Annals of Nuclear Energy 63 (2014) 751–762

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

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Multi-group formulation of the temperature-dependent resonance scattering model and its impact on reactor core parameters

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Guillermo Ibarra

Nuclear Engineering Research Seminar, March 24th, 2020

Slowing Down Equation

Brief Introduction

$$\Sigma_t(E')\phi(E') = \int_0^{\infty} P(E \to E')\sigma_s(E)\phi(E)dE$$

$$\Sigma_t(E')\phi(E') = \int_0^\infty P(E \to E')\sigma_s(E)\phi(E)dE$$

$$\Sigma_t(E')\phi(E') = \int_{E'}^{E'/\alpha} \frac{\sigma_s(E)}{(1-\alpha)E}\phi(E)dE$$

$$\sigma_s(E)P(E \to E') = \begin{cases} \frac{\sigma_s(E)}{E(1-\alpha)}, & \alpha E \le E' \le E, \\ 0, & otherwise. \end{cases}$$

History of the Resonance Scattering Model

- Ouisloumen and Sanchez (1990) - RSM
- Rothenstein, 2004; Dagan, 2004 - $S(\alpha, \beta)$ tables
- Becker et al. (2009b) - Doppler broadened rejection correction (DBRC) approach

Summary of Results with the Mosteller Benchmark

Table 1
Summary of results performed using the resonance scattering model applied to the Mosteller benchmark.

#	Researcher(s)	Energy range	Nuclei	Method	CODE	LIBRARY	Fuel	Δk (pcm)	FTC diff. (%)[1]
1	Becker et al., 2009c	<210 eV	^{238}U	SVT vs. DBRC	MCNP5	JEFF3.1	UOX	–	8–16[2]
				SVT vs. DBRC			MOX[a]		
				SVT vs. DBRC			MOX[b]		
2	Sunny et al., 2012	<210 eV	^{238}U	DBRC	MCNP5	ENDF/B-VII	UOX	6 ± 25–194 ± 40	4.2 ± 0.3–15.2 ± 1.0
3	Sunny 2013	<210 eV	^{238}U	DBRC	MCNP5	ENDF/B-VII	UOX	20 ± 40–271 ± 41	8.8 ± 0.6–25.1 ± 1.7
4	Mori and Nagaya, 2009	>4.5 eV	^{238}U, ^{235}U	ASY vs. WCM	MVP-2	JENDL-3.3	UOX	72 ± 8–222 ± 14	7.2 ± 0.1–11.7 ± 0.2
5	Zoia et al., 2013	<210 eV	^{238}U	SVT vs. DBRC	TRIPOLI-4	ENDF/B-VII	UOX	66 ± 13–225 ± 14	6.2 ± 0.2–12.8 ± 0.3
6		<210 eV	^{238}U	SVT vs. WCM		ENDF/B-VII	UOX	77 ± 13–274 ± 18	8.7 ± 0.2–15.6 ± 0.4
7		0.1 eV–1 keV	^{238}U	SVT vs. DBRC		CEAV5.1	UOX	59 ± 6–232 ± 7	9.6 ± 0.1–12.7 ± 0.2
8		0.1 eV–1 keV	All nuclei	SVT vs. DBRC		CEAV5.1	UOX	62 ± 6–233 ± 7	9.3 ± 0.1–12.4 ± 0.1
9		0.1 eV–1 keV	^{238}U	SVT vs. DBRC		CEAV5.1	MOX[a]	67 ± 7–177 ± 6	7.0 ± 0.1–9.1 ± 0.1
10		0.1 eV–1 keV	All nuclei	SVT vs. DBRC		CEAV5.1	MOX[a]	108 ± 7–222 ± 6	8.0 ± 0.1–11.2 ± 0.1
11		0.1 eV–1 keV	Actinides	SVT vs. DBRC		CEAV5.1	MOX[a]	113 ± 7–232 ± 6	7.5 ± 0.1–11 ± 0.1
12	Ono et al., 2012	4–200 eV	Not specified	Deterministic	Not specified	Not specified	UOX	50–200	9.3–10.1[3]
13		4–200 eV					MOX[a]	70–160	6.5–7.2[4]
14	Lee et al., 2009	<1000 eV	^{238}U	ASY vs. WCM	CASMO-5[5]	ENDF/B-VII	UOX	59–212	9.2–9.8
15	Ghrayeb et al.	<20 MeV	Actinides	Deterministic	DRAGON	ENDF/B-VII	UOX	68–208	8.6–9.8
16	(current work)	<20 MeV	^{238}U				UOX	68–205	8.6–9.7
17		<20 MeV	^{238}U				MOX[a]	74–165	6.2–7.9
18		<20 MeV	Actinides				MOX[a]	115–216	7.5–8.7
19		<20 MeV	^{238}U				MOX[b]	89–187	6.9–9.6
20		<20 MeV	Actinides				MOX[b]	109–218	7.7–9.8

[1] FTC Diff.$(\%) = \frac{FTC_{ASY} - FTC_{RSM}}{FTC_{ASY}} \times 100$, see Eq. (8) for FTC.
[2] The FTC differences for each enrichment case were not individually documented.
[3] The difference in the Doppler reactivity coefficient were calculated manually and vary from the numbers reported in their paper.
[4] Based on Pu_2O_2 content of 4 wt.%, and 8 wt.% (their 20 wt.% cases was excluded due to a typo in their paper).
[5] The resonance integral data was calculated using their Monte Carlo Slowing Down code: MCSD code and supplied to CASMO-5.
[a] Reactor-Recycle MOX fuel.
[b] Weapons-Grade MOX fuel.

Formulation

Ousilomen and Sanchez, 1990:

$$\sigma_{sn}^{T}(E \to E') = \frac{\beta^{5/2}}{4E} e^{\frac{E}{kT}} \int_0^\infty t \sigma_s^{\text{tab}} \left(\frac{\beta k T}{A} t^2 \right) e^{-\frac{t^2}{A}} \Psi_n(t) dt$$

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For isotropic scattering:

$$\sigma_{s_0,g\to g'}^{T} = \frac{1}{\delta_g \delta_g'} \int_{E_g}^{E_{g+1}} dE \int_{E_{g'}}^{E_{g'+1}} dE' \sigma_{s_0}^{T}(E \to E')$$

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For within group scattering:

$$\sigma_{s_0,g\to g'}^{T} = \frac{1}{\delta_g \delta_g} \int_{E_g}^{E_{g+1}} dE \left\{ \int_{E_g}^{E} dE' \sigma_{s_0}^{T}(E \to E') + \int_{E}^{E_{g+1}} dE' \sigma_{s_0}^{T}(E \to E') \right\}$$

Test Implementation

Multi-group implementation of the scattering kernel with $\delta_g < 10^{-3} eV$

$$\delta_g \rightarrow 0, \delta_{g'} \rightarrow 0 \Rightarrow \sigma^T_{s_0, t \rightarrow g'} \approx \sigma^T_{s_0}(\overline{E}_g \rightarrow \overline{E}_{g'});$$

$$\overline{E}_g, \overline{E}_{g'} = \frac{E_{g+1} + E_g}{2}, \frac{E_{g'+1} + E_{g'}}{2}$$

Scattering kernel of ^{238}U at 1000 K

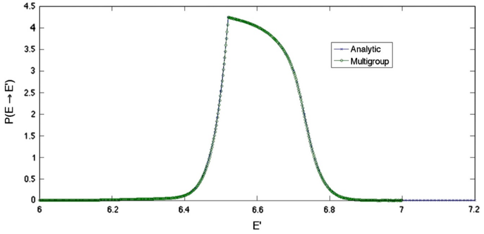

Fig. 1. Scattering kernel of ^{238}U at 1000 K for neutron starting at energy 6.52 eV.

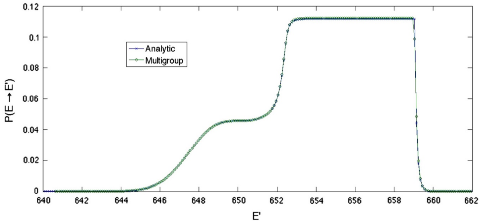

Fig. 2. Scattering kernel of ^{238}U at 1000 K for neutron starting energy of 659.05 eV.

Comparison with NJOY

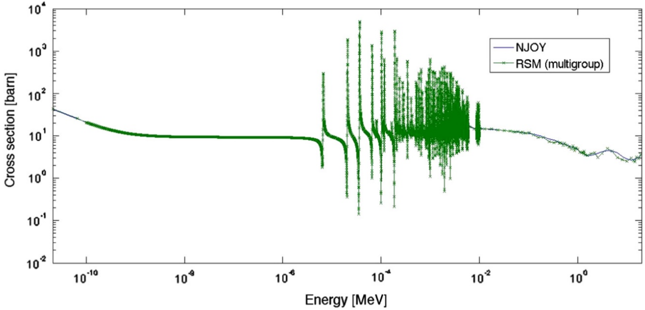

Fig. 3. The elastic cross section for ^{238}U at 900 K comparing NJOY multi-group results with those of the RSM using the same energy group structure.

Multi-group RSM with Mosteller Benchmark

- Using DRAGON Code, Marleau et al., 2010

Multi-group RSM with Mosteller Benchmark

- Using DRAGON Code, Marleau et al., 2010
- Scattering matrices generated with RSM calculation combined with NJOY data

Multi-group RSM with Mosteller Benchmark

- Using DRAGON Code, Marleau et al., 2010
- Scattering matrices generated with RSM calculation combined with NJOY data
- Fuel temperature coefficient:

$$FTC = \left(\frac{1}{k_{HZP}} - \frac{1}{k_{HFP}} \right) \frac{1 \times 10^5}{\Delta T}$$

Mosteller UOX benchmark, RSM kernel applied only to ^{238}U

Table 2
Fuel temperature coefficients for the Mosteller UOX benchmark with uranium enrichments ranging from 0.711% to 5.0% and the RSM kernel applied only to ^{238}**U**.

wt (%)	*k* (asymptotic kernel)			*k* (RSM kernel only for ^{238}U)			FTC diff (%)
	HZP	HFP	FTC	HZP	HFP	FTC	
0.711	0.6621394	0.6560206	−4.70	0.6614598	0.6548324	−5.10	−8.62
1.6	0.9562254	0.9478355	−3.09	0.9553188	0.9461777	−3.37	−9.25
2.4	1.0939660	1.0847290	−2.59	1.0929660	1.0828760	−2.84	−9.52
3.1	1.1716930	1.1620540	−2.36	1.1706490	1.1601060	−2.59	−9.66
3.9	1.2341210	1.2242040	−2.19	1.2330470	1.2221950	−2.40	−9.70
4.5	1.2694110	1.2593600	−2.10	1.2683240	1.2573230	−2.30	−9.72
5.0	1.2936360	1.2835050	−2.03	1.2925430	1.2814540	−2.23	−9.72

Mosteller UOX benchmark, RSM kernel applied to all heavy nuclides

Table 3
Fuel temperature coefficients for the Mosteller UOX benchmark with uranium enrichments ranging from 0.711% to 5.0% and the RSM kernel applied for all the heavy nuclei.

wt (%)	*k* (RSM kernel for all uranium nuclei)			FTC diff (%)
	HZP	HFP	FTC	
0.711	0.6614576	0.6548296	−5.10	−8.63
1.6	0.9553133	0.9461702	−3.37	−9.27
2.4	1.0929570	1.0828640	−2.84	−9.56
3.1	1.1706380	1.1600910	−2.59	−9.70
3.9	1.2330470	1.2221950	−2.40	−9.70
4.5	1.2683090	1.2573000	−2.30	−9.81
5.0	1.2925260	1.2814290	−2.23	−9.81

FTCs, RSM kernel applied to all heavy nuclides

Table 4
Fuel temperature coefficients for the Mosteller Reactor-Recycle MOX fuel benchmark with 1–8 wt.% PuO_2 and the RSM kernel applied to all the heavy nuclei.

MOX composition (PuO_2 wt.%)	*k* (asymptotic kernel)			*k* (RSM kernel)			FTC diff. (%)
	HZP	HFP	FTC	HZP	HFP	FTC	
1.0	0.9407429	0.9312128	−3.63	0.9395729	0.9292448	−3.94	−8.74
2.0	1.0183990	1.0076460	−3.49	1.0171230	1.0055030	−3.79	−8.43
4.0	1.0759170	1.0644960	−3.32	1.0746340	1.0623330	−3.59	−8.05
6.0	1.1057560	1.0942010	−3.18	1.1045310	1.0921170	−3.43	−7.76
8.0	1.1297120	1.1181500	−3.05	1.1285580	1.1161660	−3.28	−7.48

Table 5
Fuel temperature coefficients for the Mosteller Weapons-Grade MOX fuel benchmark with 1–6 wt.% PuO_2 and the RSM kernel applied to all the heavy nuclei.

MOX composition (PuO_2 wt.%)	*k* (asymptotic kernel)			*k* (RSM kernel)			FTC diff. (%)
	HZP	HFP	FTC	HZP	HFP	FTC	
1.0	1.0838630	1.0748170	−2.59	1.0827770	1.0728730	−2.84	−9.79
2.0	1.1765110	1.1656680	−2.64	1.1753040	1.1635420	−2.87	−8.79
4.0	1.2472990	1.2352440	−2.61	1.2460520	1.2330640	−2.82	−8.04
6.0	1.2847710	1.2725020	−2.50	1.2835640	1.2703840	−2.69	−7.71

FTCs, RSM kernel applied only to ^{238}U

Table 6
Fuel temperature coefficients for the Mosteller Reactor-Recycle MOX fuel benchmark with 1–8 wt.% PuO_2 and the RSM kernel applied to ^{238}U only.

MOX composition (PuO_2 wt.%)	HZP	HFP	FTC	FTC diff. (%)
1.0	0.9398723	0.9296191	−3.91	−7.87
2.0	1.0175060	1.0059940	−3.75	−7.33
4.0	1.0750620	1.0628910	−3.55	−6.81
6.0	1.1049570	1.0926810	−3.39	−6.46
8.0	1.1289670	1.1167140	−3.24	−6.18

Table 7
Fuel temperature coefficients for the Mosteller Weapons-Grade MOX fuel benchmark with 1–6 wt.% PuO_2 and the RSM kernel applied to ^{238}U only.

MOX composition (PuO_2 wt.%)	HZP	HFP	FTC	FTC diff. (%)
1.0	1.0828870	1.0730010	−2.84	−9.57
2.0	1.1755180	1.1637980	−2.86	−8.35
4.0	1.2463530	1.2334410	−2.80	−7.35
6.0	1.2838850	1.2707980	−2.67	−6.88

FTCs, RSM kernel applied to individual nuclei

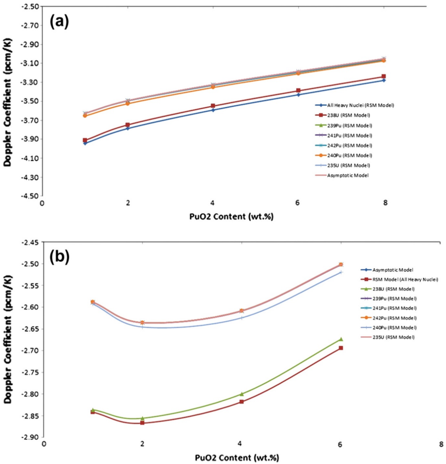

Fig. 4. Fuel temperature coefficient for the (a) Reactor-Recycle MOX fuel pin and (b) Weapons-Grade MOX fuel pin when applying the RSM to individual nuclei.

Mini

Table 8
The up-scattering percentage contribution of each nucleus towards the eigenvalue for Mosteller Reactor-Recycle MOX fuel benchmark with 1–8 wt.% PuO_2 at 600 K.

MOX composition (PuO_2 wt.%)	^{238}U	^{235}U	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	74.51	0.09	0.04	2.59	22.58	0.19
2.0	70.15	0.16	0.08	6.13	23.33	0.16
4.0	66.85	0.39	0.23	11.65	20.72	0.16
6.0	65.60	0.49	0.33	15.19	18.23	0.16
8.0	64.84	0.78	0.52	17.75	15.93	0.17

Table 9
The up-scattering percentage contribution of each nucleus towards the eigenvalue for Mosteller Reactor-Recycle MOX fuel benchmark with 1–8 wt.% PuO_2 at 900 K.

MOX composition (PuO_2 wt.%)	^{238}U	^{235}U	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	81.17	0.07	0.03	1.65	16.95	0.14
2.0	77.30	0.14	0.09	4.07	18.25	0.14
4.0	74.62	0.28	0.14	8.00	16.83	0.14
6.0	73.54	0.39	0.24	10.64	15.05	0.15
8.0	73.12	0.56	0.31	12.53	13.39	0.10

Table 10
The up-scattering percentage contribution of each nucleus towards the eigenvalue for Mosteller Weapons-Grade MOX fuel benchmark with 1–6 wt.% PuO_2 at 600 K.

MOX composition (PuO_2 wt.%)	^{238}U	^{235}U	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	89.87	0.18	0.00	0.00	9.76	0.18
2.0	82.41	0.33	0.00	0.00	17.10	0.17
4.0	75.98	0.64	0.00	0.00	23.21	0.16
6.0	73.59	0.91	0.00	0.00	25.33	0.17

Table 11
The up-scattering percentage contribution of each nucleus towards the eigenvalue for Mosteller Weapons-Grade MOX fuel benchmark with 1–6 wt.% PuO_2 at 900 K.

MOX composition (PuO_2 wt.%)	^{238}U	^{235}U	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	93.51	0.15	0.00	0.00	6.18	0.15
2.0	88.08	0.28	0.00	0.00	11.49	0.14
4.0	82.90	0.51	0.00	0.00	16.46	0.14
6.0	80.80	0.71	0.00	0.00	18.40	0.09

Neutron Flux Near Third Resonance of ^{238}U

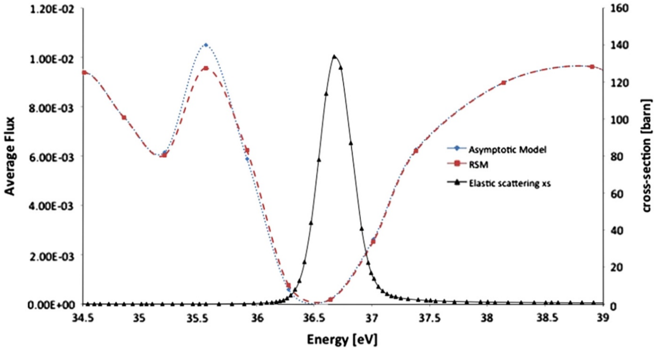

Fig. 5. Neutron flux of the fuel region for UO_2 pin-cell at 0.711 wt.% enrichment at 600 K near the third resonances of ^{238}U, 36.68 eV, using the RSM (dashed curve) and the traditional asymptotic (dotted curve) model. The elastic scattering cross section is also plotted (solid curve).

Relative Differences

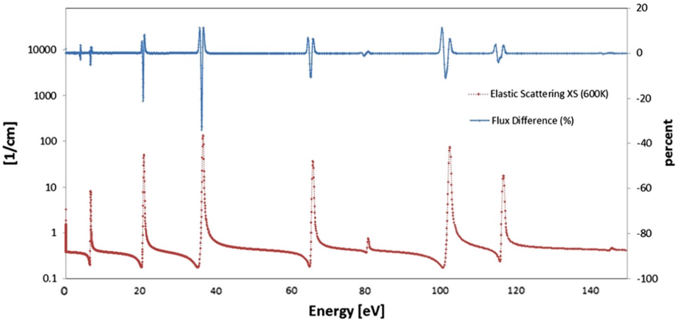

Fig. 6. Relative difference in flux (%, solid curve above) between the asymptotic model and the resonance scattering model plotted against the macroscopic cross-section of the fuel (dotted curve below). Where the flux is almost zero, the relative error is very large (which cannot be seen in Fig. 5 due to the scale in that figure).

Comparison of Works with the Mosteller Benchmark

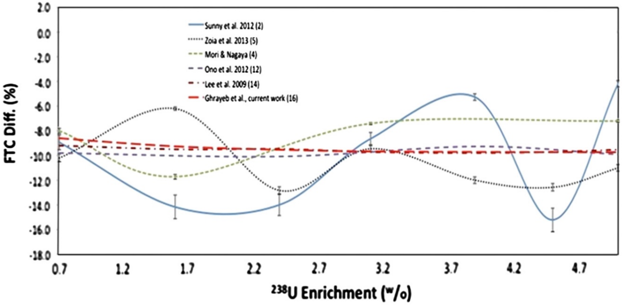

Fig. 7. Comparison of the FTC differences for UOX Mosteller benchmark. The results of Ghrayeb et al. (long dashed curve) and Lee et al. 2009 (dash dot curve) compare relatively well against each other showing a nearly constant behavior in FTC difference with respect to ^{235}U enrichment. However, there is no consensus among the work of others to show consistency in FTC difference with respect to ^{235}U enrichment. The numbers in parentheses correspond to the first column of Table 1.

Summary of Main Aspects, TLDR

- Temperature-dependent resonance scattering and up scattering effects are considered in slowing down calculation.

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- In the case of the UO_2 fuel, the contribution of up-scattering was overwhelmingly due to ^{238}U.
- When using RSM instead of asymptotic model, in case of UO_2 fuel, change in eigenvalues varies from 68 to 208 pcm.
- In the case of the weapons-grade MOX fuel the largest and most significant contribution to resonance up-scattering after that of ^{238}U is that of ^{241}Pu, which is responsible for as much as 25% of up-scattering

Thanks!
Questions?