Critical analysis of the effective delayedneutron fraction calculation routes by deterministic and Monte Carlo codes.

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OECD/NEA 11th Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation (11IEMPT)

1-5 November 2010 San Francisco

Introduction

- ✓ Theoretical analysis
- **\checkmark** Standard and Monte Carlo β_{eff} formulations
- ERANOS formalism and calculation set up
- ERANOS results
- Conclusions

Introduction

- The increasing use of Monte Carlo codes in the field of nuclear reactors calculation and the studies on ADS have renewed the interest in the theoretical and computational evaluation of the main integral parameters characterizing subcritical systems.
- Some particular parameters, as the effective delayed neutron fraction, are evaluated in Monte Carlo codes by formulations which do not require the calculation of the adjoint flux.
- The assessment of the various formulations of the effective delayed neutron fraction is crucial for the system evaluation, since it plays an important role in determining its dynamic characteristics.
- This work is focused on a theoretical and computational analysis about how the different β_{eff} definitions are connected.

Introduction

- Theoretical results show how the Monte Carlo formulation of β_{eff} may be connected to the classical definition, interpreting the classical one through a reactivity evaluation based on an "improved" first order approach of perturbation theory.
- The computational analysis is carried out in a coherent and consistent way, using the same deterministic code (ERANOS) and neutron data library (JEFF 3.1) for the β_{eff} evaluation.
- The GUINEVERE system is selected as a relevant test case for ADS technology. The GUINEVERE experience, mainly devoted to the issues concerning on-line reactivity monitoring in ADS, will be performed by using a modified lay-out of the VENUS critical facility located at the Belgium SCK•CEN Molsite, coupling the subcritical core facility to a deuteron accelerator delivering, by a continuous or pulsed beam, 14 MeV neutrons by deuterium-tritium reactions.

Let us take as *reference* system the following eigenvalue problem:

$L\phi = \omega F\phi$

With **L** loss operator, **F** fission operator and $\omega = 1/k$.

If a perturbation $\delta \mathbf{F}$ is introduced:

$$\mathbf{L}\boldsymbol{\varphi}^* = [\boldsymbol{\omega} + \boldsymbol{\delta}\boldsymbol{\omega}][\mathbf{F} + \boldsymbol{\delta}\mathbf{F}]\boldsymbol{\varphi}^*$$

Following the exact approach of Perturbation Theory (PT), i.e. considering the adjoint problem corresponding to the *reference* system:

$$\mathbf{L}^{+}\boldsymbol{\varphi}^{+} = \boldsymbol{\omega}\mathbf{F}^{+}\boldsymbol{\varphi}^{+}$$

we obtain:

$$\frac{\delta\omega}{\omega + \delta\omega} = 1 - \frac{k^*}{k} = -\frac{\langle \phi^+ \delta \mathbf{F} \phi^* \rangle}{\langle \phi^+ \mathbf{F} \phi^* \rangle}$$

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If we follow the first order PT approach, while retaining the second order term $\delta\omega\delta F\phi$, we obtain the "improved" first order formulation:

$$\frac{\delta\omega}{\omega + \delta\omega} = 1 - \frac{k^*}{k} \cong -\frac{\langle \phi^+ \delta \mathbf{F} \phi \rangle}{\langle \phi^+ \mathbf{F} \phi \rangle}$$

If the perturbation is $\delta F = -F_d$, with F_d as delayed neutrons fission operator, the perturbed system can be written as:

$$\mathbf{L}\boldsymbol{\varphi}_{\mathrm{p}} = \boldsymbol{\omega}_{\mathrm{p}} \left[\mathbf{F} - \mathbf{F}_{\mathrm{d}} \right] \boldsymbol{\varphi}_{\mathrm{p}}$$

with the perturbed flux given by the prompt flux ϕ_p and $\omega_p{=}1/k_p.$

We have:

$$1 - \frac{k_p}{k} = \frac{\langle \varphi^+ \mathbf{F}_{\mathbf{d}} \varphi_p \rangle}{\langle \varphi^+ \mathbf{F} \varphi_p \rangle} \cong \frac{\langle \varphi^+ \mathbf{F}_{\mathbf{d}} \varphi \rangle}{\langle \varphi^+ \mathbf{F} \varphi \rangle} = \beta_{eff}$$

PT "improved" first order formulation

The effective delayed neutron fraction β_{eff} is an "*improved*" PT first order formulation of the formula 1-(k_p/k), widely used in Monte Carlo codes as β_{eff} estimator.

Standard and Monte Carlo β_{eff} formulations

Effectiveness of delayed neutrons:



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Current Monte Carlo (MC) calculations approximate β_{eff} by:



unperturbed

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We have:

(1)
$$\beta_{eff}^{MC} = 1 - \frac{k_p}{k} = \sum_{m} \sum_{i} \overline{\nu}_{d,i}^{(m)} \frac{\langle \langle \phi^+(\mathbf{r}, E) \chi_{d,i}^{(m)}(E) \rangle \Sigma_{f}^{(m)}(\mathbf{r}, E') \phi_p(\mathbf{r}, E') \rangle_{E'} \rangle_{E} \rangle_{F}}{\sum_{m} \langle \langle \phi^+(\mathbf{r}, E) \chi^{(m)}(E) \rangle \nabla_{f}^{(m)}(E') \Sigma_{f}^{(m)}(\mathbf{r}, E') \phi_p(\mathbf{r}, E') \rangle_{E'} \rangle_{E} \rangle_{F}}$$

(2) $\beta_{eff} = \sum_{m} \sum_{i} \overline{\nu}_{d,i}^{(m)} \frac{\langle \langle \phi^+(\mathbf{r}, E) \chi_{d,i}^{(m)}(E) \rangle \Sigma_{f}^{(m)}(\mathbf{r}, E') \phi(\mathbf{r}, E') \rangle_{E'} \rangle_{E} \rangle_{F}}{\sum_{m} \langle \langle \phi^+(\mathbf{r}, E) \chi_{d,i}^{(m)}(E) \rangle \nabla_{f}^{(m)}(\mathbf{r}, E') \phi(\mathbf{r}, E') \rangle_{E'} \rangle_{E'} \rangle_{E} \rangle_{F}}$

The classical β_{eff} definition given in (2) is an "improved" PT first order approximation of the relationship 1-(k_p/k) given in (1). The coherent prompt flux ϕ_p to be used in the β_{eff} definition given in (1) is the eigenfunction of:

$$\begin{split} \mathbf{\Omega} \cdot \nabla \phi_{p}(\mathbf{r}, E) + \Sigma_{t}(\mathbf{r}, E) \phi_{p}(\mathbf{r}, E) &= \\ \frac{1}{k_{p}} \sum_{m} \left[\chi^{(m)}(E) < \nu^{(m)}(E') \Sigma_{f}^{(m)}(\mathbf{r}, E') \phi_{p}(\mathbf{r}, E') >_{E'} - \sum_{i} \chi^{(m)}_{d,i}(E) \overline{\nu}_{d,i}^{(m)} < \Sigma_{f}^{(m)}(\mathbf{r}, E') \phi_{p}(\mathbf{r}, E') >_{E'} \right] \\ + < \Sigma_{s}(\mathbf{r}, E' \rightarrow E) \phi_{p}(\mathbf{r}, E') >_{E'} . \end{split}$$

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The other way round. If we calculate k_p and ϕ_p by:



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The following β_{eff} formulation is adopted in ERANOS:



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$$\beta_{eff} = \sum_{m} \sum_{i} \overline{\nu}_{d,i}^{(m)} \xrightarrow{\left\{ \sum_{g} \phi_{g}^{+}(\mathbf{r}) \right\}} \overline{\chi}_{d,i,g} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) >_{\mathbf{r}}} \frac{\left\{ \sum_{g} \phi_{g}^{+}(\mathbf{r}) \right\}}{\left\{ \sum_{g} \phi_{g}^{+}(\mathbf{r}) \right\}} \overline{\chi}_{g} \sum_{m} \sum_{g'} \nu_{g'}^{(m)} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) >_{\mathbf{r}}} \frac{\left\{ mproved' \text{ PT first order formulation} \right\}}{\left\{ p_{eff}^{MC} = 1 - k \right\}} \sum_{i} \overline{\nu}_{i}^{(m)} \frac{\left\{ \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{g} \sum_{m} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \right\}}{\left\{ \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{g} \sum_{m} \sum_{g'} \nu_{g'}^{(m)} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \right\}}.$$

$$\Omega \cdot \nabla \phi_{p,g}(\mathbf{r}) + \Sigma_{i,g}(\mathbf{r}) \phi_{p,g}(\mathbf{r}) = \frac{1}{k_{p}} \sum_{g'} \sum_{g'} \overline{\chi}_{g} \nu_{g'}^{(m)} - \sum_{i} \overline{\chi}_{d,i,g} \overline{\nu}_{d,i}^{(m)}} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) + \sum_{g'} \Sigma_{s,g' \rightarrow g}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \sum_{g'} \overline{\gamma}_{g'} \nabla_{g'}^{(m)} - \sum_{i} \overline{\chi}_{d,i,g} \overline{\nu}_{d,i}^{(m)}} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) + \sum_{g'} \sum_{s,g' \rightarrow g} (\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \sum_{g'} \overline{\gamma}_{g'} \nabla_{g'}^{(m)} \sum_{g'} \overline{\gamma}_{g'} \nabla_{g'}^{(m)} \sum_{g'} \overline{\gamma}_{g'}^{(m)} \nabla_{g'}^{(m)} \sum_{g'} \sum_{g'} \overline{\gamma}_{g'}^{(m)} \sum_{g'} \sum_{$$

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$$\overline{\overline{\chi}_{p,g}} = \frac{\sum_{m} \left[\overline{\chi}_{g} \overline{v}^{(m)} - \sum_{i} \overline{\chi}_{d,i,g} \overline{v}^{(m)}_{d,i} \right] \sum_{g'} \Sigma^{(m)}_{f,g'} \psi_{g'}}{\sum_{m} \left[\overline{v}^{(m)} - \sum_{i} \overline{v}^{(m)}_{d,i} \right] \sum_{g'} \Sigma^{(m)}_{f,g'} \psi_{g'}},$$

$$\overline{2 \cdot \nabla \phi_{p,g}(\mathbf{r}) + \Sigma_{t,g}(\mathbf{r}) \phi_{p,g}(\mathbf{r})} = \frac{1}{k_{p}} \overline{\chi}_{p,g} \sum_{m} \left[\overline{v}^{(m)} - \sum_{i} \overline{v}^{(m)}_{d,i} \right] \sum_{g'} \Sigma^{(m)}_{f,g'} (\mathbf{r}) \phi_{p,g'}(\mathbf{r})$$

$$-\sum_{g'} \Sigma_{s,g' \rightarrow g}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}).$$

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2)

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The corresponding β_{eff} formulation is:

$$\beta_{eff} = \sum_{m} \sum_{i} \overline{\nu}_{d,i}^{(m)} \frac{<\sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{d,i,g} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) >_{\mathbf{r}}}{<\sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{g} \sum_{m} \overline{\nu}^{(m)} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) >_{\mathbf{r}}}$$



$$\beta_{eff}^{MC} = \boxed{1 - \frac{k_p}{k}} = \sum_{m} \sum_{i} \overline{\nu}_{d,i}^{(m)} \frac{\langle \sum_{g} \phi_g^+(\mathbf{r}) \overline{\chi}_{d,i,g} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \rangle_{\mathbf{r}}}{\langle \sum_{g} \phi_g^+(\mathbf{r}) \overline{\chi}_g \sum_{m} \overline{\nu}_{m'}^{(m)} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{p,g'}(\mathbf{r}) \rangle_{\mathbf{r}}}$$

Now all the equations sides can be calculated by ERANOS

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ERANOS results

Simplified RZ model of the GUINEVERE start-up (at critical) configuration. Dimensions, not in scale, are given in cm.



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ERANOS transport calculations

Neutron data library JEFF 3.1 - 49 energy groups - P_0 transport approximation - Angular quadrature S_4

	Family	1	2	3	4	5	6	7	8	Sum
U ₂₃₅	Abundance *	0.0340 ⁽¹⁾	0.1501 ⁽¹⁾	0.0992 ⁽¹⁾	0.2001 ⁽¹⁾	0.3122 ⁽¹⁾	0.0932 ⁽¹⁾	0.0872 ⁽¹⁾	0.0240 ⁽¹⁾	1
	β **	0.00022	0.00099	0.00065	0.00132	0.00205	0.00061	0.00057	0.00016	0.00657
	v _d	0.00055	0.00245	0.00162	0.00326	0.00509	0.00152	0.00142	0.00039	0.01630 ⁽²⁾
U ₂₃₈	Abundance	0.0084 ⁽³⁾	0.1040 ⁽³⁾	0.0375 ⁽³⁾	0.1370 ⁽³⁾	0.2940 ⁽³⁾	0.1980 ⁽³⁾	0.1280 ⁽³⁾	0.0931 ⁽³⁾	1
	β **	0.00014	0.00175	0.00063	0.00231	0.00496	0.00334	0.00216	0.00157	0.01687
	v _d	0.00039	0.00484	0.00174	0.00637	0.01367	0.00921	0.00595	0.00433	0.04650 ⁽⁴⁾

Delayed neutron data

* Yellow background indicates data from literature. No background indicates derived data.

** $\beta = \overline{v}_d / \overline{v}$ values are obtained from mean v values for U_{235} and U_{238} in the GUINEVERE core region.

⁽¹⁾ Note CEA DEN/CAD/DER/SPRC/LEPH 06-204. Data are adapted (to have 1 as summation) from Progress in Nuclear Energy, Vol 41, Number 1-4 2002 (ISSN 0149-1970), pag. 266 (U₂₃₅ fast spectrum).

⁽²⁾ Progress in Nuclear Energy, Vol 41, Number 1-4 2002 (ISSN 0149-1970), pag. 405 (recommended values U₂₃₅ fast spectrum).

⁽³⁾ Note CEA DEN/CAD/DER/SPRC/LEPH 06-204. Data are from Progress in Nuclear Energy, Vol 41, Number 1-4 2002 (ISSN 0149-1970), pag. 268 (U₂₃₈ fast spectrum).

⁽⁴⁾ Progress in Nuclear Energy, Vol 41, Number 1-4 2002 (ISSN 0149-1970), pag. 405 (recommended values U₂₃₈ fast spectrum).

ERANOS results

$$\beta_{eff} = \sum_{m} \sum_{i} \overline{v}_{d,i}^{(m)} \frac{\langle \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{d,i,g} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \rangle_{\mathbf{r}}}{\langle \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{g} \sum_{m} \sum_{g'} \langle v_{g'}^{(m)} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \rangle_{\mathbf{r}}} \rightarrow 723 \text{ pcm}$$

$$\beta_{eff} = \sum_{m} \sum_{i} \overline{v}_{d,i}^{(m)} \frac{\langle \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{d,i,g} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \rangle_{\mathbf{r}}}{\langle \sum_{g} \phi_{g}^{+}(\mathbf{r}) \overline{\chi}_{g} \sum_{m} \overline{v}_{g'}^{(m)} \sum_{g'} \Sigma_{f,g'}^{(m)}(\mathbf{r}) \phi_{g'}(\mathbf{r}) \rangle_{\mathbf{r}}} \rightarrow 731 \text{ pcm}$$

$$732 \text{ pcm}$$

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ERANOS results

Total and prompt fluxes, together with spectral differences $\Delta = (\phi_{p,g} - \phi_g)/\phi_g$.



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Conclusions

- When evaluating β_{eff} by the formula 1-(k_p/k), the *quality* of the obtained result depends on the *quality* of the description of the delayed neutron emission assumed in the k_p prompt calculation.
- Great detail is given in ERANOS to the characteristics of the delayed neutron emission through the β_{eff} formulation, and it is not possible to set up a prompt calculation having the same quality of the delayed neutron emission description available in the β_{eff} formulation.
- Following the perturbation theory approach, a rigorous relationship may be established between the β_{eff} evaluation by the formula 1-(k_p/k), used in Monte Carlo codes, and the corresponding β_{eff} calculation by the classical formulation involving direct and adjoint fluxes.
- The classical formulation can be considered an "improved" PT first order formulation of the formula $1-(k_p/k)$.
- By means of a refined computational analysis carried out in a coherent and consistent way, i.e. using the same deterministic code ERANOS and neutron data library JEFF 3.1 for the β_{eff} evaluation in different ways, the theoretical analysis is numerically confirmed.

- Both theoretical and numerical results confirm the effectiveness of the β_{eff} evaluation by the MC formula 1-(k_p/k), at least in cases where spectral differences between total and prompt fluxes are negligible with respect to the value of the functionals entering the classical β_{eff} formulation.
- For other material configurations more investigations are needed to obtain a detailed quantification of the effects involved.