

## Explicit decay heat calculation in the nodal diffusion code DYN3D

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**Abstract** - 3D reactor dynamic code DYN3D was developed for analysis of transients and accident scenarios. The residual radioactive decay heat plays an important role in some of accident scenarios and in DYN3D it is taken into account by a model based on German national standard DIN Norm 25463. The applicability of this model is limited to a low enriched uranium dioxide fuel for light water reactors. This paper describes the new general decay heat model implemented in DYN3D. The radioactive decay rate of each nuclide in each spatial node is calculated and the cumulative released heat is used to obtain the decay power spatial distribution for any time step. Such explicit approach is based on first principles and is free from approximations which limit its applicability. The proposed method is verified against Monte Carlo reference calculations.

## I. INTRODUCTION

Coupling of neutron kinetics codes with plant thermo-hydraulic codes is widely used for analysis of complicated transient and accident scenarios where both 3D neutronics and thermal feedbacks from plant components and safety systems play an essential role.

DYN3D is a 3D nodal reactor dynamic code developed at the Helmholtz-Zentrum Dresden-Rossendorf, mainly for transients, but also for steady-state and fuel cycles analyses in LWR cores with hexagonal or square fuel assemblies [1]. It can be coupled with system codes such as ATHLET [2] and RELAP5 [3].

Simulation of residual decay heat is important in a number of accident scenarios such as loss of coolant, main steam line break, station blackout, etc.

DYN3D calculates node-wise decay heat power by applying methodology described in German normative document DIN Norm 25463 [4, 5]. The fission products of four fissile isotopes  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{241}\text{Pu}$  are divided into 24 groups, each having a characteristic decay constant. Decay heat power is calculated individually for each node taking into account local power history. Due to applied approximations the model is suitable for decay heat calculation for UOX fuel in LWRs with a maximum initial enrichment of 4.1%. However, if this methodology is applied to other fuel types, it introduces large uncertainty into the results [6].

This work presents an explicit approach that accounts for the decay heat, recently implemented in DYN3D. This method relies on “first principles” – it utilizes detailed information about nuclide content and does not require approximations or assumptions about initial fuel content and its evolution with depletion. Thus, the proposed method is general and not limited to particular fuel types.

This paper describes the depletion and the decay heat methodology implemented in DYN3D, briefly describes Serpent Monte Carlo code which was used to obtain reference solution and demonstrates the results of code-to-code verification.

## II. CODES AND METHODS

### 1. Serpent

SERPENT 2 is a continuous energy MC neutron transport code with burnup capabilities developed at VTT research center in Finland [7]. The code was developed as an alternative to deterministic lattice physics codes for generation of homogenized multi-group material properties (XS) for reactor analyses using nodal codes.

The code has a number of features that dramatically reduce CPU time required for its execution, among them unified energy grid [8] and the use of Woodcock delta-tracking [9] of particles.

Serpent features a built-in decay and depletion solver, which applies matrix exponential method to solve Bateman decay and depletion equations. Decay and transmutation paths are formed and the nuclides selected for the calculation (about 1500 in typical LWR fuel depletion) automatically. Radioactive decay data and energy-dependent fission yields and isomeric branching ratios for neutron reactions are read from ENDF format data libraries. The matrix exponential is solved utilizing Chebyshev Rational Approximation (CRAM) method, which was proven to be fast and accurate for transmutation matrixes [10].

In this work Serpent 2.1.26 with JEFF-3.1 isotopic library was used to obtain the reference solutions for the examined test cases and to generate homogenized macro- and microscopic cross sections for DYN3D.

## 2. DYN3D

DYN3D couples dynamic neutron flux solution with coolant and fuel temperature fields obtained by thermo-hydraulic solver. The neutronic solver utilizes the nodal expansion method to solve multi-group diffusion or SP3 equations in rectangular, hexagonal or trigonal geometries, with pin-power reconstruction capabilities. Thermo-hydraulic solver simulates two-phase flow in parallel channels, coupled by the core mass flow or pressure drop as boundary conditions. Four-equation model is used to obtain the coolant temperature and density distributions, heat fluxes, heat transfer regimes and DNBR. The model includes thermal properties of water-steam as well as helium and liquid sodium coolants. The fuel rod model is used to obtain the fuel temperature profiles and contains burnup-dependent thermal properties of uranium dioxide.

The range of DYN3D applicability is greatly extended by multi-physics coupling with system codes like ATHLET [2] and RELAP [3], CFD code ANSYS CFX and FLICA4 [11], sub-channel thermal hydraulics SUBCHANFLOW [12] and fuel performance code TRANSURANUS [13].

## 3. Hybrid microscopic depletion in DYN3D

Nodal codes such as DYN3D spatially discretize a reactor core into nodes, which could be axial layers of fuel assembly or a part of fuel assembly. The neutronic properties are considered homogeneous within each node and are obtained from a few-group homogenized macroscopic cross section (XS) library, which are pre-generated using a lattice code. XS-libraries parametrize dependence of homogenized material neutronic properties with respect to operational parameters (fuel and coolant temperatures, boron concentration, control rod presence, etc.) and burnup.

The actual nuclide content of nuclear fuel depends on the node position in the reactor core and local operational history (i.e. history of the local temperatures, power and control rod insertion during fuel burnup). To account for the actual local nodal nuclide content, the hybrid microscopic depletion method was recently developed and implemented in DYN3D [14].

DYN3D obtains the local nuclide content for each node at the end of each time step  $\Delta t$  by solving the Bateman equation in matrix form by computing the matrix exponential:

$$\mathbf{N}(t + \Delta t) = e^{\mathbf{A}\Delta t}\mathbf{N}(t) \quad (1)$$

where  $\mathbf{N} = [N_1 \dots N_n]$  is local nuclide vector for a given time point. The operator  $\mathbf{A}$  represents the transmutation matrix which depends on the rates of neutron induced and decay reactions. The matrix exponential is solved using fast and accurate CRAM [10] method.

DYN3D tracks about 1200 nuclides and utilizes complete decay and depletion chains. Currently, the depletion solver considers 5 types of neutron reactions:  $(n,\gamma)$ ,  $(n,\text{fission})$ ,  $(n,2n)$ ,  $(n,3n)$ , and  $(n,\alpha)$ . Homogenized few-group *microscopic* cross sections for the considered reactions are generated by a lattice transport code along with homogenized few-group *macroscopic* XS and included in the few-group cross section library utilized by DYN3D.

The local nuclide content is used to improve the accuracy of the node's homogenized cross sections:

$$\Sigma_j^{actual} = \Sigma_j^{SA} + \sum_i (\sigma_{ij}^{actual} N_i^{actual} - \sigma_{ij}^{SA} N_i^{SA}) \quad (2)$$

where

$i$  – is the isotope index;

$j$  – the reaction index (absorption or fission);

$\Sigma^{SA}$  – the homogenized macroscopic XS calculated by the lattice code in a single assembly (SA) model;

$\Sigma^{actual}$  – the homogenized macroscopic XS corrected with local nuclide content;

$\sigma^{SA}$  – the homogenized microscopic XS of nuclide  $i$  calculated by the lattice code;

$\sigma^{actual}$  – the homogenized microscopic XS of nuclide  $i$  corrected with local fissile content;

$N_i^{SA}$  – the concentration of nuclide  $i$  calculated at the nominal depletion conditions;

$N_i^{actual}$  – the local concentration of nuclide  $i$  calculated by the nodal code.

The values calculated by the lattice code provided to DYN3D in the XS-library are the homogenized XS  $\Sigma^{SA}$  and  $\sigma^{SA}$ , parametrized against burnup and instantaneous operational parameters, while the reference nuclide content  $N^{SA}$  is parametrized against burnup only.

## 4. Explicit decay heat model in DYN3D

The fact that DYN3D tracks the full set of nuclides during all depletion and decay steps allows explicit calculations of important fuel characteristics such as decay heat power in each node:

$$P^n(t) = \sum_i N_i^n(t) \lambda_i q_i \quad (3)$$

where

$P^n(t)$  – the decay heat power in node  $n$  at time  $t$ ;

$N_i^n(t)$  – the concentration of nuclide  $i$  in node  $n$ ;

$\lambda_i$  and  $q_i$  – the decay constant and energy release per decay of the nuclide  $i$ , respectively. The sum in Eq.(3) is over the entire set of nuclides in the node.

The decay constants, fission yield data, and energy released per decay of each nuclide are included in an internal DYN3D library of physical constants.

### III. RESULTS

A verification of the new decay heat power calculation capability has been performed using simple fuel pin test models with various fuel materials. DYN3D results were benchmarked against the reference Serpent Monte Carlo solution.

The first considered test case is a BWR UOX fuel pin with reflective boundary conditions. The depletion and decay calculations were performed with DYN3D employing homogenized macro- and microscopic XS generated by Serpent 2 Monte Carlo code. The obtained XS library was used to simulate different depletion and outage scenarios.

Four-step depletion and decay history used in the calculations is illustrated in Figure 1 (top): a) first depletion period of 520 days at 120% of nominal power; b) 60 days outage; c) second depletion period of 60 days at nominal power; and finally d) decay period of 10 years.

The neutron multiplication factor calculated by Serpent and deviation of DYN3D results are shown in Figure 1 (bottom). Application of the hybrid microscopic depletion method keeps the errors in DYN3D multiplication factor below 50 pcm.

The results of the decay heat power calculations depicted in Figure 2 show excellent agreement between DYN3D and Serpent. For the entire simulated time period, from minutes to 10 years, DYN3D is able to reproduce the reference decay heat power and its components within 0.5%.

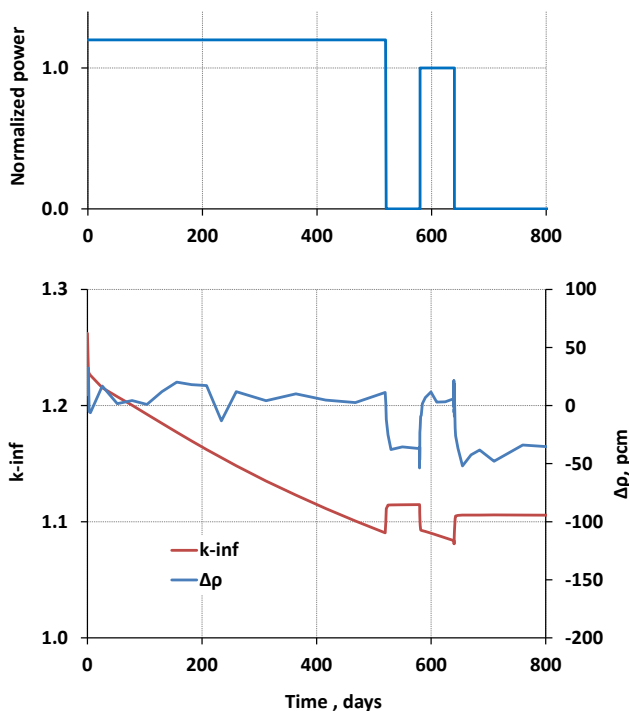


Fig. 1. Power history and multiplication factor in test case.

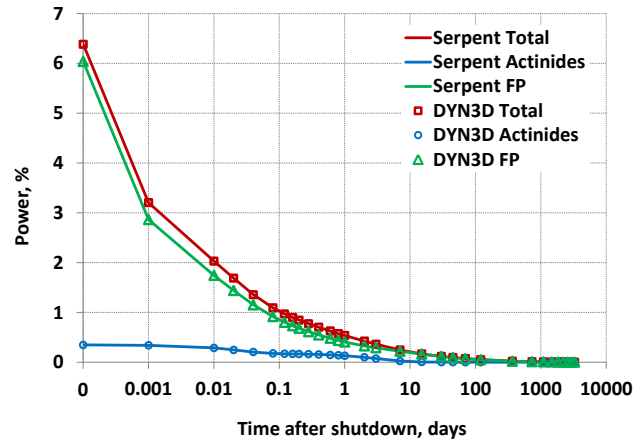


Fig. 2. Decay heat power after shutdown in BWR UOX test case.

The decay heat power depends on fuel burnup level, as illustrated in Figure 3. The decay heat produced by the same BWR fuel pin after depletion up to 10, 20, 30, and 50 MWd/kgHM was calculated by DYN3D and compared with Serpent reference. Figure 3 shows the relative difference from the decay heat after 50 MWd/kgHM. Different burnup accumulated just before shutdown results in up to 10% difference in the first hours and an order of magnitude in the long term (years).

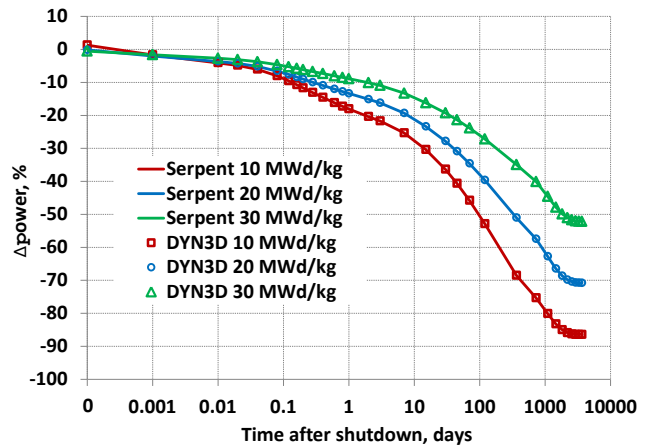


Fig. 3. Decay heat power dependence on fuel burnup.

Since the fuel nuclide content depends on a local depletion history, the decay heat power depends on depletion history as well, as illustrated in Figure 4. The BWR fuel pin was depleted up to 50 MWd/kgHM under nominal power and fuel temperature, but the “top” node with water density of 400 kg/m<sup>3</sup>, while the “bottom” node with water density of 700 kg/m<sup>3</sup>. Figure 4 shows the relative difference between decay heat after shutdown produced in these “top” and “bottom” nodes. Depletion with different coolant density results in 4-5% difference in the decay heat in the initial few hours and about 10% in longer time scales.

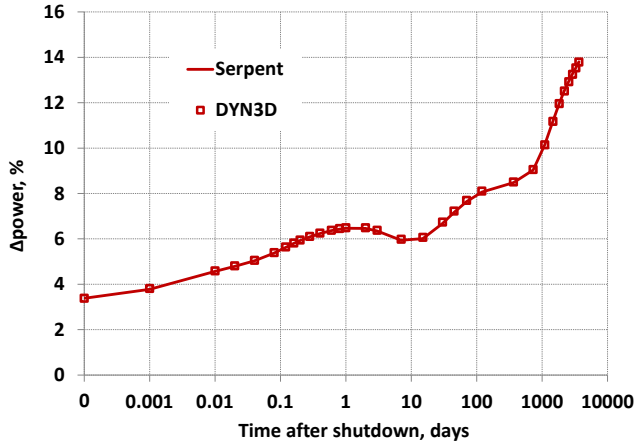


Fig. 4. Decay heat power dependence on depletion conditions.

To demonstrate the applicability of the proposed method to other types of fuel, a depletion and decay heat of PWR MOX and UOX fuel pin were simulated. Both fuel pins were depleted under nominal conditions up to 50 MWd/kgHM. Figure 5 demonstrates the decay heat power (in percent of the nominal power) after shut down and its components from actinides and fission products (FP).

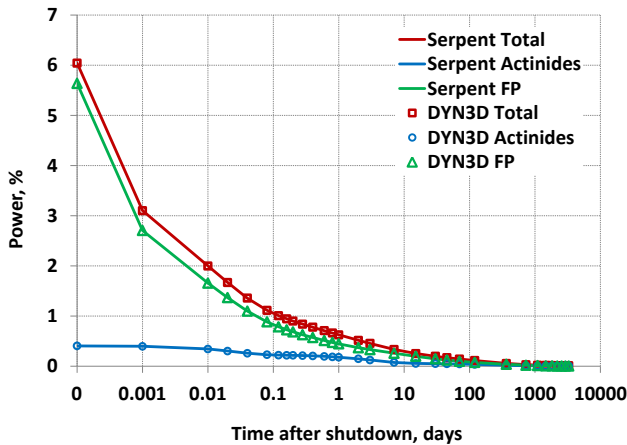


Fig. 5. Decay heat power after shutdown in PWR MOX test case.

Figure 6 illustrates the difference in decay heat power generated by PWR MOX in comparison with PWR UOX. Both fuel pins share the same geometry and were depleted under nominal power to 50 MWd/kgHM before shutdown. Power produced in MOX fuel is about 4% higher in first hours and almost double in longer time scale.

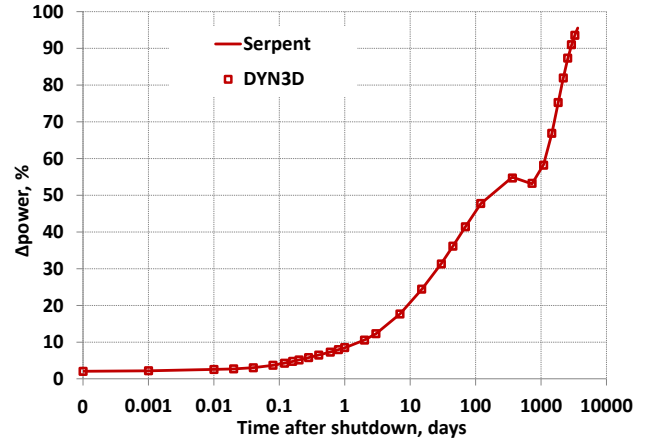


Fig. 6. Difference in decay heat power generated by PWR MOX and UOX.

#### IV. CONCLUSIONS

Reactor dynamics code DYN3D, often coupled with plant thermo-hydraulic codes such as ATHLET or RELAP, is used to simulate transients and accidents scenarios. The radioactive decay heat generated by nuclear fuel after shutdown plays an important role in a number of accident scenarios. The decay heat model implemented in DYN3D so far is based on the German national standard DIN Norm 25463 (1990) and its applicability is limited to LWR fuel up to 4.1% enrichment.

This paper proposes a general methodology of the decay heat calculation by accounting explicitly for the heat from the decay of each nuclide in the fuel. This method relies on “first principles” and does not involve any assumptions about the fuel content or operational history. Therefore, its range of applicability is not restricted to any particular fuel type. Detailed nuclide content, required for the decay heat calculation, is calculated by DYN3D using recently implemented depletion solver.

The presented method was verified against Serpent 2 Monte Carlo reference solution in 2D infinite lattice test cases with BWR UOX and PWR UOX and MOX fuel cells. In all test cases, the deviation of DYN3D decay heat power from Serpent 2 reference is within 0.5%.

The test results have also shown notable sensitivity of the decay heat production to the operational history and burnup accumulated before shutdown as well as on initial fuel composition. DYN3D calculates nodal nuclide content during fuel cycle simulation, taking into account the local operational history of each node. Thus, DYN3D is able to accurately estimate 3D decay heat power distribution in a core during transients as well as in long term storage.

The future work will be focused on the verification of the method on realistic test cases.

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