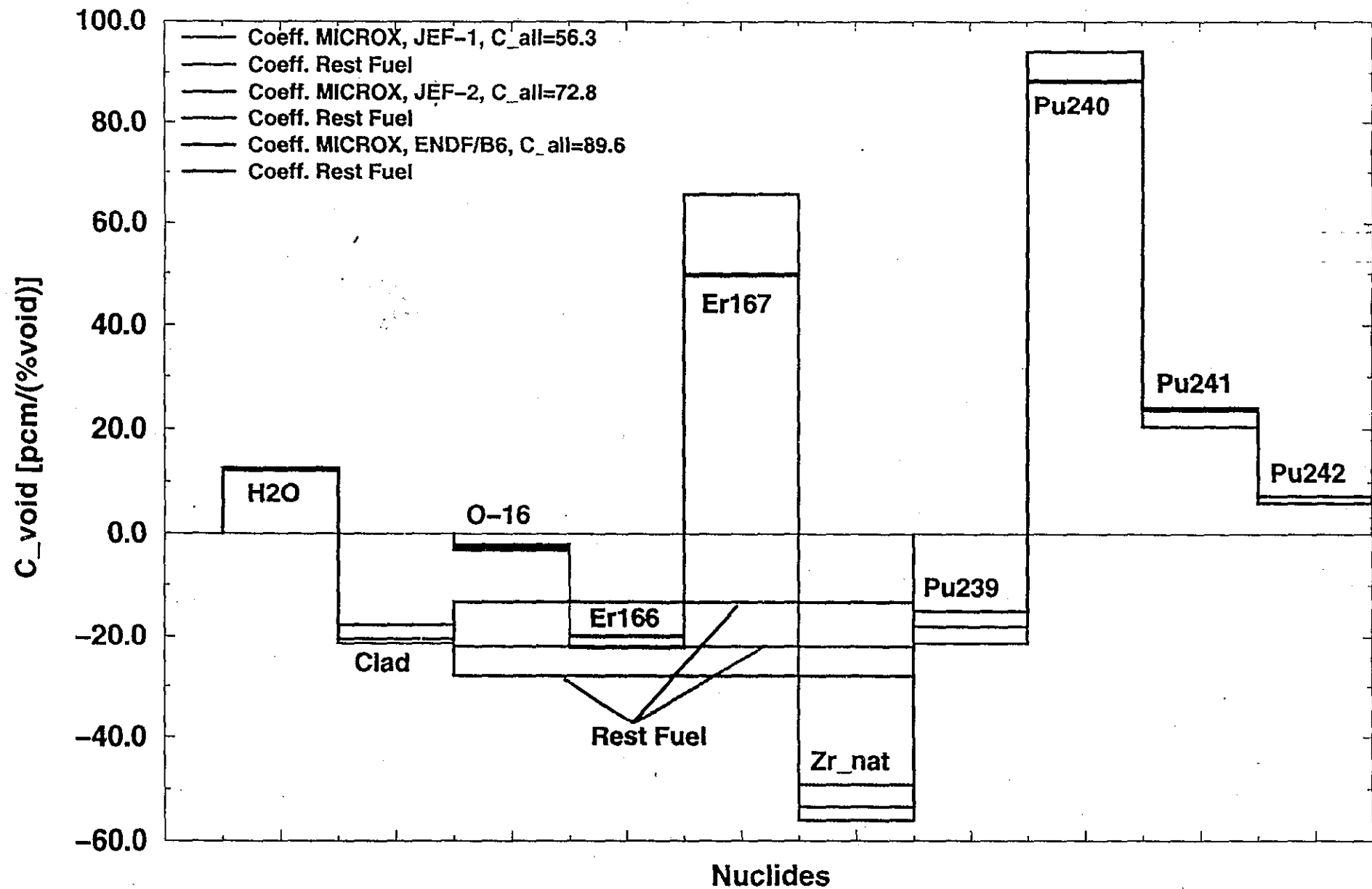
A : Absorption Rates

k_1 : initial Eigenvalue

Void Coefficient for 0 to 95% void for Fuel-1 with WG-Pu separated into the contributions of the nuclides

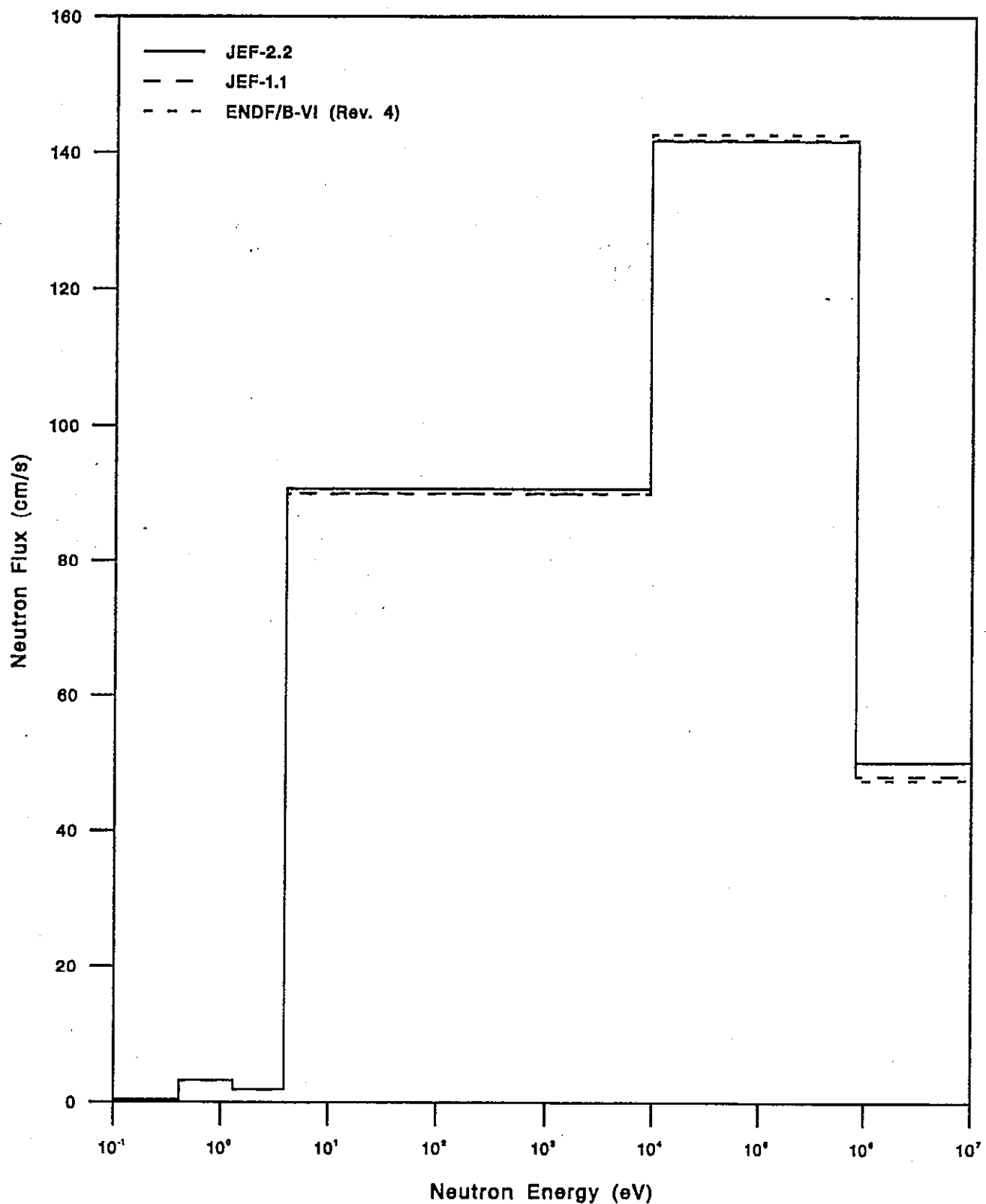


Void Coefficient for 0 to 95% void for Fuel-3 separated into the contributions of the nuclides



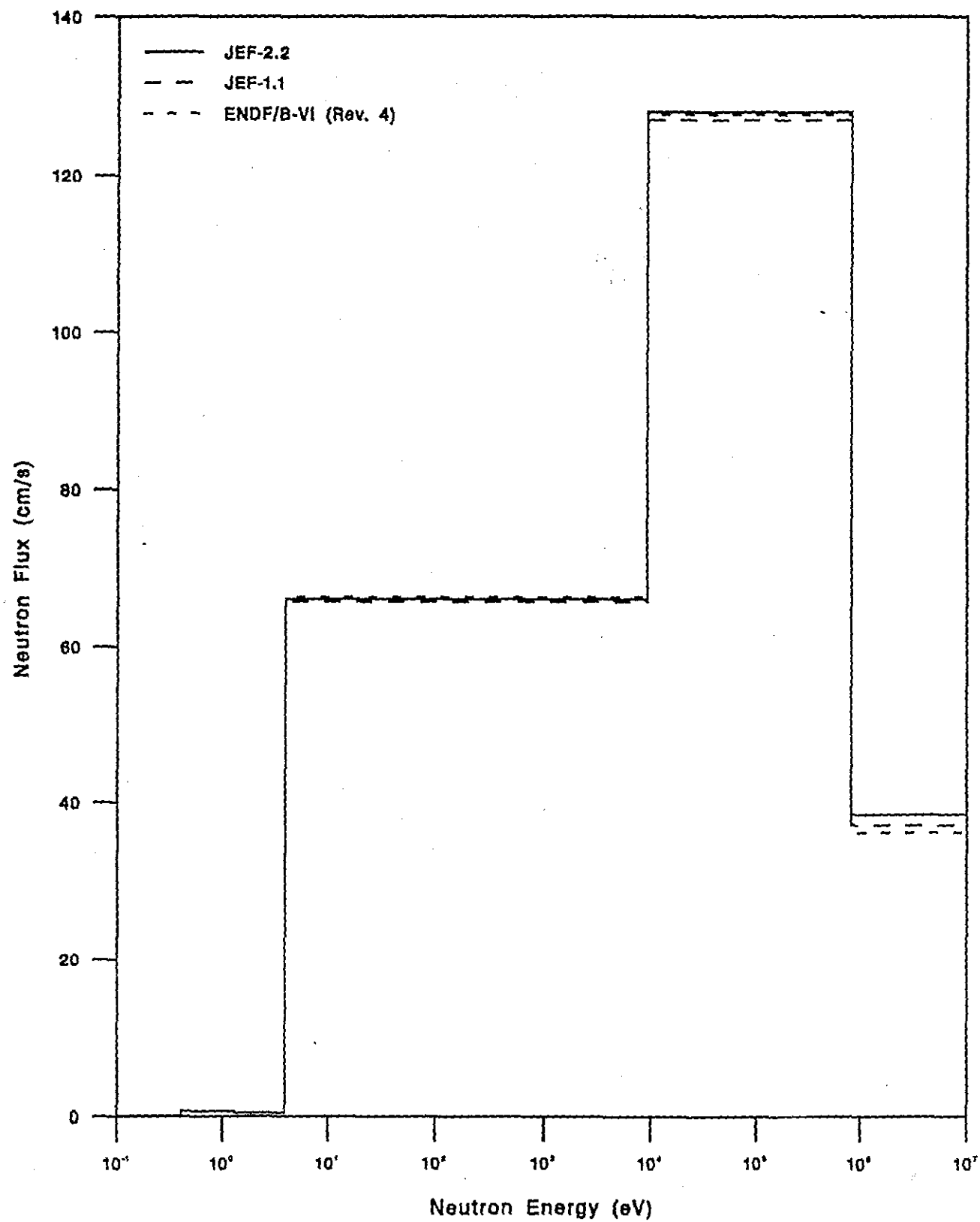
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Total Flux in 6 Groups (WG1, 95% Void)



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Total Flux in 6 Groups (RG3, 95% Void)



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We observe:

- Zr-nat =====> Zr-Isotopes:
The computed void coefficient slightly decreases.
- JEF-1.1 =====> JEF-2.2 =====>
ENDF/B-VI (Rev. 4):
The computed void coefficient **increases**.
- This **increase** becomes **bigger** when **increasing the voided fraction** (resonance range becomes more important), and
- is **significantly larger** for cells with **erbium**.

We find:

- **JEF-1.1 =====> JEF-2.2:**

- The **increase** of the void coefficient is mostly **due to ^{239}Pu , and zirconium** (in both the fuel and the clad).

- **JEF-2.2 =====> ENDF/B-VI (Rev. 4):**

- The **increase** is due to (^{167}Er ,) ^{240}Pu , and ^{239}Pu .

- However, the **contribution of zirconium decreases** and is similar to that obtained using JEF-1.1 data.

Results (Fuel Temperature Coefficient)

for RG3 from 600 to 900 degree C			
Data	JEF-1.1	JEF-2.2	JEF-2.2 (Zr-Isos)
pcm/degree C	-1.608	-1.618	-1.621

Results (at EOL)

Effects against results with pure JEF-1.1 data			
Δk_{∞} WG1 0 % Void (pcm)	Δk_{∞} RG3 0 % Void (pcm)	Δk_{∞} RG3 95 % Void (pcm)	$\Delta(\text{Void Coeff.})$ RG3 (pcm/ % Void)
JEF-2.2 data			
-442	-418	+775	+12

Results at EOL

- No additional deviations induced by fission product and minor actinide cross sections.
- These deviations are **smaller** than at **BOL**, due to the burn-up of ^{239}Pu .

Summarising Results

PSI-BOXER ("JEF-1.1")	-66
CEA-APOLLO (JEF-2.2)	-33

New calculations with MICROX-2

BOXER-Simulation	-54
JEF-1.1 (Zr-nat from ENDF/B-IV)	-48
JEF-1.1 (Zr-Isotopes)	-42
JEF-1.1	-39
JEF-2.2 (Zr-Isotopes)	-30
JEF-2.2	-26
ENDF/B-VI (Rev. 4)	-23

Example: Void Coefficient from 0 to 95 %
Void (pcm/% Void) for WG1

Concluding Remarks

- The computed k_{∞} -values for the normal situation (0 %-void) agree better than the k_{∞} -values for the voided case.
- Correct calculation of the void coefficient (for "high" voided fraction $\geq \sim 90\%$)
====> **Uncertainties** in the data for zirconium, erbium, ^{239}Pu , and ^{240}Pu must be reduced.