Critical Mass Determination with the European Scheme (JEF2, ECCO and ERANOS)

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Introduction

The new cell code ECCO /1/ uses the subgroup method to treat the resonance self-shielding, this being particularly suitable for calculations involving complex heterogeneous structures. Libraries have been generated /2/ from JEF2 evaluations with the processing codes NJOY /3/ and CALENDF /4/ for use in ECCO and contain sub-group parameters to represent the resonance structure of the cross-sections.

An explicit P1 treatment of leakage with appropriate self-shielding treatment has been introduced in ECCO, therefore avoiding any transport approximation.

A simplified but accurate treatment of blankets is performed taking into account the neutron source from the core.

Effective cross sections and matrices are then used in SN P1 Transport calculations with the BISTRO code of ERANOS.

For the calculation of the sensitivities required for the cross section adjustment studies, perturbation theory calculations are performed within ERANOS using the diffusion theory option.

The whole scheme has been used for the analysis of MASURCA clean core critical masses.

Reference ECCO calculations

ECCO prepares self shielded cross sections and matrices with both the subgroup method within each fine group and the slowing down treatment in many groups (1968 groups)

The ECCO reference route treats the heterogeneous geometry in fine groups (1968) for the 37 most important nuclides. Less important nuclides are coming from the broad group libraries (172 or 33).

These calculations are very accurate as the fine group plus sub-group scheme has been set up to represent accurately the reaction thresholds and the resonances in any situation narrow or wide.

The elements ordered by importance of their contribution to the inelastic slowing down are U238, Fe, Na, Pu239 and Cr. The energies of their first important inelastic levels are the following ones:

U238	45KeV
Fe56	845KeV
Na	440KeV
Pu239	8KeV
Cr52	1.46MeV

The fine group scheme is representing accurately these thresholds.
On the other hand, the absorption resonances of heavy nuclides have the following characteristics:

	Pu239	U238
Capture width	40meV	23meV
Spacing	3.2 to 9.6 eV	23eV
Resolved resonances	0 to 1KeV	0 to 10Kev
Statistical resonances	1KeV to 30 KeV	10KeV to 300 KeV

Adopting a uniform lethargy grid, 80000 points in energy would be required to describe U238 in the full resonance energy range and only 32256 points between 7466eV and 4eV. 200000 points would be required to represent all the elements present in Fast Reactors.

The sub-group method enables the calculation of these resonances taking account the resonance structure of heavy nuclides by means of probability table parameters and by assuming the neutron source to be uniform in lethargy in a fine group.

The self shielding formula for a standard effective cross section σ_{x_i}, where x can be the total (Legendre order 0), capture, fission, elastic or inelastic for each group g, is the following:

$$\tilde{\sigma}^g_{xi} = \frac{\sum_j S^g_j \sum_k \alpha^g_k \, \sigma^g_{x_k} \, p_{ij}\left(\Sigma^g_{t_k}\right)}{\sum_j S^g_j \sum_k \alpha^g_k \, p_{ij}\left(\Sigma^g_{t_k}\right)}$$

where S^g_j is the source in the current group and in region j.

α^g_k is the probability in group g to find the partial cross section $\sigma^g_{x_k}$

to which corresponds the total cross section $\sigma^g_{t_x}$

(used to calculate the macroscopic cross section $\Sigma^g_{t_k}$ in each region).

$p_{ij}\left(\Sigma^g_{t_k}\right)$ is the reduced collision probability for this subgroup k within the group g.

The self shielding of the total Legendre order one cross section (as well as order one of the elastic cross section) has a different formulation coming from the fact that this type of cross section has a current weighting:

$$\tilde{\sigma}_{tr_i} = \frac{\sum_j S_j \sum_k \alpha_k \, \sigma_{tr_k} \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)}{\sum_j S_j \sum_k \alpha_k \sum_l p_{il}\left(\Sigma_{t_k}\right) p_{lj}\left(\Sigma_{t_k}\right)}$$

The flux and current are calculated with the self shielded cross sections and matrices in a P1 consistent approximation:

$$\phi^g_i = \sum_j \left(-B^g \, J^g_j + S^g_{fj} + \sum_{g'} \Sigma^{g' \to g}_{s_{o,j}} \, \phi^{g'}_j \right) p_{ji}\left(\Sigma^g_t\right)$$

$$J^g_i = \sum_j \left((B^g/3) \, \phi^g_j + \sum_{g'} \Sigma^{g' \to g}_{s_{1,j}} \, J^{g'}_j \right) p_{ji}\left(\Sigma^g_t\right)$$

Effective cross sections and matrices are condensed and smeared to provide effective cross sections and matrices in the user required group scheme.

One can distinguish wide and narrow resonances depending on their width compared to the energy loss through scattering. This mean energy loss is the smallest for scattering by heavy nuclides. Translated into lethargy gain the value for U238 is almost constant and equal to 0.008. This compares well with the fine group width 1/120 = 0.0083 and explains the fact that 3/4 of the neutrons having a collision escape from the group.

If the resonance is wide, it is treated explicitly with the cross sections themselves, the resonance in that case having a width larger than the group.

If the resonances are narrow, they are represented by the probability tables, and a use of the subgroup method can be applied in a very accurate way.

The method to calculate the resonance self-shielding has been checked by comparison with an independent code TRAMP /5/ which uses a group scheme, fine enough to represent the resonance structure without the need for sub-group data (group widths of 1/960 in lethargy in the lower energy range and 1/3840 in the higher resonance range). For a PWR cell ($U238\ O_2 + H_2O$) with one fuel zone, the U238 capture rate for a range in energy from 6.16 eV to 7466 eV is calculated by ECCO only 0.33% higher than the result of TRAMP.

Finally, the fact that the balance is preserved in ECCO through condensation and smearing is providing a final internal validation of ECCO algorithms, and enables us to track back the origin of discrepancies in evaluations. Note that the same calculational scheme could be used for thermal reactor problems and for shielding applications.

BISTRO SN Calculations

Different methods are available in ERANOS for reactor calculations, one of these being the BISTRO SN code. This code is a finite difference code with a highly efficient convergence algorithm.

The SN BISTRO calculation is performed in P1 and as all SN transport codes requires only one total cross section.

The calculation has been performed using the Legendre order one total cross section $\Sigma_{t_1}^g$ that is, the current averaged value, for each region of the spatial description of the reactor, each of them being treated by independent fundamental mode ECCO calculations.
The within group scattering term is corrected for the use of this single total cross section in this way:

$$\Sigma_0^{*g\to g} = \Sigma_0^{g\to g} - \Sigma_{t_0}^g + \Sigma_{t_1}^g$$

where $\Sigma_0^{g\to g}$ and $\Sigma_{t_0}^g$ are the flux averaged values.

The standard type of calculations have often been performed using the transport corrected P0 method. A comparison with the SN transport P1 inconsistent method has been done. In that case, the within group term has been corrected for the use of the transport cross section in this way:

$$\Sigma_0^{*g\to g} = \Sigma_0^{g\to g} - \Sigma_{t_0}^g + \Sigma_{tr}^g$$

A correction for the mesh effect has been performed using the following procedure based on the assumption that the mesh error is proportional to the square of the mesh width:

$$\varepsilon_n = a_x h_{xn}^2 + a_y h_{yn}^2 + a_z h_{zn}^2$$

- a first calculation is performed with a standard mesh of around 1.5cm, it gives a
  $K_{effective} = K_n$
- a second calculation is performed with a half mesh size, it gives a
  $K_{effective} = K_{2\,n}$

The extrapolated value is then obtained with this formulation:

$$K_\infty = \frac{4 * K_{2n} - K_n}{3}$$

The same type of formulation has been used for the extrapolation to S_∞ for the angular distribution discretization.

Results

The critical masses being analysed with this procedure are the MASURCA clean cores. These cores have been chosen to qualify the fast reactor scheme and the nuclear data associated with it by minimising the errors which might be introduced in the modelling of the core. Here, the cores are described in RZ geometries, corrections for cylindrisation but also corrections for end caps and coolant channels having been introduced in the experimental value at the time of the realisation of the experiment.

The mesh correction has been calculated for the R2 core with 60cm high (R260: table 1). It has been found so small that it has been neglected for the other cores, the other having a larger size even less sensitive to the mesh effect.

The extrpolation to S_∞ for the angular distribution discretization has been done in the same way. S8 gives very good answers which need very little correction.

The results of the comparison between calculations with P1 moments and calculations with a transport cross section without P1 moments are presented in table 3 for the various cores. The higher the enrichment, the larger the magnitude of the correction. The P1 consistent option is not a negligeable effect (402 pcm for ZOCO1) and cannot be neglected. In figure 1, the P1 correction is presented as a function of $K^* - 1$, the leakage fraction for the core. This effect is negative in fast reactor cores and is representative of classical types of approximation used for defining the transport cross-section.

Finally, the (E-C)/C values for the MASURCA clean cores have been listed after all mentioned corrections (table 4). Although, they are not satisfactory, one can assume that no bias effect has been introduced in the calculation. In figure 2, values are presented as a function of $K^* - 1$, the leakage fraction for the core. Uranium enriched cores have negative (E-C)/C values, plutonium cores have positive (E-C)/C values except ZONA2(PECORE). This core is particular in the way that it has a radial reflector.

Conclusion

The recent developments of the sub-group method for the European Cell Code ECCO offer the possibility to calculate the resonance self-shielding in complex geometries and temperature distributions with excellent accuracy. Together with the BISTRO SN code, it provides an accurate route for the analysis of critical cores. With this route, the critical mass determination of MASURCA clean cores has been done and enables the possibility of doing accurate cross section adjustment studies.

References

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Table 1 Mesh correction for the R260 critical mass

S8 P1 Inconsistent	K*	K*-1	B^2	Fine Mesh *	Standard Mesh	Mesh correction
R260	1.66834	0.66834	2.30E-03	1.00964E+00	1.00960E+00	4

* Fine Mesh = Standard Mesh / 2 in each direction

Table 2 SN correction for the critical masses

	K*	K*-1	B^2	S4	S8	S ∞	Correction SN
R260	1.66834	0.66834	2.30E-03	1.01E+00	1.00765E+00	1.00749E+00	64
R1	1.50814	0.50814	1.64E-03	1.01E+00	1.00717E+00	1.00704E+00	53
R290	1.66808	0.66808	2.30E-03	1.01E+00	1.00714E+00	1.00686E+00	113
R3	1.27669	0.27669	8.23E-04	1.01E+00	1.00502E+00	1.00492E+00	41
ZOCO1	1.81421	0.81421	4.66E-03	1.00E+00	9.99960E-01	9.99573E-01	155
ZONA2	1.87040	0.87040	2.27E-03	1.01E+00	1.01130E+00	1.01109E+00	83
ZONA3	1.28434	0.28434	7.14E-04	1.00E+00	1.00073E+00	1.00063E+00	41
Z2	1.85434	0.85434	2.53E-03	1.00E+00	9.99430E-01	9.99230E-01	80
Z3	1.23703	0.23703	7.09E-04	1.00E+00	1.00061E+00	1.00051E+00	39
MAS1AP	1.64820	0.64820	3.93E-03	9.97E-01	9.96700E-01	9.96450E-01	100
MAS1B	1.61148	0.61148	4.11E-03	1.00E+00	1.00411E+00	1.00387E+00	96
R212NA	1.68902	0.68902	2.05E-03	1.01E+00	1.00786E+00	1.00770E+00	63

Table 3 P1 correction for the critical masses

	K*	K*-1	B^2	P1 consistent	P1 inconsistent	Correction P1
R260	1.66834	0.66834	2.30E-03	1.00749E+00	1.00943E+00	-194
R1	1.50814	0.50814	1.64E-03	1.00704E+00	1.00842E+00	-138
R290	1.66808	0.66808	2.30E-03	1.00686E+00	1.00885E+00	-199
R3	1.27669	0.27669	8.23E-04	1.00492E+00	1.00625E+00	-133
ZOCO1	1.81421	0.81421	4.66E-03	9.99573E-01	1.00359E+00	-402
ZONA2	1.87040	0.87040	2.27E-03	1.01109E+00	1.01416E+00	-306
ZONA3	1.28434	0.28434	7.14E-04	1.00063E+00	1.00208E+00	-145
Z2	1.85434	0.85434	2.53E-03	9.99230E-01	1.00174E+00	-251
Z3	1.23703	0.23703	7.09E-04	1.00051E+00	1.00192E+00	-141
MAS1AP	1.64820	0.64820	3.93E-03	9.96450E-01	9.99270E-01	-282
MAS1B	1.61148	0.61148	4.11E-03	1.00387E+00	1.00620E+00	-233
R212NA	1.68902	0.68902	2.05E-03	1.00770E+00	1.00968E+00	-197

Table 4 (E-C)/C with the European Code System JEF2/ECCO/ERANOS

	Fuel/Coolant	Enrichment	K*	K*-1	B^2	P1 consistent	Exp. value	(E-C)/C
R260	U metal/Na	30%	1.66834	0.66834	2.30E-03	1.00749E+00	1.00272E+00	-473
R1	U metal/Na	23%	1.50814	0.50814	1.64E-03	1.00704E+00	1.00093E+00	-606
R290	U metal/Na	30%	1.66808	0.66808	2.30E-03	1.00686E+00	1.00174E+00	-508
R3	U metal/Na	16%	1.27669	0.27669	8.23E-04	1.00492E+00	1.00099E+00	-391
ZOCO1	PuO2	18%	1.81421	0.81421	4.66E-03	9.99573E-01	1.00824E+00	867
ZONA2	PuO2/Na	25%	1.87040	0.87040	2.27E-03	1.01109E+00	1.00263E+00	-837
ZONA3	PuO2/Na	13%	1.28434	0.28434	7.14E-04	1.00063E+00	1.00113E+00	50
Z2	Pu metal/Na	25%	1.85434	0.85434	2.53E-03	9.99230E-01	1.00265E+00	342
Z3	Pu metal/Na	13%	1.23703	0.23703	7.09E-04	1.00051E+00	1.00335E+00	284
MAS1AP	Pu metal/C	25%	1.64820	0.64820	3.93E-03	9.96450E-01	1.00135E+00	492
MAS1B	U metal/C	30%	1.61148	0.61148	4.11E-03	1.00387E+00	1.00236E+00	-150
R212NA	U metal/Na+Void	30%	1.68902	0.68902	2.05E-03	1.00770E+00	1.00277E+00	-490

figure 1 P1 Consistent - P1 Inconsistent

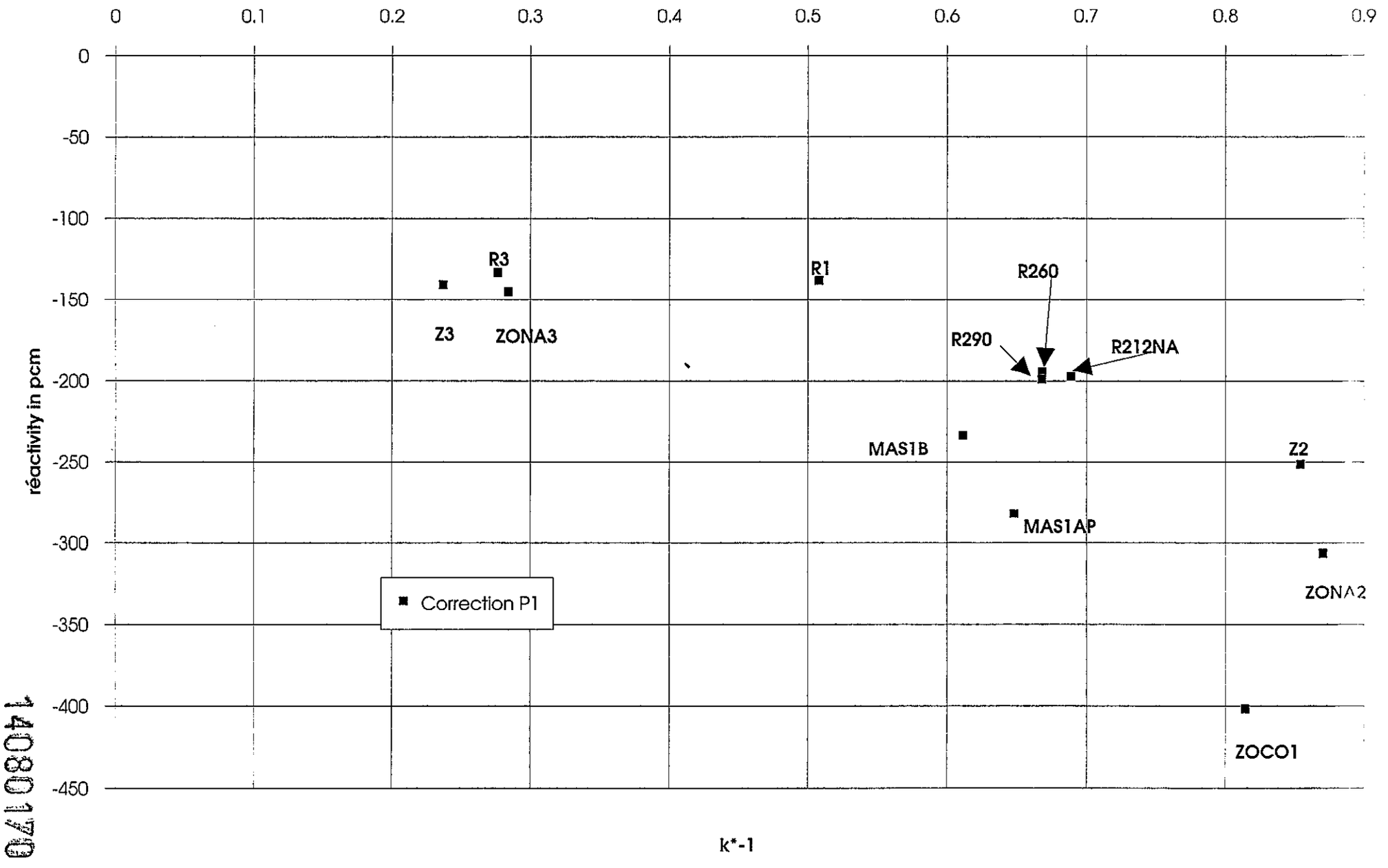

figure 2 Experiment JEF2 Calculation Discrepancies for Critical Masses