

FISPACT-II

Self shielding of resonant channels

Probability tables, sub-group method

Applications: black n-absorber, LWR fuel cycle

Jean-Christophe Sublet



CALENDF probability tables are used to model dilution effects in the computation of the effective cross-sections

cal-mt	description	mt in set
2	elastic scattering	2
101	absorption (no outgoing neutron)	102 103 107
18	fission total	18
4	inelastic scattering (emitting one neutron)	4 11
15	multiple neutron production (excluding fission)	5 16 17 37

$$\sigma_{\text{eff}}(x, n) = \sigma_{\text{eff}}(g, x, n) \text{ and } p(x, n) = p(g, x, n)$$

where

g = energy group number

x = macro-partial (or total) index

n = quadrature index

Cross section, PT distribution, discretization

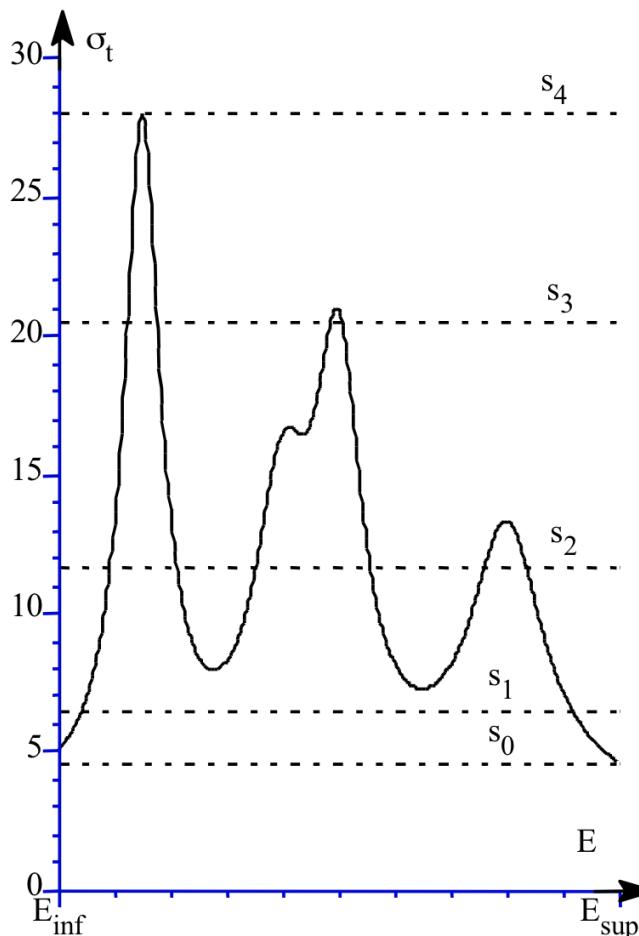
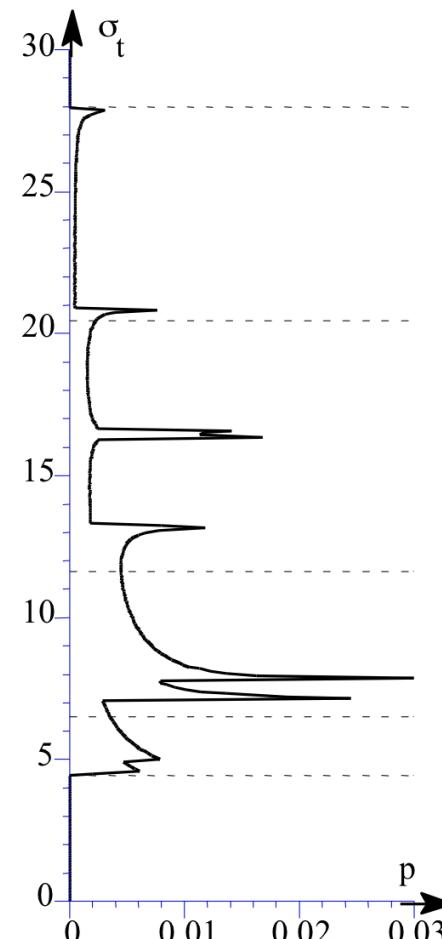
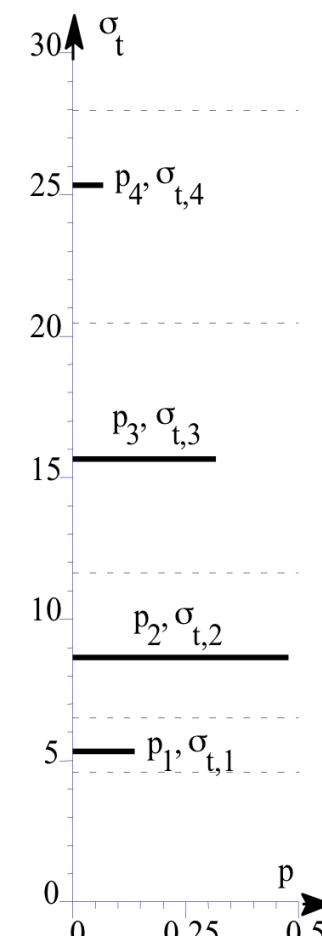


Fig. 1a Cross section versus energy



1b Exact PT distribution



1c PT discretisation

$$\frac{1}{G} \int_{E_{\text{inf}}}^{E_{\text{sup}}} \sigma_t^n(E) dE = \int_{\sigma_{\min}}^{\sigma_{\max}} p(\sigma_t) \sigma_t^n d\sigma_t = \sum_{i=1}^{i=N} p_i \sigma_{t,i}^n$$



Padé approximant and Gauss Quadrature

The moments having been computed, the probability table is established:

$$\begin{aligned} I(z) &= \int \frac{p(x)}{1 - zx} dx = \underbrace{M_0 + M_1 z + M_2 z^2 + \dots + M_{2N-1} z^{2N-1}}_{2N \text{ moments}} + R_{2N} z^{2N} \\ &= \frac{b_0 + b_1 z + b_2 z^2 + \dots + b_{N-1} z^{N-1}}{\underbrace{1 + a_1 z + a_2 z^2 + \dots + a_N z^N}_{Q_{N,N-1} = \text{PADE approximant}}} + R'_{2N} z^{2N} \\ &= \frac{b_0 + b_1 z + \dots + b_{N-1} z^{N-1}}{\prod_{i=1}^N (1 - zx_i)} + R'_{2N} z^{2N} = \underbrace{\sum_i \frac{p_i}{1 - zx_i}}_{p_i, x_i = \text{quad.table}} + R'_{2N} z^{2N} \end{aligned}$$

The second line is the Padé approximant that introduces an approximate description of higher moment order



Effective cross section and moment

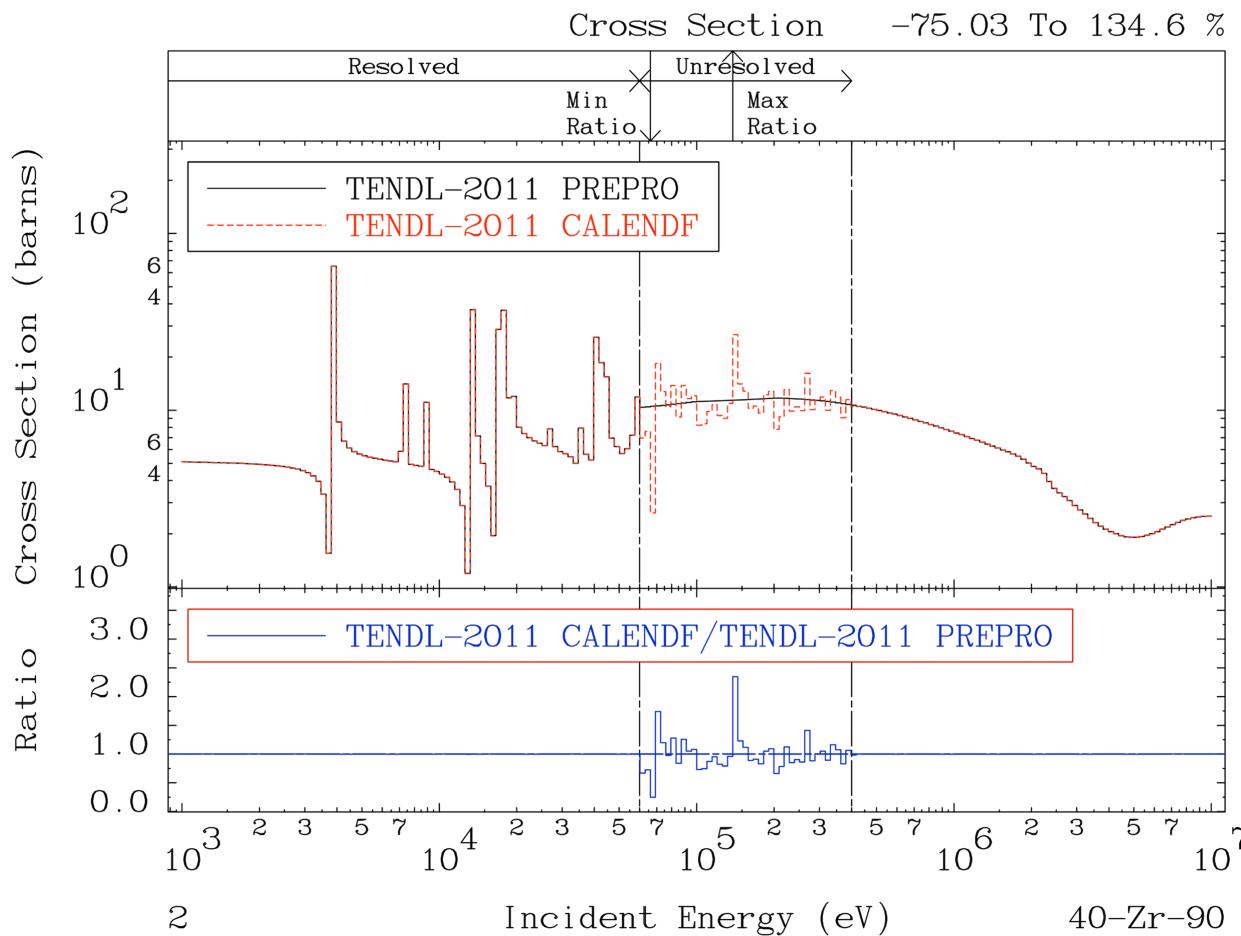
The effective cross section can be calculated from either the pointwise cross section or the probability table as follows:

$$\sigma_{x,eff,quad.}(\sigma_d) = \frac{\sum_{i=1}^{i=N} \frac{p_i \sigma_{x,i}}{\sigma_{t,i} + \sigma_d}}{\sum_{i=1}^{i=N} \frac{p_i}{\sigma_{t,i} + \sigma_d}}$$

When the dilution is infinite this formula becomes:

$$\sigma_{x,eff,quad.} = \sum_{i=1}^{i=N} p_i \sigma_{x,i}$$

Effective cross sections comparison



From 0.1 eV to the end of the URR

Uniquely accessible SSF's in the URR !!

Self Shielding Factor

The probability tables from CALENDF are used in conjunction with fine 709 or 1102 group data. They are given at 3 temperatures: 293.6, 600 and 900 Kelvin



The dilution $d(p; g)$ for a given nuclide p and energy group g is computed using a weighted sum over all the nuclides, $q = 1; Q$ in the mixture. The first approximation for the fraction f_q uses the total cross-sections :

$$d^{(0)}(p, g) = \sum_{\substack{q=1 \\ p \neq q}}^Q \frac{f_q \sigma^{LIB-tot}(q, g)}{f_p}$$

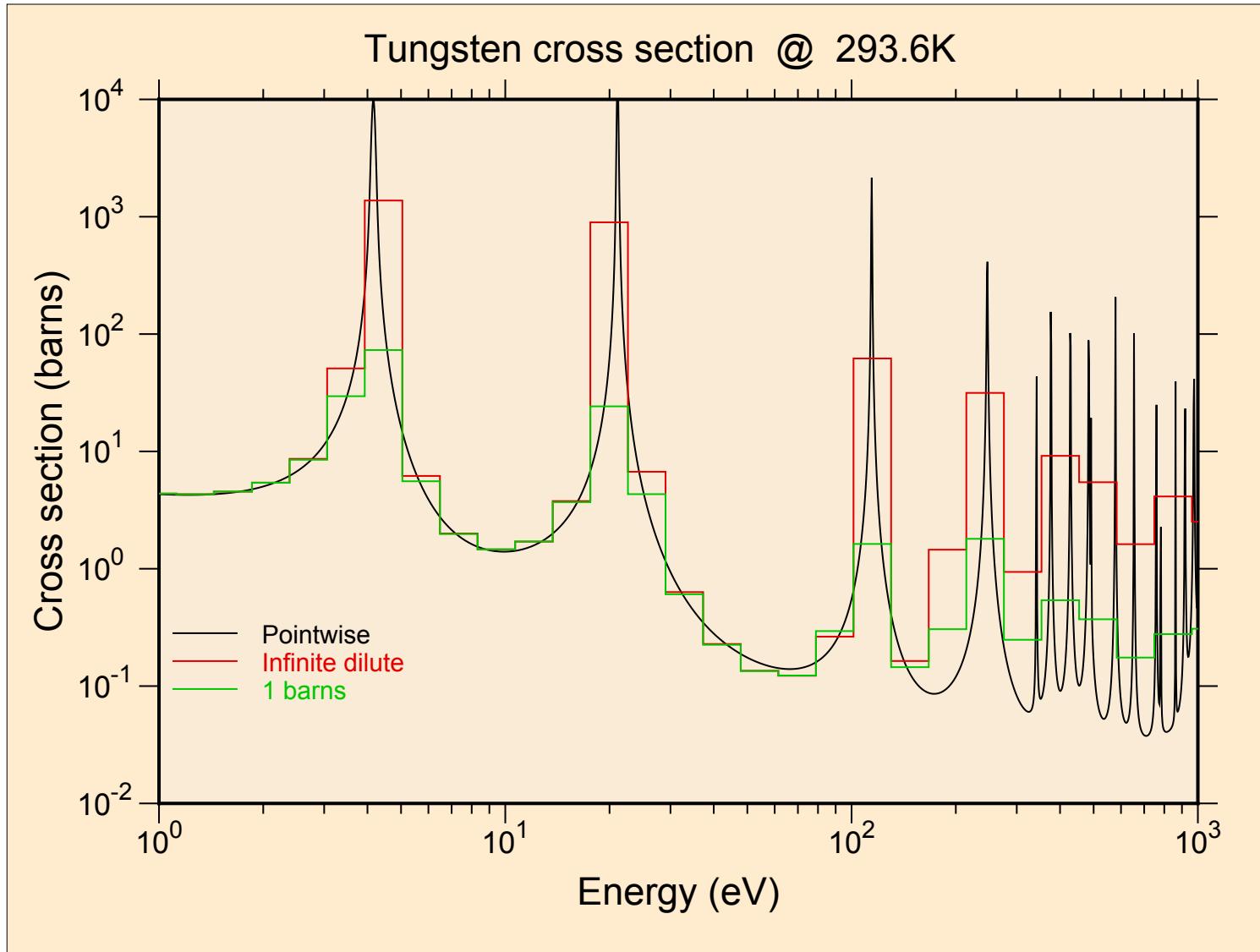
where

$$\sigma^{LIB-tot}(p, g) = \sum_{y=1}^Y \sigma^{LIB}(p, g, y)$$

Over the energy range for which the probability table data are available, the above approximation is iteratively refined using:

$$\begin{aligned} S^{(i)}(g) &= \sum_{q=1}^Q f_q \sigma^{LIB-tot}(q, g) \left(\frac{\sigma^{tot}(q, g, d^{(i)}(q, g))}{\sigma^{tot}(q, g, \infty)} \right) \\ d^{(i+1)}(p, g) &= \frac{S^{(i)}(g)}{f_p} - \sigma^{LIB-tot}(p, g) \left(\frac{\sigma^{tot}(p, g, d^{(i)}(p, g))}{\sigma^{tot}(p, g, \infty)} \right) \end{aligned}$$

Effective cross section: dilution effects





- **CALENDF-2010**

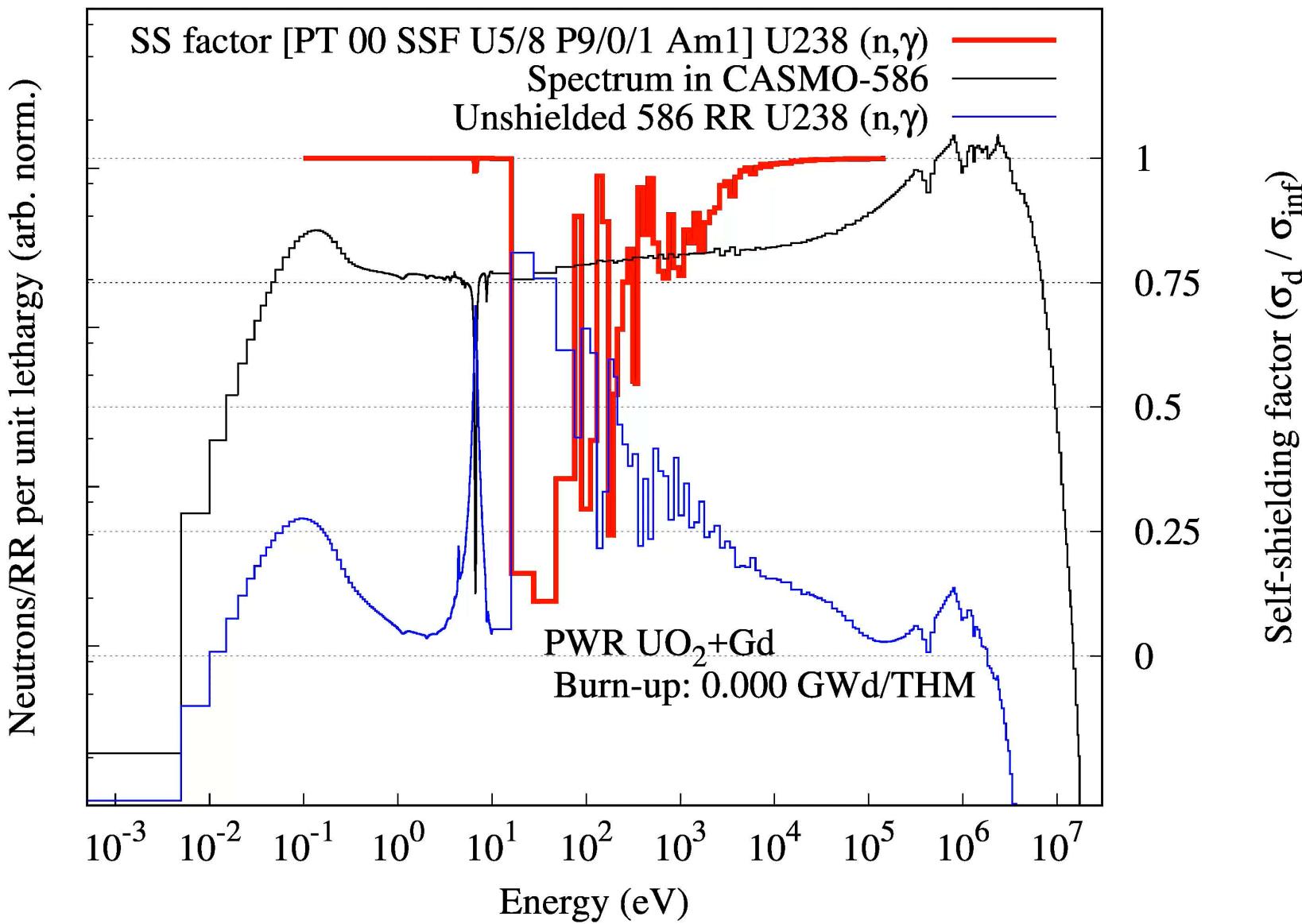
- 0 Kelvin run
- Single temperature pendf, statistical resonance in the URR
- Single temperature Probability Tables
- PT in the RR and URR from 0.1 eV to the end of the URR for each target isotopes
- Group structure 615 @ 10 eV, 900 @ 5 MeV

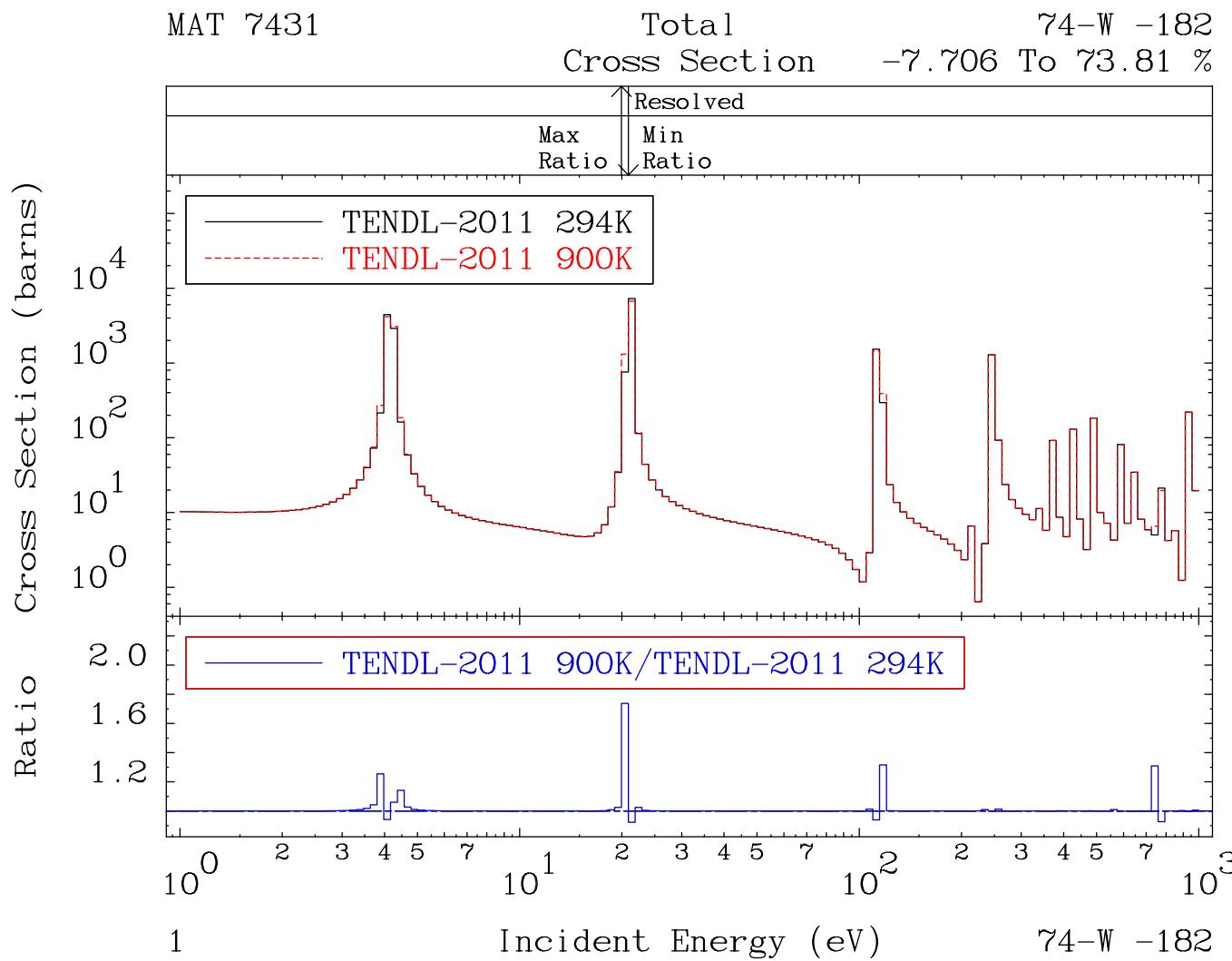
Those PT tables as they are stored can be used by either FISPACT-II and TRIPOLI-4.9. They allow self-shielding treatment in the URR to be accounted for (300 pcm on Bigten @ 20-150 KeV)



- Pointwise forms, Temperature dependent
- 1102 Groupwise, T and sigma zeroes dependent, PT's SSF
- Variance and covariance (on cross section)
- MF-2 resonance widths for shielding
- Matrices: n-n, n-g, n-prod and recoil
- All partials and total Kerma (7), dpa (4), gas production (5)

- For FISPACT-II & SPECTRA-PKA nuclear data forms, groupwise with probability tables, uncertainty, n-prod/recoil matrices, responses

LWR UO₂ + GD assembly



Giant resonances dominate the reaction rate

The effect is not negligible around the resonances



- Collaboration with PSI, using modern CASMO-SIMULATE to compare inventory predictions for variety of assemblies:
 - BWR and PWR with mix of UO₂, MOX, Gd
 - Includes Takahama, Atrium-10, TMI-1, Beznau

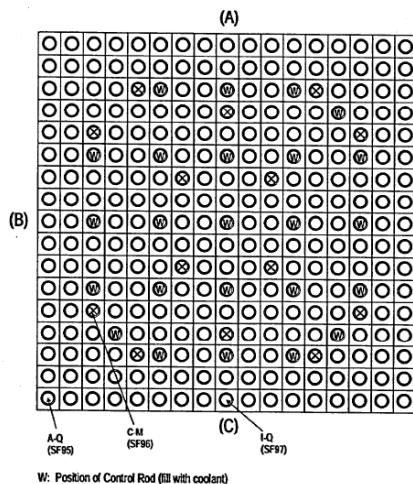


Figure 1 Positions of assay fuel rods in Takahama-3 assemblies NT3G23 and NT3G24

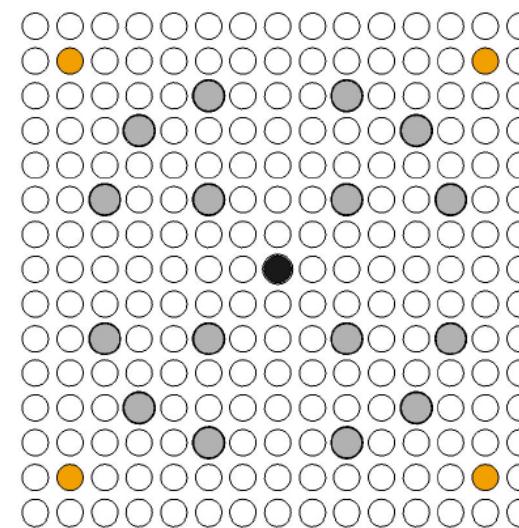
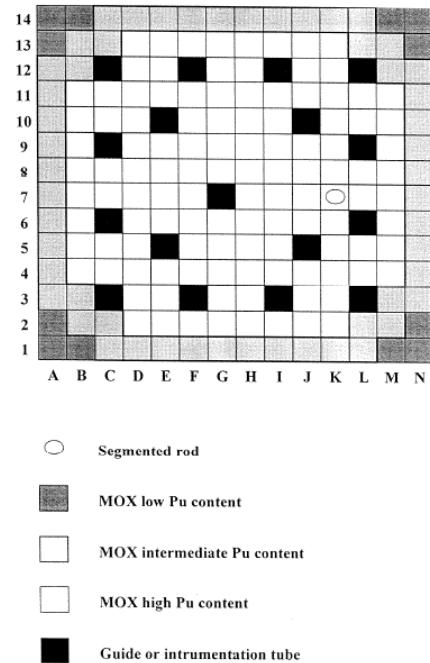
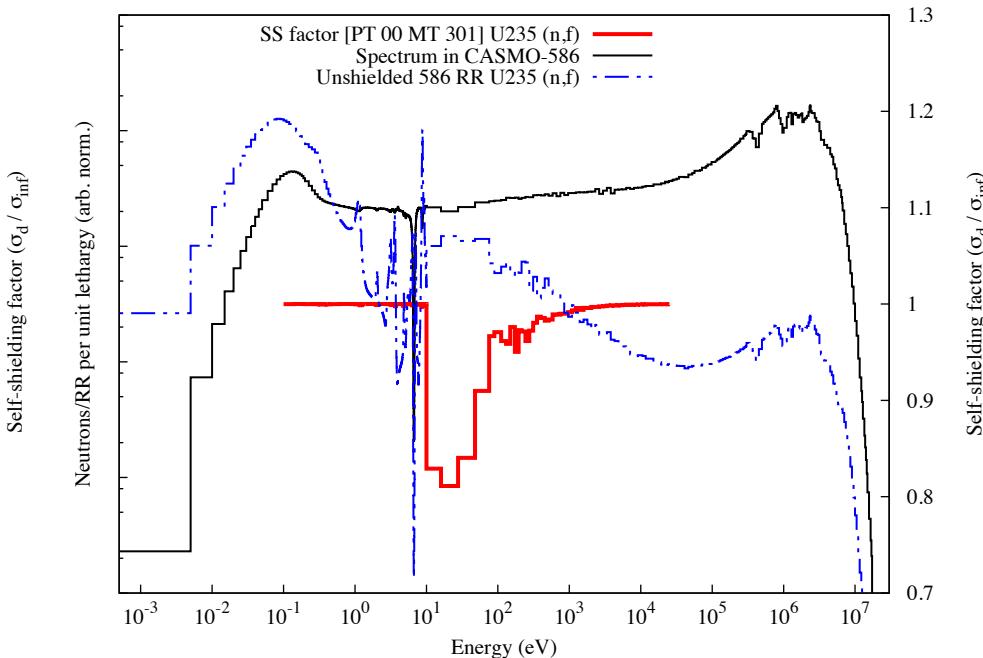
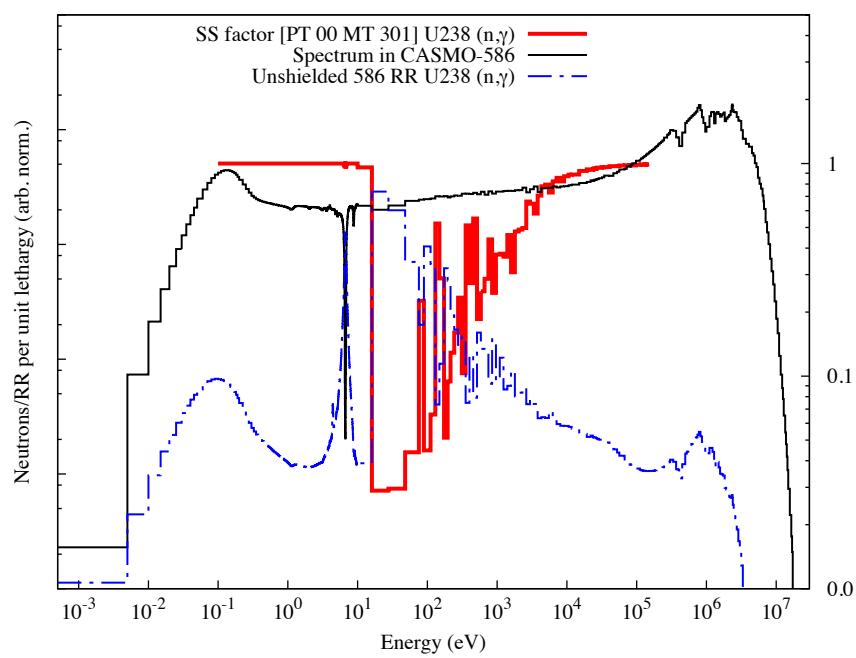


Figure 28: TMI-1 Fuel Assembly Layout

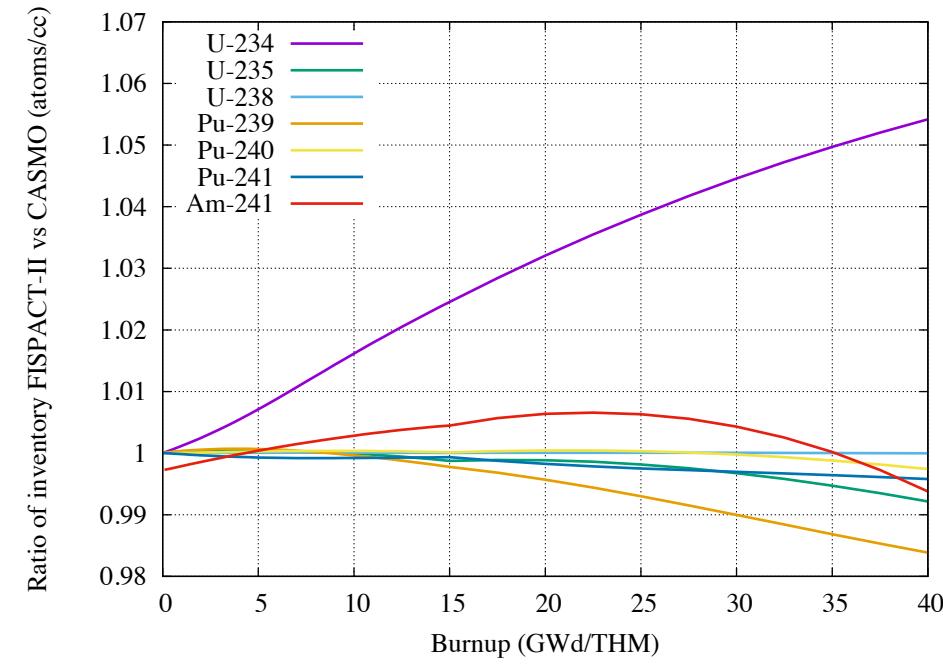
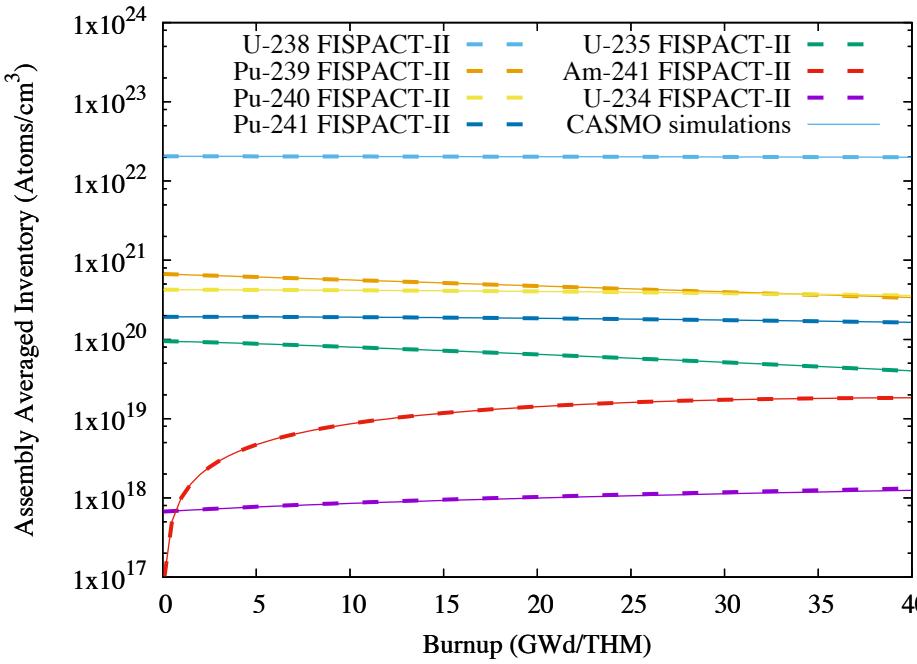


- Added 586 CASMO data for ENDF/B-VII.1, with CALENDf PTs for self-shielding. Applied to major actinides, but can in principle apply to any nuclide
- Left:** U8 capture RR and SSFs **Right:** U5 fission RR+SSFs

Note: CASMO 586 treatment of <10 eV requires no SSFs! No so for >10 eV, where significant SS occurs and must be accounted for.



- In all examples, normalisation using POWER keyword of FISPACT-II (normalising flux based on full Kerma) to CASMO power density, converted to W/cc.
- Ratios are to CASMO simulation, following the spectra changes over 40 GWd/te, **below:** BWR MOX simulation





- A proper characterization of the neutron spectra for irradiated samples is vital to get even close to real transmutation rate in simulations
 - Without this correct treatment of the neutron fields the reaction rates (and hence transmutation rates) for key capture reactions are much greater
 - The thermal part of the neutron spectrum is very important and must be correctly predicted
- Simulations in node with more realistic neutron spectra give daughter production rates that are in very good agreement with experimental measurements