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McSAFER

High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors

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D3.3: Advanced transient heat deposition models for Ants nodal solver including dynamic decay heat

Summary

One of the main objectives of the McSAFER project is to estimate the added benefit of using beyond the state-of-the-art high fidelity methods for reactor core physics compared to state of the art reduced order methods. This will be achieved by modelling the same small modular reactor (SMR) transients using high fidelity and reduced order methods.

Ants reduced order (nodal diffusion) solver within the Kraken framework constitutes one such reduced order solver as part of the two steps Serpent-Ants calculation chain that aims to provide full core neutronics solution based on the pre-calculated (micro-group constants) data from Serpent, continuous-energy Monte Carlo particle-transport code.

The availability of an advanced thermal energy deposition model in the time-dependent calculations to be conducted in the project is a must to produce accurate power distributions in transient or accident scenarios and design-basis parameters definition.

An explicit decay heat methodology, and its optimization via depletion system compression method, is proposed within the future needs of Ants calculations simulations to be conducted in Task 3.2 of the McSAFER project.

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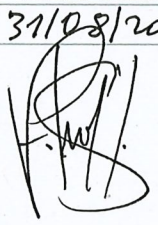
Signatures			

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Introduction

Ants reduced order (nodal diffusion) solver [1] within the Kraken framework [2] constitutes part of the two steps Serpent-Ants calculation chain that aims to provide full core neutronics solution based on the pre-calculated (micro-group constants) data from Serpent [3], continuous-energy Monte Carlo particle-transport code.

Ants will be applied as a state-of-the-art reduced order neutronics solver to provide nodal level results for the NuScale SMR core transients in WPs 3 and 5 of the McSAFER project.

For such simulations an advanced thermal energy deposition model in time-dependent calculations is a must to produce accurate power distributions in transient or accident scenarios and design-basis parameters definition.

Thermal energy deposition models in nuclear reactors: background

1.1. Energy deposition rates: overview

The total energy released by a fission event has several prompt and delayed energy contributors [4]. Although, primarily, the recoverable energy is released instantaneously as kinetic energy from fission products and fission neutrons, prompt gamma rays or energy, from the subsequent neutron capture. Only a part of it is emitted after as, radioactive decay of fission products and radioactive nuclei due to neutron capture as delayed beta and gamma rays. After a period of steady power history, of the order of magnitude of days, its equilibrium is reached. Consequently, its time dependence is no longer represented in reactor core solvers aside from the decay heat production during reactor shutdown or post-accident scenarios. Some transient scenarios, i.e., a slow transient due to core depletion and a fast transient, such as a reactivity-initiated accident (RIA), might question such simplification.

1.1. Decay heat model: overview

The decay heat is the thermal energy release through the radioactive decay of fission products and nuclides produced by the neutron capture in fission products and actinides produced by the neutron capture in heavy metals. It constitutes the second largest source of thermal power within the reactor and thus, it should be accurately modelled at any time of the reactor operation. It plays an important role, not only in the analysis of transient/accident scenarios, e.g. loss of coolant, main steam line break, etc., but also as a safety design parameter, e.g. spent fuel storage, final disposal sites, etc.

Table 1: Energy deposition contributors [4].

1.	Fission a) Kinetic energy of Fission Products b) Prompt and Decay Beta Particle Energy
2.	Neutron Capture a) Kinetic Energy of Charged Particles b) Decay Beta Particle Energy c) Nuclear Recoil
3.	Neutron Scattering a) Nuclear Recoil Following Elastic Scattering Interactions b) Nuclear Recoil Following Inelastic Scattering and Subsequent Nuclear De-Excitation
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5.	Photon Transport
6.	Photon Interactions a) Photoelectric Absorption b) Compton Scattering c) Pair Production d) Photonuclear Reactions

Time-dependent thermal energy deposition modeling

The traditional evaluation of the thermal power [5] either in steady-state or time-dependent calculations accepts equilibrium delayed power, forsaken the time-dependence of the decay power from the precursors.

The power at time t due to the energy release from neutron fission and capture rates, and is normalized to produce the true thermal power of the reactor,

$$P(t) = F(t)\sum_j V_j\left(\sum_i q_{f,i}N_i(t)\sum_g \sigma_{f,g,i,j}\phi_{g,j}(t) + \sum_i q_{c,i}N_{i,j}(t)\sum_g \sigma_{c,g,i,j}\phi_{g,j}(t)\right) \quad (1)$$

where:

$F(t)$ flux normalization factor
$q_{f,i}$ direct fission energy release for isotope i
$q_{c,i}$ recoverable energy per neutron capture for isotope i
V_j volume of material region j

$N_{i,j}$	number density of isotope i in material region j
$\phi_{g,j}$	neutron flux of energy group g in region j
$\sigma_{f,g,i,j}$	microscopic fission cross section
$\sigma_{c,g,i,j}$	$\sigma_{a,g,i,j} - \sigma_{f,g,i,j}$, microscopic capture cross section
$\sigma_{a,g,i,j}$	microscopic absorption cross section
$P(t)$	thermal power of the reactor

** Approximately 7% of the total recoverable fission energy constitutes the delayed term.

1.2. General methodology

The reactor thermal power, $P(t)$, can be written as the sum of a prompt component $P_p(t)$, and a delayed component $P_d(t)$.

$$P(t) = P_p(t) + P_d(t) \quad (2)$$

For an isotope, iso, the fraction γ_i^f and γ_i^c correspond, respectively, to the fission and capture energy release some time after the fission or capture event. This way, the prompt thermal power, $P_p(t)$, can be written as,

$$P_p(t) = F(t) \sum_j V_j \sum_i \sum_{x=f,c} (1 - \gamma_i^x) q_{x,i} N_{i,j}(t) \times \sum_g \sigma_{x,g,i,j} \phi_{g,j}(t) \quad (3)$$

To determine the delayed thermal power, $P_d(t)$, two main approaches can be followed. A general approach is to lump the numerous components of the delayed heat source into a relatively small number of “groups” (*multi-group* methodology). On the other hand, a rigorous calculation based on a detailed fuel inventory for each time step, where each contributor is explicitly represented (*explicit* methodology), tracks independently all the nuclides involved within the calculation. The fidelity and the computational cost and memory demand are proportional.

Following the *multi-group* methodology is described as it is the most common approach within (reduced order) neutronics solvers, and its extension to the explicit representation does not involve major changes besides the number of independent nuclides or ”groups”.

The *multi-group* approach is similar to the treatment of delayed neutron precursors. The characterization of each “group” is based on the half-lives of the delayed heat groups. Defining $C_{m,i,j}^x$ as the concentration of the delayed heat group m of isotope i at region j for the induced reaction x and, being the balance equation that $D_{m,i,j}^x$ satisfies given by,

$$\frac{dC_{m,i,j}^x(t)}{dt} = F(t) V_j \gamma_{m,i}^x q_{x,i} N_i(t) \sum_g \sigma_{x,g,i,j} \phi_{g,j}(g) - \lambda_{m,i}^x C_{m,i,j}^x(t) \quad (4)$$

where $\gamma_{m,i}^{x}$ and $\lambda_{m,i}^{x}$ are the yield and decay constants of the delayed heat group m. Thus, $\sum_m \gamma_{m,i}^{x}$ represents γ_i^x in Eq. (3). Giving $C_{m,i,j}^{x}$, the delayed power is defined as,

$$P_d(t) = \sum_j \sum_i \sum_{x=f,c} \sum_m \lambda_{m,i}^{x}\, C_{m,i,j}^{x}(t) \qquad (5)$$

Eq. (1) should be substituted by Eqs. (2)-(5) to solve for the time dependence of delayed energy. Let's note that Eq. (4) has the same form as the delayed neutron precursor equation. The analytical solution, assuming a constant delayed heat source $S_{m,i,j}^{x} = FV_j\gamma_{m,i,}^{x}q_{x,i}N_{i,j}\sum_g \sigma_{x,g,i,j}\phi_{g,j}$ within a standard burnup time step or sub-step (t_1, t_2), results into,

$$C_{m,i,j}^{x}(t) = C_{m,i,j}^{x}(t_1)\exp\left(-\lambda_{m,i}^{x}(t-t_1)\right) + \frac{S_{m,i,j}^{x}}{\lambda_{m,i}^{x}}\left[1-\exp\left(-\lambda_{m,i}^{x}(t-t_1)\right)\right], \qquad t_1 \le t \le t_2 \qquad (6)$$

The predictor-corrector time integrator relaxes the previously assumed hypothesis referred to the delayed heat source $S_{m,i,j}^{x}$.

The definition of the average $C_{m,i,j}^{x}$ over a time step Δt used for the flux normalization is given as,

$$\bar{C}_{m,i,j}^{x} = \frac{1}{\Delta t \lambda_{m,i}^{x\ 2}}\left(\left[S_{m,i,j}^{x} - \lambda_{m,i}^{x}C_{m,i,j}^{x}(t_1)\right]\exp\left(-\lambda_{m,i}^{w}\Delta t\right) + \lambda_{m,i}^{x}C_{m,i,j}^{x}(t_1) + \lambda_{m,i}^{x}S_{m,i,j}^{x}\Delta t - S_{m,i,j}^{x}\right) \qquad (7)$$

Consequently, the flux normalization factor is described as,

$$F(t) = \frac{P(t) - \sum_j \sum_i \sum_{x=f,c} \sum_m \lambda_{m,i}^{x}\bar{C}_{m,i,j}^{x}}{\sum_j V_j \sum_i \sum_{x=f,c}\left(1-\gamma_i^x\right)q_{x,i}N_{i,j}(t)\sum_g \sigma_{x,g,i,j}\phi_{g,j}(t)} \qquad (8)$$

The coupled system defined by Eq. (8) and Eq. (4) is iterated to solve for $F(t)$ and $C_{m,i,j}^{x}(t)$. The converged normalization factor F is used within the depletion calculation in the current step.

The methodology considers two approximations: (i) Eq. (6) assumes that the delayed energy source $S_{m,i,j}^{x}$ is a constant within a time step under the framework of a predictor-corrector depletion calculation; (ii) Eq. (8) uses a time-averaged $\bar{C}_{m,i,j}^{x}$ to estimate the average delayed power over a time step.

The normalization factor F is derived from the steady-state calculation, being constant throughout the transient. However, at each time-step, the thermal power is updated. Eqs. (2)-(6) model the delayed power explicitly, leading to a constant $S_{m,i,j}^{x}$ within the time step. Finally, the flux at the end of the time step is used to compute the new $S_{m,i,j}^{x}$.

1.3. Multi-group delayed heat data

The constants for the *multi-group* delayed heat data, analogously to the associated data to the delayed neutron precursors, can be obtained by fitting the energy release as a function the emission time. The delayed heat data can be derived from, e.g., the ANS-5.1 decay heat standard for LWRs [6], which provides either tabular data at discrete cooling times or exponential fit of the tabular data.

The standard relies on the direct fission of four fissile isotopes (^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu). There is no independent data from the neutron capture absorber, only for the overall fission products. In such scenario, it could be assumed the capture energy is prompt, i.e., $\gamma_i^c = 0$.

$$P_{dh}(t) = \sum_{m=1}^{M=23} \alpha_m \exp(-\lambda_m t) \quad (9)$$

Eq. (9) represents the decay heat power at t seconds after a fission pulse from a fissionable isotope. The solution of integrating Eq. (9) over time is the total delayed heat release after a fission pulse.

$$E_{dh} = \int_0^{\infty} P_{dh}(t)dt = \sum_{m=1}^{M=23} \frac{\alpha_m}{\lambda_m} \quad (10)$$

Based on the previously described delayed heat model and the total direct fission energy release for fissionable isotope q_m, the delayed yield γ_m is defined as,

$$\gamma_m = \frac{\alpha_m}{\lambda_m q_m} \quad (11)$$

Other standards, such DIN Norm 25463 [7] or *multi-group* curve-fitting methodologies, e.g. Dunn's approach [8], implemented in reactor core simulators, produce similar overall decay heat estimate depending on the assumption consider in the formulation.

Thermal energy deposition in Ants: decay heat model

1.4. Explicit methodology

Modelling the reactor physics behavior with a reduced order solver, e.g., nodal diffusion solver, in fuel cycle simulations requires tracking the nuclide concentrations at such spatial and angular discretization without losing accuracy. The spatial homogenization methodology envisions preserving the reaction rates of a high-fidelity heterogeneous transport solver evaluation, e.g., Serpent, when performing a calculation with a low-fidelity homogenous solver, e.g., Ants.

The *explicit* methodology for delayed energy thermal deposition allows an accurate prediction of the decay heat evolution for any reactor system, e.g. thermal and fast, and fuel type, without the imposed assumptions derived from the semi-empirical correlations defined over a limited range of burnup and fuel types characterizing the *multi-group* methodology [9].

Ants accounts for the spatial nuclide composition at a local operational history during burnup, at the end of each time step Δt, by solving the full set of Bateman equations, Eq. (12). It computes the matrix exponential using a built-in depletion solver based on the Chebyshev Rational Approximation Method, CRAM [10] (for $\mathbf{N} = [N_j]$ the local (j-region) nuclide composition vector and, $\mathbf{A}$ the transmutation matrix, including neutron-induced and decay reactions).

$\mathbf{N}(t + \Delta t) = \exp(\mathbf{A}\Delta t)\mathbf{N}(t)$	(12)

The number of tracked nuclides and transmutation chains is not fixed in Ants. It is defined by the lattice code depletion calculation used to generate the homogenized cross section data, aka. Serpent. By evaluating the contribution of the full set of nuclides during all depletion and decay steps, Ants allows an explicit calculation of the local (j-region) nuclide decay heat $\mathbf{P}_{dh} = [P_{dh,j}]$ as,

$\mathbf{P}_{dh}(t) = \sum_i \mathbf{N}_i(t)\lambda_i q_i$	(13)

where:

$\mathbf{P}_{dh}(t)$	local decay heat rate vector at time t
$\mathbf{N}_i(t)$	local isotope i concentration vector at time t
λ_i	decay constant for isotope i
q_i	energy release per decay for isotope i

The decay constants and the energy released per decay for each nuclide are obtained from the radioactive decay data file based on a given nuclear data evaluation. Ants calculates the local fuel nuclide compositions on the run using the actual local fluxes and the pre-calculated microscopic cross sections, dependent on the local operational parameters.

1.5. Micro-group constant generation

Analogously, to a homogenized macroscopic cross section $\Sigma_{x,g}$ for reaction x and for a volume V to be homogenized [11], defined a scalar neutron flux ϕ,

$\Sigma_{x,g} = \frac{\int_{E_g}^{E_{g-1}} \int_V \Sigma_x(r,E)\,\phi(r,E)dVdE}{\int_{E_g}^{E_{g-1}} \int_V \phi(r,E)dVdE}$	(14)

a microscopic cross section for a nuclide i aims to preserve the reaction rate between the heterogeneous and homogeneous representation of the same volume [12]. Nonetheless, macroscopic cross sections homogenization is based on the whole volume V for all nuclides, while in the case of microscopic cross sections, the homogenization is only performed for a volume $\omega \in V$. The microscopic cross section $\sigma_{x,g,i}$ is defined as within the reaction rate equation balance as,

$$\sigma_{x,g,i}\bar{N}_i\bar{\phi}_g = \frac{1}{\int_V dV}\int_{E_g}^{E_{g-1}}\int_{\omega} \sigma_{x,i}(r,E)N_i(r)\phi(r,E)dVdE \quad (15)$$

Defining the nuclide number density smeared to the homogenized volume $\bar{N}_i$ as,

$$\bar{N}_i = \frac{1}{\int_V dV}\int_{\omega} N_i(r)dV \quad (16)$$

and the average neutron flux $\bar{\phi}_g$ in the homogenized volume calculated as

$$\bar{\phi}_g = \frac{1}{\int_V dV}\int_{V} \phi(r,E)dV \quad (17)$$

From Eqs. (15)-(17), the homogenized microscopic cross section is written as follows,

$$\sigma_{x,g,i} = \frac{1}{\bar{N}_i\bar{\phi}_g}\frac{1}{\int_V dV}\int_{E_g}^{E_{g-1}}\int_{\omega} \sigma_{x,i}(r,E)N_i(r)\phi(r,E)dVdE \quad (18)$$

A uniform nuclide density distribution in ω is assumed for $N_i(r) = 0$ in all ω, and consequently Eq. (*18*) can be written as,

$$\sigma_{x,g,i} = \frac{1}{\bar{\phi}_g}\frac{1}{\int_V dV}\int_{E_g}^{E_{g-1}}\int_{\omega} \sigma_{x,i}(r,E)\phi(r,E)dVdE \quad (19)$$

The homogenized microscopic cross sections are calculated by Serpent for the given nuclide(s) and reaction(s).

1.6. Dynamic decay heat model implementation

The *explicit* decay heat model via CRAM solver in Ants provided the pre-calculated micro-depletion data by Serpent does not constitute an additional feature itself in steady-state simulations due to it is a natural outcome from a depletion calculation.

Ants time-dependent formulation solves at discretized time intervals the diffusion equation, following the homogenized neutron flux evolution due to space and time power variations. The depletion solver updates the nuclide compositions computing the full set of Bateman equations built on the micro-depletion data within the coupled system of diffusion and Bateman equations at each time interval, given the flux from the predictor-corrector time integrator scheme.

The computed compositions define the delayed thermal energy deposition (decay heat) at the subsequent time interval.

The *explicit* decay heat methodology based on a full depletion system might constitute an overhead in the calculation time and memory resources while its complexity is usually unnecessary for most reactor physics applications. Ants nodal diffusion solver main aims to perform daily-basis analysis, being the computation speed a key factor. To not deviate from the real solution, a depletion system compression and performance optimization system will be evaluated.

1.7. Depletion compression and performance optimization system

The depletion system compression methods project the original complex depletion system into more compact ones while preserving the intended accuracy. The optimization system is built as a representative case (and depletion step) that considers the neutronics-depletion coupling effects via setting neutronics and target nuclides and decay heat precursors accuracy thresholds [13].

The depletion compression system incorporates three operations: (i) deletion of a reaction channel; (ii) deletion of a nuclide; and (iii) reduction of a decay nuclide; and its subsequent effects on each other. The significance analysis evaluates the accuracy degradation in a specific depletion region caused by the compressed system is based on neutron flux, cross section and number density data from the representative problem under the original depletion system.

To characterize the decay heat within a depletion compression system, the methodology should include the target nuclide specification and the decay heat precursors to identify the major contributors within the heavy metal nuclides and fission products irradiation-effect nuclides via non-linear fitting of delayed neutron emission and fission product decay heat release.

1.8. Current status and future work

Over the recent years, under the framework of The Finnish Research Programme on Nuclear Power Plant Safety 2019-2022, the SAFIR2022/LONKERO project has extended the Ants steady-state multi-group diffusion capabilities in rectangular and hexagonal geometries using the AFEN and FENM methods to depletion calculation via micro-depletion and, recently, to time-dependent modelling.

The implementation of the proposed *explicit* decay heat methodology, and its optimization via depletion system compression method, is scheduled within the future needs of the Ants calculations to be conducted in WP3 and WP5 of the McSAFER project.

References

[1] V. Salhlberg und A. Rintala, „Development and first results of a new rectangular nodal diffusion solver of Ants," in *PHYSOR 2018*, American Nuclear Society, pp.3861-3871, 2018.

[2] V. Valtavirta, V. Hovi, H. Loukusa, A. Rintala, V. Sahlberg, R. Tuominen und J. Leppänen , „Kraken: An upcoming Finnish reactor analysis framework," *M&C 2019,* American Nuclear Society, pp. 786-795, 2019.

[3] J. Leppänen, M. Pusa, T. Viitannen, V. Valtavirta und T. Kaltiaisenaho, „The Serpent Monte Carlo code: Status, development an applications in 2013," *Annals of Nuclear Energy,* V. 82, pp. 142-150, 2015.

[4] ANSI/ANS-19.3.4-2002 (R2017), The Determination of Thermal Energy Deposition Rates in Nuclear Reactors, American Nuclear Society Standards, 2017.

[5] Y. Liu, B. Kochunas, W. Martin und T. Downar, „Delayed fission energy effect on LWR normal operation and transients," *Annals of Nuclear Energy,* V. 128, pp. 84-93, 2019.

[6] ANSI/ANS-5.1-2014 (R2019), Decay Heat Power in Light Water Reactos, American Nuclear Society Standards, 2019.

[7] DIN Norm 25463, Berechnung der Nachzerfallsleistung der Kernbrennstoffe von Leichtwasserreaktoren, Deutsches Institut für Normung, 1990.

[8] F. E. Dunn, „Decay Heat Calculations for Transient Analysis," *Transactions of the American Nuclear Society,* V. 60, pp. 633-634, 1989.

[9] Y. Bilodid, E. Fridman, D. Kotlyar und E. Shwageraus, „Explicit decay heat calculation in the nodal diffusion code DYN3D," *Annals of Nuclear Energy,* Bd. 121, pp. 374-381, 2018.

[10] M. Pusa, „High-order Chebyshev rational approximation method and application to burnup equations," *Nuclear Science and Engineering,* V. 182, pp. 297-318, 2016.

[11] J. Leppänen , M. Pusa und E. Fridman, „Overview of methodology for spatial homogenization in the Serpent 2 Monte Carlo code," *Annals of Nuclear Energy,* V. 96, pp. 126-136, 2016.

[12] A. Rintala, V. Valtavirta und J. Leppänen, „Microscopic cross section calculation methodology in the Serpent 2 Monte Carlo code," *Manuscript submitted for publication,* 2021.

[13] K. Huang, H. Wu, Y. Li und L. Cao, „Depletion system compression method with treatment of decay heat," *Progress in Nuclear Energy,* V. 101, pp. 476-485, 2017.