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Preventing xenon oscillations in Monte Carlo burnup calculations by enforcing equilibrium xenon distribution

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ABSTRACT

Existing Monte Carlo burnup codes suffer from instabilities caused by spatial xenon oscillations. These oscillations can be prevented by forcing equilibrium between the neutron flux and saturated xenon distribution. The equilibrium calculation can be integrated to Monte Carlo neutronics, which provides a simple and lightweight solution that can be used with any of the existing burnup calculation algorithms. The stabilizing effect of this approach, as well as its limitations are demonstrated using the reactor physics code Serpent.

1. Introduction

Monte Carlo burnup calculations have typically focused on two dimensional pin cell geometries, assembly segments and other geometries with relatively small dimensions. As computers and algorithms develop, calculations involving research reactors, full 3D assemblies and even simplified models of power reactors are becoming increasingly common. While most modeled geometries have been, and still are, too small or too crudely discretized for spatial oscillations to occur, applications are increasingly approaching the point where this in no longer the case.

Several widely used burnup calculation algorithms have been found to be unstable, at least in long symmetric pin cell geometries (Dufek and Hoogenboom, 2009; Dufek et al., 2013), which is sufficient to show that they cannot handle the general case. These oscillations are driven by xenon, although due to time discretization the mechanisms differ from physical xenon oscillations. Since all existing methods seem to be affected, this effectively prevents expanding Monte Carlo burnup calculations to large and detailed geometries.

Xenon oscillations can also occur in real reactors, or could, if they were not prevented by active control. Due to various approximations oscillations in numerical calculations can be much worse than they would in real reactors, but despite this, explicitly modeling the control system should help. Such solution would, however, be extremely laborious, if at all feasible in the context of Monte Carlo neutronics, and thus a simpler alternative is required.

In deterministic codes, spatial oscillations involving various quantities are dealt with by forcing equilibrium at each time step. This is done via wrapper algorithms that use multiple neutronics solutions to find the equilibrium distributions and the corresponding flux, which is then used for depletion. This approach has also been used in Monte Carlo burnup calculations (Dufek and Gudowski, 2006). However, with Monte Carlo neutronics it is also possible to efficiently calculate equilibrium xenon distributions inside the criticality source simulation (Griesheimer, 2010).

In this paper we suggest utilizing such inline equilibrium xenon calculations for stabilizing Monte Carlo burnup calculations. This provides a lightweight approach that can be used with any burnup calculation algorithm. The inherent instability of computational models used in Monte Carlo burnup calculations and the stabilizing effect of the equilibrium xenon treatment are demonstrated.

2. Theory

2.1. Xenon oscillations

^{135}Xe has a very large thermal absorption cross-section and a high cumulative fission yield giving it a profound effect on neutronics. The combined direct yield of ^{135}Xe ($T_{1/2} \approx 9.2$ h) and ^{135m}Xe ($T_{1/2} \approx 15$ min) from thermal fissions is only around 0.2%, while its precursors ^{135}Sb, ^{135}Te and ^{135}I have a combined yield of 6%. ^{135}Sb and ^{135}Te decay to ^{135}I in seconds, but ^{135}I has a

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half-life of 6.6 h. Because of this, changes in the flux affect xenon production rate with a delay, whereas removal rate, which is dominated by absorption, changes instantly.

If the flux is tilted, the immediate effect is that in the areas of high flux reactivity starts to increase as xenon is depleted and in the areas of low flux reactivity decreases as xenon builds up. These changes in reactivity reinforce the flux tilt, which in turn leads to even larger changes in reactivity. Over time ^{135}I concentrations stabilize and the xenon concentration in high flux areas starts to increase while that in the low flux decreases, eventually tilting the flux the opposite way and the cycle repeats.

Burnup calculations aiming to follow long term development use step lengths much longer than the timescale involved in physical xenon oscillations. Due to long steps ^{135}I and ^{135}Xe concentrations have time to reach saturation levels corresponding to the used flux at each step, making the physical xenon oscillation mechanism impossible. Instead, if the flux is tilted, the areas with high flux will get high xenon concentration during the following depletion step and the other way around. This in turn means that in the next neutronics solution the flux will tilt the other way, leading to an unphysical oscillation.

2.2. Equilibrium xenon calculation

All xenon driven oscillations are prevented if the xenon concentrations and neutron flux are forced to remain in equilibrium. Griesheimer (2010) has presented an algorithm that allows the equilibrium to be calculated inside a Monte Carlo criticality source simulation, providing a massive reduction in running time when compared to traditional wrapper algorithms. Another integrated equilibrium calculation algorithm based on the same principle can be found in the reactor physics code Serpent.[1] While both algorithms were designed for other purposes, they can also be used for removing oscillations in burnup calculations simply by applying them to all neutronics solutions. Since only the neutronics is affected, this can be done with any burnup calculation algorithm.

The equilibrium calculation in Serpent is performed during a criticality source simulation by recalculating the concentrations of ^{135}I and ^{135}Xe after each source cycle using the flux and cross-sections tallied during that cycle. This is done separately for each fissile material region. The new concentrations are then used during the next source cycle and so on. The result is a continuous iteration between neutronics and the equilibrium concentration of ^{135}I and ^{135}Xe, performed as the transport simulation is run. This means that the concentrations of these two nuclides change through all inactive and active cycles.

The concentrations of ^{135}I and ^{135}Xe are calculated by assuming that ^{135}Xe and its precursors are in a secular equilibrium with the actinides, and that the neutron capture rates of the precursors of ^{135}Xe are insignificant compared to radioactive decay. With these approximations, the concentrations become:

$$n_{\mathrm{I}} = \frac{\gamma_{\mathrm{I}} \Sigma_{\mathrm{f}} \Phi}{\lambda_{\mathrm{I}}} \tag{1}$$

and

$$n_{\mathrm{X}} = \frac{\gamma_{\mathrm{X}} \Sigma_{\mathrm{f}} \Phi}{\lambda_{\mathrm{X}} + \sigma_{\mathrm{X}} \Phi}, \tag{2}$$

where n_{I} and n_{X} are the concentrations of ^{135}I and ^{135}Xe, respectively, γ_{I} and γ_{X} (which includes γ_{I}) their cumulative fission yields, λ_{I} and λ_{X} their decay constants, Σ_{f} is the macroscopic total fission cross-section of the material, σ_{X} the microscopic capture cross-section of ^{135}Xe, and Φ the total flux.

All results, including the cross-sections and flux used in depletion calculations, are tallied as before over all active cycles. The concentrations of ^{135}I and ^{135}Xe are collected by averaging over the iterated concentrations from all cycles. The concentrations of all other nuclides, including the daughters of ^{135}I and ^{135}Xe still come from depletion calculations.

The fission yields used in the equations are fission rate weighted averages of the values for each actinide. The data is typically provided for three incident neutron energies: 0.0253 eV, 400 keV and 14.0 MeV. Even though the energy dependence is taken into account in Serpent burnup calculations, the equilibrium xenon model always uses the data corresponding to the lowest energy.

While the algorithm has produced good results, its correctness and possible improvements remains a topic of future study: There has been no theoretical analysis on its validity, and the estimate of Eq. (2) for ^{135}Xe concentrations is known to be biased (Griesheimer, 2010). Because the updates in the algorithm of Serpent uses only one source cycle worth of statistics, the bias might become an issue in some cases despite being insignificant in the algorithm of Griesheimer (2010).

3. Numerical test calculations

The base case for all tests is a single PWR pin cell identical to the one used by Dufek and Hoogenboom (2009). Fuel pin diameter is 0.82 cm, cladding outer diameter 0.95 cm and there is no gas gap. Lattice pitch is 1.26 cm. The cell is 4 m long and divided into eight 50 cm long axial segments. The segments are numbered 1–8 starting from one end. Reflective boundary conditions are used at all boundaries, including the vertical direction. The cladding is pure zirconium at 600 K and the coolant light water with density of 0.7 g/cm^3 at 600 K. Fuel density is 10 g/cm^3, temperature 900 K and their average enrichment 3.1 wt.%. To break the symmetry, this base case is varied by increasing enrichment in segments 1–4, and lowering it in segments 5–8. The enrichments are selected so that the average remains at 3.1 wt.%. For example, with 0.4 pp (percentage points) difference the enrichments are 3.3 wt.% and 2.9 wt.%. Mean linear power is kept constant at 16 kW/m.

Burnup calculations consisting of 480 steps of 15 min, 40 steps of 3 h, 20 steps of 6 h, 10 steps of 12 h or 10 steps of 1, 2, 4, 8, 16, 30, 60 or 120 d were performed with enrichment differences of 0, 0.1, 0.4, 0.8, and 1.6 pp using the default CE/LI predictor–corrector burnup algorithm (Isotalo and Aarnio, 2011a) of Serpent. The calculations with 15 min steps used version 2.1.9 of Serpent with 1000 inactive and 5000 active cycles of 1000 neutrons, while all other calculations used version 2.1.10 with 1000 inactive and 5000 active cycles of 5000 neutrons.[2] All calculations used the same JEFF 3.1.1 based nuclear data libraries, and were repeated five times with different random number sequences to get an idea of the magnitude of statistical variation.

Additional test calculations, and their results, are described in Sections 3.3 and 3.4. Section 3.5 describes the differences, or lack of, in results obtained with other burnup algorithms.

3.1. Short steps without equilibrium xenon

Step lengths under 1 d are well below those typically used in burnup calculations. These calculations were done to demonstrate that it is impossible, not just unpractical, to avoid the oscillations simply by reducing step lengths and thus to show that a stabilizing scheme is really required. Since reducing step lengths should only

[1] For a complete and up-to-date description of the Serpent code, see http://montecarlo.vtt.fi.

[2] Equilibrium xenon calculation was added to Serpent 2 in version 2.1.10. There are no other changes that affect the results.