

# Development of Multigroup Cross Section Generation Code MC<sup>2</sup>-3 for Fast Reactor Analysis

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# Background

- Under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) of U.S. DOE, an integrated, advanced neutronics code system is being developed to allow the high fidelity description of a nuclear reactor and simplify the multi-step design process
  - Development of UNIC with unstructured finite element mesh capabilities on a large scale of parallel computation environment
  - Integration with thermal-hydraulics and structural mechanics calculations
- As part of this effort, an advanced multigroup cross section generation code named MC<sup>2</sup>-3 is being developed
  - The ANL multigroup generation code system, ETOE-2 / MC<sup>2</sup>-2 / SDX, has been successfully used for fast reactor analysis
  - Recent studies with the ENDF/B-VII.0 data identified some improvement needs of MC<sup>2</sup>-2
    - Increased importance of resolved resonances in the ENDF/B-VII.0 data due to the extended upper energy cutoff and significantly increased number of resolved resonances required the use of RABANL for a rigorous treatment of resolved resonances
    - Use of RABANL is limited to the relatively low energy range where the isotropic source approximation is valid

## ETOE-2 / MC<sup>2</sup>-2 / SDX

- ETOE-2
  - Generate MC<sup>2</sup> libraries by processing ENDF/B data, including ultrafine group smooth cross sections (2,082 groups with constant lethargy from 20 MeV to 0.4 eV)
  - Screen out wide resonances to smooth cross sections
  - Convert the resolved resonances in the Reich-Moore formalism to those in the multipole formalism
- MC<sup>2</sup>-2
  - Self-shield unresolved and resolved resonances using the generalized resonance integral method based on the narrow resonance (NR) approximation
  - Perform the consistent P1 or B1 transport spectrum calculations
    - Multigroup method for above resolved resonance energy range
    - Continuous slowing down method for the resolved resonance energy range
  - RABANL option for the hyperfine group slowing-down calculation based on isotropic elastic scattering (applicable below ~tens keV)
- SDX
  - Perform the 1D integral transport calculation to account for the local heterogeneity effects

#### MC<sup>2</sup>-2/SDX vs. MC<sup>2</sup>-3



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## Changes and Improvements in MC<sup>2</sup>-3

- Numerical integration of resolved resonances with pointwise cross sections based on the NR approximation
  - Reconstruction of pointwise cross sections with Doppler broadening
  - Optionally, use of PENDF files from NJOY
- Multigroup spectrum calculation with the consistent P<sub>1</sub> transport equation for the entire energy range
- New capability of treating anisotropic inelastic scattering
- Self-shielding of resonance-like cross sections above the resonance energy for intermediate-weight nuclides (Fe, Cr, Ni, etc.)
- 1D transport calculation with ultrafine (2082) or user-defined groups (SDX capability)
- 1D hyperfine (> ~100,000) group transport calculation
  - MOC solver with higher-order anisotropic scattering in the LS and CMS (up to ~1 MeV)

$$\sigma_{sl}^{i}(g \to g') = \frac{1}{\psi_{lg}} \int_{u_{g'-1}}^{u_{g'}} du' \int_{u_{g-1}}^{u_{g}} du \frac{\psi_{l}(u)\sigma_{s}^{i}(u)e^{-(u'-u)}P_{l}(\mu_{s}^{i})}{(1-\alpha_{i})} \sum_{n=0}^{N} (2n+1)f_{n}^{i}(u)P_{n}(\mu_{c}^{i})$$

- Inline cross section generation as a module of UNIC
  - Standalone version for conventional multi-step analyses
- FORTRAN 90/95 memory structure

## **Critical Experiments**

Δk in pcm from Monte Carlo results



## C/E of Fission Reaction Rate Ratios for LANL Assemblies

Assembly		Data	$\sigma^{\scriptscriptstyle U238}_{\scriptscriptstyle f}$ / $\sigma^{\scriptscriptstyle U235}_{\scriptscriptstyle f}$	$\pmb{\sigma}_{\scriptscriptstyle f}^{\scriptscriptstyle Np237}$ / $\pmb{\sigma}_{\scriptscriptstyle f}^{\scriptscriptstyle U235}$	$\sigma^{\scriptscriptstyle U233}_{\scriptscriptstyle f}$ / $\sigma^{\scriptscriptstyle U235}_{\scriptscriptstyle f}$	$\sigma_{\scriptscriptstyle f}^{\scriptscriptstyle Pu239}$ / $\sigma_{\scriptscriptstyle f}^{\scriptscriptstyle U235}$
	Experiment		$0.1643 \pm 0.0018$	$0.8516 \pm 0.013$	$1.59 \pm 0.03$	$1.4152 \pm 0.025$
GODIVA	C/E	MCNP <sup>a)</sup>	0.960	0.975	0.987	0.977
		$MC^2$ -3 <sup>b)</sup>	0.958	0.974	0.987	0.977
	Experiment		0.2133±0.0023	$0.9835 \pm 0.016$	$1.578 \pm 0.027$	$1.4609 \pm 0.013$
JEZEBEL	C/E	MCNP	0.978	0.988	0.986	0.975
		$MC^2$ -3	0.968	0.986	0.987	0.975
JEZEBEL -23	Experiment		0.2131±0.0026	$0.9970 \pm 0.015$		
	C/E	MCNP	0.989	0.984		
		$MC^2-3$	0.988	0.998		
<b>ΓΙ ΑΤΤΟΡ</b>	Experiment		$0.1492 \pm 0.0016$	$0.7804 \pm 0.01$	$1.608 \pm 0.003$	$1.3847 \pm 0.012$
-25	C/E	MCNP	0.968	0.988	0.975	0.982
		$MC^2-3$	0.966	0.988	0.975	0.982
FLATTOP -Pu	Experiment		$0.1799 \pm 0.002$	$0.8561 \pm 0.012$		
	C/E	MCNP	0.984	0.996		
		$MC^2-3$	0.970	0.992		
<b>ΓΙ ΑΤΤΟΡ</b>	Experiment		0.1916±0.0021	$0.9103 \pm 0.013$		
-23	C/E	MCNP	0.976	0.997		
-23		$MC^2$ -3	0.976	0.998		

#### C/E of Fission Reaction Rate Ratios for LANL Assemblies



## **Hyperfine-Group Spectrum Calculation**



Inner core composition of ZPR-6/6A

#### Ultrafine and Hyperfine Group Spectrum Calculation with Anisotropic Scattering Sources



#### **ZPPR-15A Critical Experiments**



120 - - 110 -	MATRIX TUBES			MATRIX TURES	
- 100 -	AXIAL REFLECTOR	MATTIA TODES			
90 - - 80 -	AMALREFLECTOR				
- 70 - 60 - 50 -	AXIALBLANKET	AXIAL BLANKET	R A D I A	RADIAL	
40 - 30 - 21 - 10 -	INNER CORE	OJTER CORE	B L A K K E T	REFLECTOR	

Loading	Experiment	VIM	M C <sup>2</sup> - 2	M C <sup>2</sup> - 3
15	1.00046	0.99985	-392	-245
16	0.99627	0.99571	-393	-244
20	0.99853	0.99742	-316	-192

\* Uncertainty: Experiment < ±0.0018, VIM < ±0.00020



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## **ZPR-6** Critical Experiments

- A full core heterogeneous reactor calculations with explicit fuel plate representation
- 50,000,000 vertices

   (~equivalent to 200 million
   PARTISN finite difference cells)
- 200+ angles with P<sub>5</sub> anisotropic scattering
- 9, 33, 70, and 230 groups
- No thermal-hydraulics considerations (i.e. clean comparison with MCNP/VIM)



Plate by Plate ZPR Geometry



## UNIC Results with MC<sup>2</sup>-3 Cross Sections

 Homogeneous cell cross sections with MC<sup>2</sup>-3 without the heterogeneity effect of fuel drawers

Energy Group	K-effective	$\Delta$ k pcm		
9	0.99513	113		
33	0.99373	-27		
116	0.99355	-45		
230	0.99344	-56		
VIM : 0.99400 ±0.00020				



Power Distribution

 Cell-averaged cross sections with the 1D slab transport calculation of MC<sup>2</sup>-3 to account for the heterogeneity effect of fuel drawers

	Energy Group	K-effective	$\Delta$ k pcm
	9	1.00007	26
VIIVI 0.99981 +0.00025	33	0.99966	-15
0.00001 20100020	116	0.99965	-16
	230	0.99966	-15
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# Summary

- New multigroup cross section generation code MC<sup>2</sup>-3 has been developed with improved methods
- Verification tests with LANL, ZPR-6, ZPPR-15A, ZPPR-21, and BFS critical experiments showed more rigorous and accurate solutions compared to MC<sup>2</sup>-2 / SDX
- 1D hyperfine-group transport calculation capability with higher-order anisotropic scattering sources is near completion
- Initial integration of MC<sup>2</sup>-3 into UNIC for inline cross section generation was accomplished
- Development of efficient algorithms for inline multigroup cross section generation is in progress