FITXS: A fast burn-up scheme based on the fitting of one-group cross-sections

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Introduction

Time evolution of the fuel composition (Bateman equations):

$$\frac{\mathrm{d}N_i}{\mathrm{d}t} = \sum_{j \neq i} (\sigma_{ji}\Phi + f_{ji}\lambda_j)N_j(t) - (\sigma_i^a \Phi + \lambda_i)N_i(t)$$

Difficulty: $\sigma = \sigma(N_1, N_2, \ldots, N_n), \quad \Phi = \Phi(N_1, N_2, \ldots, N_n)$

Common approximations:

- burn-up tables
- precalculated average cross-section sets
- parametrized cross-sections (e.g. burn-up dependent cross-section sets)

The first two methods are possibly inaccurate when the fuel composition changes greatly (e.g. Pu and/or MA multirecycling)

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The FITXS method

Common parameters used for cross-section parametrization:

- fuel burn-up or irradiation time
- initial ^{235}U enrichment
- initial Pu content in the case of MOX
- etc.

Main idea: parametrization of one-group cross-section as functions of the detailed fuel composition (atomic densities of 15-20 nuclides)

1. selection of fitting parameters
2. preparation of the cross-section databases
3. cross-section fitting

$$\sigma(N_1, N_2, \ldots, N_n) = a_0 + \sum_{i=1}^{n} a_i N_i + \sum_{i=1}^{n} \sum_{j=i}^{n} a_{ij} N_i N_j$$

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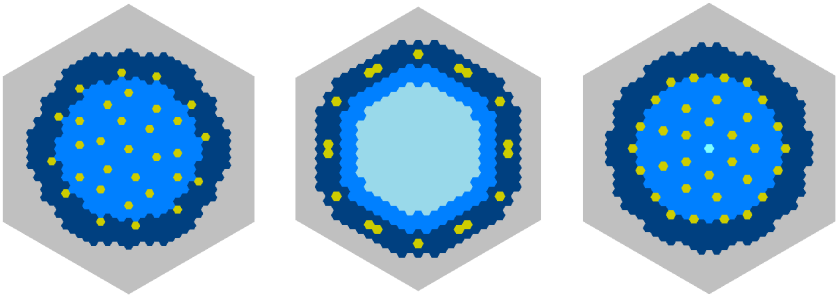
Selection of fitting parameters

- Fitting parameters were selected based on their contribution to the total reaction rates in preliminary core calculations and fuel cycle studies.

Component	GFR2400		EPR MOX	
	Parameter	Rel. reaction rate (%)	Parameter	Rel. reaction rate (%)
U	^{234}U	0.43	^{234}U	0.02
	^{235}U	0.43	^{235}U	0.75
	^{236}U	0.35	^{236}U	0.03
	^{238}U	43.1	^{238}U	23.3
Pu	^{238}Pu	2.26	^{238}Pu	0.86
	^{239}Pu	36.0	^{239}Pu	35.8
	^{240}Pu	7.80	^{240}Pu	15.0
	^{241}Pu	2.54	^{241}Pu	12.5
	^{242}Pu	0.73	^{242}Pu	2.72
MA	^{237}Np	1.59	^{237}Np	0.07
	^{239}Np	0.04	^{239}Np	0.01
	^{241}Am	2.62	^{241}Am	1.59
	^{242m}Am	0.34	^{242m}Am	0.08
	^{243}Am	0.85	^{243}Am	1.16
	^{244}Cm	0.34	^{242}Cm	0.01
	^{245}Cm	0.21	^{244}Cm	0.22
FP	Total FP	0.33	Total FP	5.84
			^{135}Xe	0.76
			^{149}Sm	0.51
Total		99.9		99.9

Preparation of fast reactor cross-section databases



(a) GFR2400 (b) ELSY (c) ESFR

- three-dimensional SCALE 6.0 KENO-VI core models
- inner (middle) and outer fuel regions with different Pu content
- two-step homogenization (elementary cell + fuel assembly)

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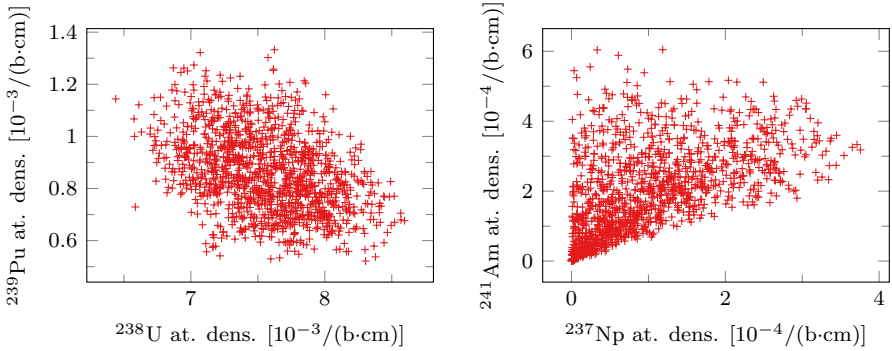
Preparation of fast reactor cross-section databases

Random sampling of the fuel composition:

- 10-25% Pu, 0-10% MA, rest U
- average fission product composition
- actinide isotopic composition also randomly sampled
- preliminary k_{eff} fitting for rejection method (k_{eff} betwen 0.9 and 1.15)



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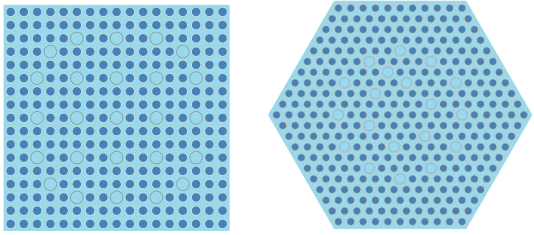
Preparation of thermal reactor MOX cross-section databases



(a) EPR (b) VVER-1200

- three-dimensional SCALE 6.0 KENO-VI fuel assembly models with reflective BCs
- MOX fuel with average pin composition
- Goal: analysis of fast reactor Pu recycling in thermal reactors

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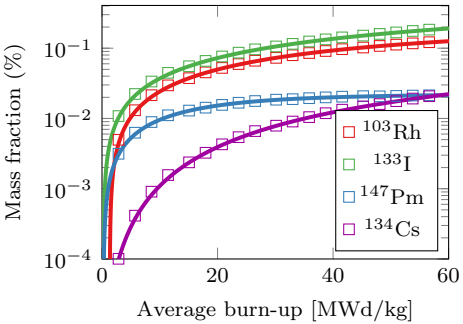
Preparation of thermal reactor MOX cross-section databases

Random sampling of the fuel composition:

- 5-12% Pu, 0-1% MA, rest U
- fission product composition fitted as 4th order polynomial function of the burn-up
- ^{135}Xe and ^{149}Sm sampled with uniform composition
- linear decrease assumed for boric acid concentration



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Cross-section fitting procedure

The following second-order polynomials were fitted on the cross-sections (and the k_{eff}):

$$\sigma(N_1, N_2, \ldots, N_n) = a_0 + \sum_{i=1}^{n} a_i N_i + \sum_{i=1}^{n} \sum_{j=i}^{n} a_{ij} N_i N_j$$

Applying the above equation on every fuel composition in the database:

$$\mathrm{M}\underline{a} = \begin{bmatrix} 1 & N_1^{(1)} & N_2^{(1)} & \ldots & N_{n-1}^{(1)} N_n^{(1)} \\ 1 & N_1^{(2)} & N_2^{(2)} & \ldots & N_{n-1}^{(2)} N_n^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & N_1^{(m)} & N_2^{(m)} & \ldots & N_{n-1}^{(m)} N_n^{(m)} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1,n} \end{bmatrix} = \underline{\sigma}$$

The least squares solution can be obtained by solving the Gaussian normal equation:

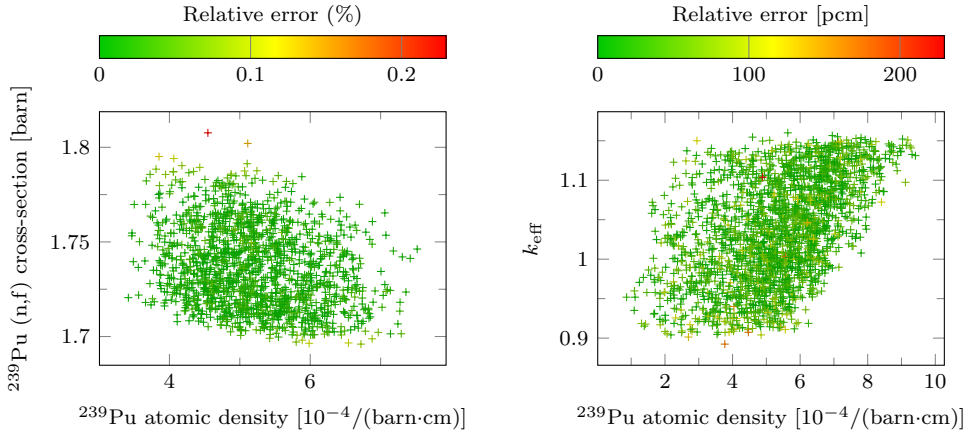
$$(\mathrm{M}^{\mathrm{T}}\mathrm{M})\underline{a} = \mathrm{M}^{\mathrm{T}}\underline{\sigma}$$

Provided that the columns of M are linearly independent:

$$\underline{a} = \mathrm{M}^{+}\underline{\sigma} = (\mathrm{M}^{\mathrm{T}}\mathrm{M})^{-1}\mathrm{M}^{\mathrm{T}}\underline{\sigma}$$

Fitting results

- The fitted polynomials describe (n,f) and (n,γ) cross-sections and the k_{eff} with average relative error around 0.1%.



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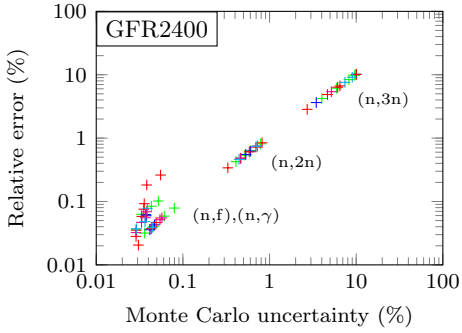
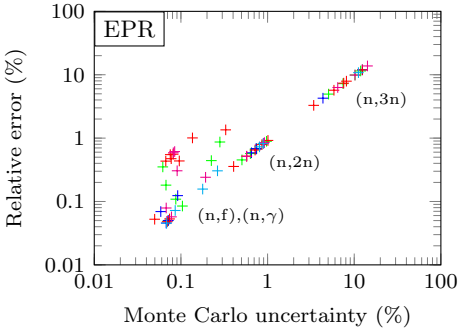
Fitting results

- Typical fitting errors are in the order of magnitude of the Monte Carlo uncertainties (but not below).





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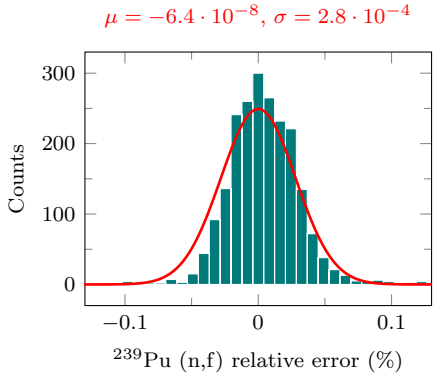

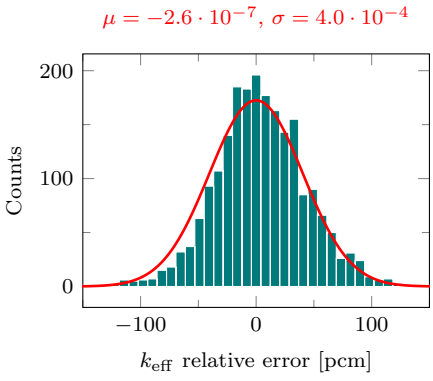

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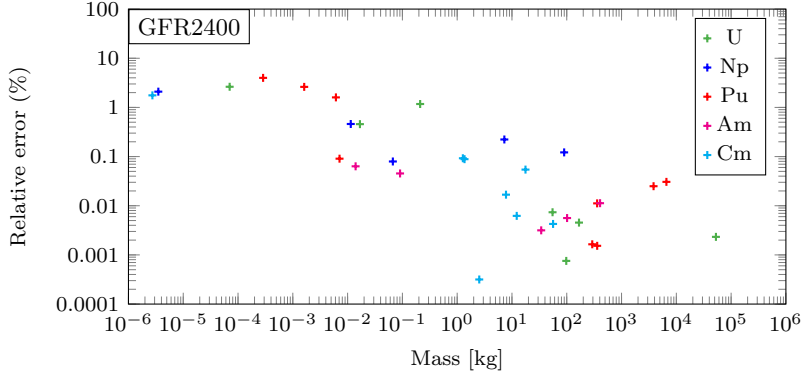
Verification

Comparison of burn-up calculations with FITXS and SCALE 6.0 cross-sections:



- Very good agreement between FITXS and SCALE 6.0 results for fast reactors

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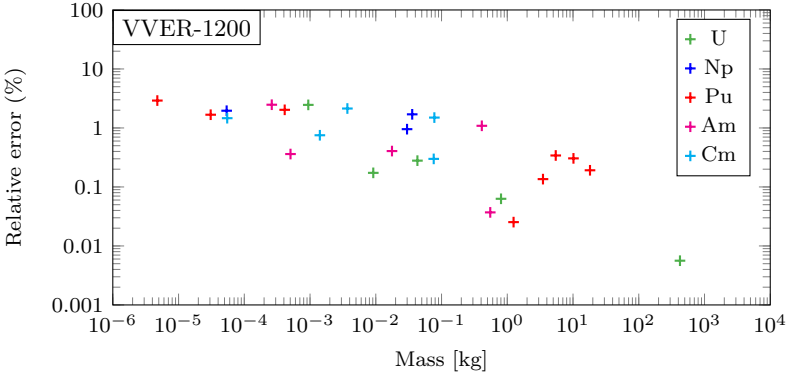

- Acceptable agreement between FITXS and SCALE 6.0 results for MOX fuel assemblies

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Further development plans

- alternate fitting methods (for thermal MOX fuel assemblies)
- cross-section database preparation with pure deterministic calculations
- perform fittings for reactivity coefficients
- optimization of the fitting domain

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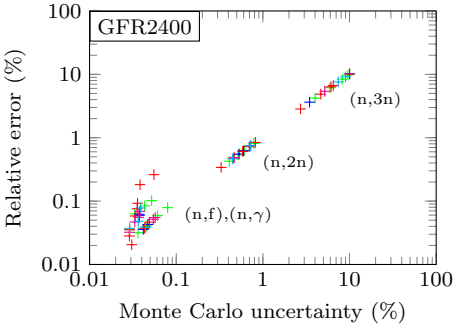
Preliminary results with neural network fitting

Preliminary fitting with neural networks performed on the GFR2400 database based on:

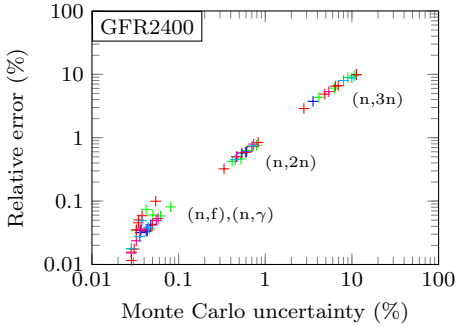
B. Leniau et al. "A neural network approach for burn-up calculation and its application to the dynamic fuel cycle code CLASS". *Annals of Nuclear Energy* 81 (2015), pp. 125-133.

- tanh sigmoid transfer function, Levenberg-Marquardt training
- (n,f) and (n,γ) cross-sections: 2 hidden layers of 16 and 12 neurons
- (n,2n) and (n,3n) cross-sections: 1 hidden layer of 16 neurons

polynomial fitting



neural network



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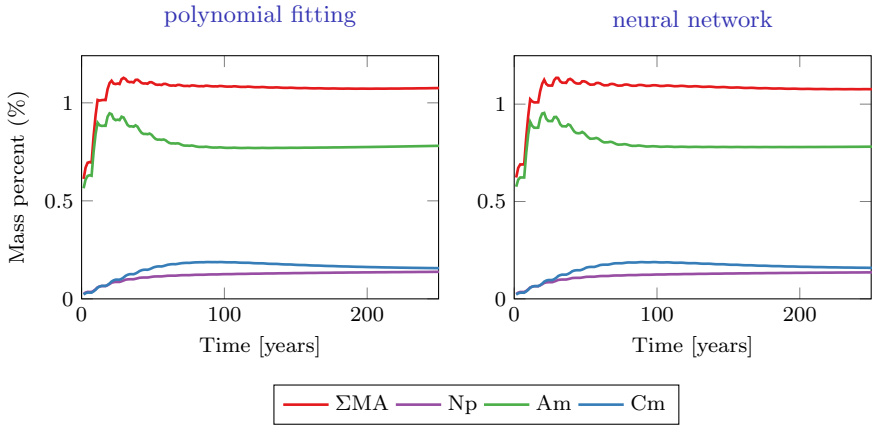
- Good agreement between closed fuel cycle simulation results with polynomial fitting and neural networks



Summary

- The FITXS method is based on the fitting of one-group cross-sections as functions of the detailed fuel composition.
- Gen-IV fast reactor and Gen-III thermal reactor MOX burn-up models were developed.
- The fitted polynomials describe important cross-sections and the k_{eff} with relative error well below 1%.
- Results of the FITXS burn-up models showed good agreement with SCALE 6.0 burn-up results.
- The models were integrated in the SITON v2.0 code developed at MTA EK and another simulation program developed at BME NTI.
- Possibilities for improvement are investigated in the case of thermal reactors.

Related publications:

Máté Halász, Máté Szieberth, Sándor Fehér. "FITXS: A fast and flexible burn-up scheme based on the fitting of one-group cross-sections". *Annals of Nuclear Energy* 104 (2017), pp. 267-281.

Áron Brolly, Máté Halász, Máté Szieberth, Lajos Nagy, Sándor Fehér. "Physical model of the nuclear fuel cycle simulation code SITON". *Annals of Nuclear Energy* 99 (2017), pp. 471-483.

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