Normalization in KCODE calculation

Dear MCNP list members,

We have encountered an interesting problem working with MCNP which we would like to share with you. It seems that the method of normalization suggested in the MCNP manual may not yield correct results in KCODE cases. We believe, though we might be wrong, that the correct way of normalization includes a division by keff as well. Since in most cases keff is rather close to 1, the issue only becomes apparent in particular cases with very low or high multiplication factors. As this problem may have serious consequences under certain conditions (eg. when calculating infinite lattices with reflective/periodic boundaries when keff may be quite different from 1), we would like to ask for your kind help resolving the "mistery".

In order to demonstrate the problem, we made a simple calculation in KCODE for an infinite „U-reactor" with various enrichments (an input is provided for an enrichment of 25% (^{235}U) in the Appendix). The results can be seen in the following tables.

Column number	Column 1	Column 2	Column 3	Column 4
Enrichment [n%]	Flux[1]	$\nu\sigma_f\Phi$[2]	$\sigma_f\Phi$[3]	ν[4]
100	1.86E+00	5.96E+00	2.33E+00	2.56E+00
50	3.14E+00	5.49E+00	2.16E+00	2.54E+00
25	4.95E+00	4.73E+00	1.87E+00	2.53E+00
10	7.76E+00	3.46E+00	1.36E+00	2.54E+00

Column 5	Column 6	Column 7	Column 8	Column 9	Column 10
Enrichment [n%]	k_{eff}	F6:N,P	P [MeV/fission neutron]	ν*P [MeV/fission][5]	ν*P/k_{eff} [MeV/fission]
100	2.27905	1.06E+00	157.63	404.32	177.41
50	2.07819	9.83E-01	146.30	371.99	179.00
25	1.78939	8.55E-01	127.16	322.19	180.06
10	1.3063	6.35E-01	94.50	240.10	183.80

[1] Calculated with F4 tally
[2] Calculated with F4 tally with multipliers -7 and -6
[3] Calculated with F4 tally with multiplier -6
[4] Calculated from the previous two columns
[5] Calculated from the previous column and the mass of the cube

Column 1, 2, 3, 6, 7 were extracted from the MCNP outputs. Effective nubar values displayed in *Column 4* were calculated by dividing *Column 2* by *Column 3*. *Column 7* shows the energy deposition values produced by F6 tallies. *Column 8* was obtained from *Column 7* by multiplying it with the mass of the cell. According to the MCNP documentation [1, page 2-175] ("... An MCNP tally in a criticality calculation is for one fission neutron being born in the system at the start of a cycle. The tally results must be scaled either by the total number of neutrons in a burst or by the neutron birth rate to produce, respectively, either the total result or the result per unit time of the source. ...") these values are normalized for one fission neutron. In order to show energy released from one fission event (displayed in *Column 9*), *Column 8* was multiplied by the corresponding nubar values. The numbers obtained are well above the widely accepted values, and they vary significantly with k_{eff}. However, values in

Column 10, which were obtained by dividing *Column 9* by keff, are in the range of expectations.
MCNP solves the static eigenvalue equation of neutrons:

$$\frac{1}{k_{eff}}\hat{P}\varphi=\hat{D}\varphi \qquad (1)$$

where P and D are the production and destruction operators, respectively. The documentation, as cited earlier, explains that tally values are provided for one fission neutron, i.e.

$$\int \hat{P}\varphi dx=1 \qquad (2)$$

where x stands for $E,\vec{r},\vec{\Omega}$ and integration is extended for the whole domain of the variables.
According to [1, page 2-79 and page 2-175] tally values are normalized as follows:

$$\mathrm{F4}=\frac{1}{w}\sum_{i,V}\frac{W_i T_i}{V} \qquad (3)$$

where the sum is for every track in the cell for all active cycles, using the notations of the MCNP documentation. The normalization factor is [1, page 2-175]:

$$w=N\left(I_t-I_c\right) \qquad (4)$$

Using $W_{s,k}=\frac{N}{M_k}$, where k indexes the active cycles during the calculation and M_k is the number of source neutrons induced in the cycle [1, page 2-161 and 2-175], we can obtain from (4):

$$w=N\left(I_t-I_c\right)=\sum_k M_k W_{s,k} \qquad (5)$$

where $W_{s,k}$ is the source particle weight in the kth active cycle.
Thus, with the equation given on top of page 2-161 we obtain:

$$w=\sum_k M_k W_{s,k}=\sum_k\left(\sum_j n_j\right)W_{s,k}=\sum_k\left(\sum_j\left\lfloor\frac{1}{k_{eff}^{c,est}}W_j\bar{\nu}\frac{\sigma_f}{\sigma_t}+\text{random number}\right\rfloor\right)W_{s,k}\,, \qquad (6)$$

where $k_{eff}^{c,est}$ is the collision estimator of k_{eff} from the previous cycle.
The $\frac{1}{k_{eff}^{c,est}}$ included in Eq. 6 suggests that tallies are normalized for $\int\frac{1}{k_{eff}}\hat{P}\varphi dx=1$ and not for Eq. 2. This coincides with our calculational results in *Column 10*.

What is your opinion regarding our problem?

Best regards,

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References ☺

[1] J. F. Briesmeister, MCNPTM-A General Monte Carlo N-Particle Transport Code, Version 4C, April 10, 2000.

Appendix. Input for the calculations

```
Infinite 235U reactor for normalization testing
c
c Cells
c
c Rest of the World
1    0           1:-2:3:-4:5:-6              imp:n,p=0
c U cube
2    1   -18.6   -1 2 -3 4 -5 6              imp:n,p=1

c
c Surfaces
c
1  -2  px       1.0
2  -1  px      -1.0
3  -4  py       1.0
4  -3  py      -1.0
*5     pz       1.0
*6     pz      -1.0

c
c Data cards
c
mode n p
kcode 1000 1.0 25 100
ksrc 0 0 0
m1
       92235.60c      0.24999
       92238.60c      0.75001
f6:n,p 2
fc6:n,p Prompt heat deposition
c
c Tally with  nu_sigma_f multiplier
c
f14:n 2
fm14:n 1.0 1 -7 -6
fc14:n Multiplier nu_sigma_f
c
c Tally with  sigma_f multiplier
c
f24:n 2
fm24:n 1.0 1 -6
fc24:n Multiplier sigma_f
c
c Tally for flux
f34:n 2
fc34:n Flux
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