# **DRAFT**

# **Oxygen Potential Scattering**

C J DEAN

Reactor Physics Shielding & Criticality Department Plant Support Services Group AEA Technology Winfrith

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#### INTRODUCTION

During the development of JEF2 the Oxygen evaluation has been improved. Early WIMS libraries were developed at Winfrith and then changed as the JEF data developed. Certain evaluation related physics parameters are specified through NJOY user input. Unfortunately old NJOY decks were adapted to process the later evaluations. Important changes to the oxygen potential scattering were not made. The use of old values results in significant changes to criticality. This paper gives details of the effects and points out possible changes to the current JENDL3.2 oxygen evaluation.

## **CHOICES OF JEF EVALUATION FOR OXYGEN**

In June 1991 H Conde (JEF/DOC-342) recommended the ENDF/B-VI evaluation for oxygen be adopted for JEF2.2 in preference to an earlier recommendation (JEF/DOC-250) to use JENDL-3 data. The main reason was the improved representation of resonances at MeV energies. The JEF Scientific Coordination group approved his decision (JEF/DOC-353) and the evaluation changed. It is noted in JEF/DOC-354.

The ENDF/B-VI revision 2 and JEF2.2 O16 files contain a scattering radius (R) of 0.5562563 with a thermal (2200m/s) elastic cross section of 3.8883. Assuming the 0k 2200m/s value to be the potential scattering cross section one finds the two quantities exactly fit the formula:  $\sigma_{\text{pot}} = 4\pi R^2$ . The JENDL-3 file contains a scattering radius (R) of 0.481 with a 2200m/s cross section of 3.78b. The formula does not fit. Assuming it should and that the 2200m/s value is the evaluator's intended result, a scattering radius of ~0.548 is obtained. Is it possible that the 5 has been missed in typing?

# **PRODUCTION OF WIMS DATA LIBRARIES**

WIMS data libraries require both the scatter matrix and the potential scattering cross section. The latter quantity is used in resonance shielding (see the next section). In theory the scattering radius can depend on incident neutron energy. In most evaluations we have processed it does not. In the few where it does, we have assumed it does not as WIMS makes that assumption.

The NJOY WIMSR module requests the user to input a potential scattering value. This leaves the user to consider the problems above. We feel a default value could be calculated if the user input a negative value and that a value of -1 could be the NJOY default.

When we updated the WIMS libraries to account for Conde's recommended change we started from the previous input decks and failed to recheck and change the O16 potential scattering cross section.

## RESONANCE SHIELDING IN WIMS

WIMS resonance shielding forms a background cross section  $(\sigma_p)$  for the shieldable nuclide (j) in its environment containing other nuclides (i) thus:-

$$\sigma_{p, j} = \frac{\sum_{i} N_{i} \lambda_{i} \sigma_{pot, i}}{N_{i}} + \text{geometric effect}$$

In fact this is an approximation. In practice two close  $\sigma_p$  values are used. The oxygen  $\sigma_{pot}$  will be used in all oxide fuels! Most benchmark results will be affected. We thus studied the PWR Pincell methods benchmark (JEF/DOC-494) to get an idea of the size of the effect.

#### WIMS6 RESULTS FOR THE PWR PINCELL

Table 1 gives a breakdown of the resonance shielding formula by nuclide. Column 2 gives the number density, column 3 the Goldstein Cohen Lambda, column 4 the potential scattering cross section, and column 5 the contribution by nuclide to the overall  $\sigma_p$ . This  $\sigma_p$  value was formed by taking the two values printed in a WIMS calculation and back-fitting to the formula above which assumes a single value is used.

By using the old potential scattering cross section we shift  $\sigma_p$  by 1.967.

Figure 1 shows how the U238 absorption cross section changes with background cross section. Figure 2 highlights the region around 50 barns. One can see a change in resonance integral of ~0.38 (2%) due to the change in oxygen potential cross section.

Table 2 shows how the neutron balance changes as a result of the O16 change. The 1994 Library contains the potential scattering cross section from JENDL3.2 whereas the 1995 contains the value from JEF2.2 (ENDF/B-VI). The  $K_{\infty}$  surprisingly changes by 240 PCM. This does not correlate exactly with the changes indicated in the graph above but there are spectrum changes and probably minor changes to the U235 shielding.

It should be noted that one cannot simply apply a correction of about 0.25% to all benchmarks because as the spectra alter, the contribution of U238 absorption also changes (so does the shielding!).

# **CONCLUSIONS**

- 1) Benchmarking studies indicated problems with the 1994 WIMS JEF2.2 library.
- 2) The 1995 WIMS library uses the current JEF2.2 potential scattering data.
- 3) NJOY user input should try to avoid specifying input data which can be calculated from the nuclear data.
- 4) Quality Assurance procedures should make sure all input is checked against the current evaluation.
- 5) The JENDL3.2 O evaluators should be asked to justify their choice of scattering radius.

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 $\sigma_{p}\left(\mathsf{b}\right)$ 

Table 1. NUCLIDE CONTRIBUTIONS TO  $\sigma_{\text{p}}$ 

Nuclide	Number Density	λ	$\sigma_{ m pot}$	Contribution to $\sigma_p$	
О	0.046624	0.9726	3.8883	7.8	
U235	0.00070803	0.2	12.6106	0.079	
U238	0.022604	0.2	11.171	2.23	

Table 2. PWR PINCELL NEUTRON BALANCE FROM THE 1994 AND 1995 WIMS LIBRARIES

Nuclide	Energy Region	Absorption			Fission			Neutron Yield		
		1994	1995	PCM	1994	1995	PCM	1994	1995	PCM
Н	Fast	5.85828E-05	5.85828E-05	0						
	Resonance	1.86527E-03	1.86230E-03	0						
	Thermal	5.48915E-02	5.47825E-02	-11						
O (Fuel)	Fast	2.39611E-03	2.39611E-03	0						
	Resonance	4.37476E-07	4.36566E-07	0						
	Thermal	1.14827E-05	1.14599E-05	0						
O(Mod)	Fast	2.41092E-03	2.41092E-03	0						
	Resonance	5.32987E-07	5.32139E-07	0						
	Thermal	1.56714E-05	1.56403E-05	0						1
Zr	Fast	5.84961E-04	5.84961E-04	0						
	Resonance	2,85015E-03	2.84856E-03	0						
	Thermal	3.01828E-03	3.01229E-03	0						
U235	Fast	8.11359E-03	8.11359E-03	0	7.00627E-03	7.00627E-03	0	1.79318E-02	1.79318E-02	0
	Resonance	6.31792E-02	6.31650E-02	-4	4.06670E-02	4.06540E-02	-1	9.89530E-02	9.89214E-02	-3
	Thermal	0.57479	0.57365	-114	0.48942	0.48845	-97	1.1933	1.1909	-240
U238	Fast	5.10584E-02	5.10584E-02	0	2.93529E-02	2.93529E-02	0	8.20464E-02	8.20465E-02	0
	Resonance	0.15222	0.15366	144	1.05588E-05	1.06028E-05	0	2.62848E-05	2.63944E-05	0
	Thermal	8.25360E-02	8.23722E-02	-16	3.50973E-07	3.50277E-07	0	8.73678E-07	8.71944E-07	0
TOTALS		1.0	1.0	0	0.56646	0.56547	-99	1,39226	1,38981	-245