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Extension of the DYN3D/ATHLET code system to SFR applications: models description and initial validation

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Abstract

DYN3D is a 3D reactor dynamics code originally developed for Light Water Reactors (LWRs) analyses. In recent years, the applicability range of DYN3D was extended to coupled 3D neutronics/ thermal-hydraulics (TH) simulations of steady-states and transients in Sodium cooled Fast Reactors (SFRs) at reactor core level.

The main objective of this study is to scale up the simulation capabilities of DYN3D from SFR core to system level by coupling DYN3D with a TH system code ATHLET capable of sodium flow modeling. The paper describes the adaption and extension of the existing LWR-oriented DYN3D/ATHLET coupling to SFR analysis. This includes a description of the coupling techniques used to integrate DYN3D with ATHLET and a summary of modifications required to enable the modeling of SFR specific phenomena. The paper also presents the approach to the modeling of reactivity effects caused by the thermal expansions of the reactor components located outside the reactor core, such as reactor vessel, core support structure (strongback), control rod drive lines (CRDLs), etc. The paper also includes the description of the initial verification and validation activities of the extended DYN3D/ATHLET code system. The unprotected stage of the Phenix End-Of-Life natural convection test is used as a test case for this purpose.

1. Introduction

DYN3D (Rohde et al., 2016) is a 3D reactor dynamics code originally developed at HZDR for Light Water Reactors (LWRs) analyses. DYN3D solves the steady-state and time-dependent diffusion equations for rectangular and hexagonal geometries by means of nodal expansion methods. In transient calculations, the time derivative terms are approximated by applying implicit first order Euler method combined with the frequency (also called exponential) transformation. DYN3D is supplemented by an internal 1D thermal-hydraulics (TH) solver and fuel rod behavior module.

In recent years, the applicability range of DYN3D was extended to steady state and transient analyses of Sodium cooled Fast Reactors (SFRs). The related accomplished methodological developments include:

- Establishing of a few-group cross section (XS) generation methodology (Fridman and Shwageraus, 2013; Nikitin et al., 2015a, 2015b), which primarily relies on the use of the Monte Carlo (MC) code Serpent (Leppänen et al., 2016).
- Updating the TH solver with thermal-physical properties of sodium such as thermal conductivity, density, heat capacity and viscosity and enabling the modeling of single-phase sodium flows (Rohde et al., 2016).
- Development and implementation of the thermal-mechanical (TM) module accounting for (1) non-uniform axial fuel expansion with an independent treatment of each fuel assembly based on local TH conditions; and (2) radial diagrid expansion driven by inlet sodium temperature (Nikitin and Fridman, 2018a; E. Nikitin and Fridman, 2019a).

With the aforementioned modifications, the extended version of DYN3D can be used as a stand-alone tool for coupled 3D neutronics/TH simulations of steady-states and transients in SFRs at the *reactor core level*. In this regard, DYN3D was validated by analyzing a number of “real life” SFR experiments including the Phenix end-of-life (EOL) control rod withdrawal tests (Nikitin and Fridman, 2018b), the unprotected stage of the Phenix EOL natural convection test (Nikitin and Fridman, 2018c), the isothermal physics tests performed at the Fast Flux Test Facility (FFTF) (E. Nikitin and Fridman, 2019b), and static neutronics characterization of the Superphenix start-up tests (Ponomarev et al., 2022b). The validation activities demonstrated a generally good agreement between the measured data and the numerical results indicating a very satisfactory performance of DYN3D.

Nevertheless, DYN3D as a stand-alone tool has a limited scope of applicability, particularly in case of strong interaction between neutron kinetics (NK) and *system* TH. In principle, the system TH behavior can be mimicked by time-dependent core inlet TH boundary conditions. However, the latter are not always available. Moreover, even with proper boundary conditions, DYN3D

cannot account for reactivity effects caused by the thermal expansion of the reactor components located outside the reactor core, such as reactor vessel, core support structure (strongback), control rod drive lines (CRDLs), etc. These reactivity effects are introduced when the out-of-core (OOC) structures change their dimensions due to the temporal and spatial variations in the sodium temperature, which in turn affect the position of control rods (CRs) relative to the reactor core.

Scaling up the simulation capabilities to SFR system level requires the coupling of DYN3D with a TH system code capable of sodium flow modeling. At HZDR, the best estimate TH system code ATHLET (Austregesilo et al., 2016) was selected for this purpose. There are two main reasons which make ATHLET an apparent choice. First, recent versions of ATHLET include sodium as working fluid. Sodium related modeling capabilities of ATHLET in a stand-alone mode were successfully demonstrated on several SFR concepts including ASTRID-like SFR (Bubelis et al., 2017), ESR (Mikityuk et al., 2021), and Superphenix (Di Nora et al., 2019; Ponomarev et al., 2022a). Second, HZDR has already accumulated a considerable experience in coupling of DYN3D and ATHLET in the LWR domain. It should be noted that the development of the coupling was associated with extensive verification and validation efforts, which were based on numerous LWR dynamic benchmarks and real plant transients (Kozmenkov et al., 2015).

This paper describes the activities related to the development of a DYN3D/ATHLET code system capable to perform coupled 3D neutron kinetics/TH analysis of SFRs at the *reactor system level*. Section 2 of the paper focuses on the adaption and extension of the existing LWR-oriented DYN3D/ATHLET coupling to SFR analysis. This includes a description of the coupling techniques used to integrate DYN3D with ATHLET and a summary of modifications required to enable the modeling of SFR specific phenomena. The approach to the modeling of thermal expansions of the OOC structures affecting the position CRs is also presented.

Sections 3 covers initial verification and validation activities, which use the unprotected stage of the Phenix EOL natural convection test (Nikitin and Fridman, 2018c) as a test case. First, the DYN3D/ATHLET code system is verified against stand-alone DYN3D by analyzing the Phenix test case at the *reactor core level* (i.e. without the modelling of the OOC structures). Second, the DYN3D/ATHLET code system is used to analyze the Phenix test case at the *reactor system level* including the modeling of the OOC structures and their expansions and accounting for respective reactivity effects. The numerical results are validated against the measured data. The effect of the OOC structures on the course of the transient is also discussed. Section 4 summarizes the paper.

2. Extension of the existing DYN3D/ATHLET coupling to SFR analysis

2.1 Overview of the existing thermal expansion models in DYN3D

In coupled 3D neutronics/TH simulations, the TH feedbacks are typically realized by introducing the dependence of few-group XSs on local state variables. In the LWR analysis, the few-group XSs employed by DYN3D are parametrized with respect to local fuel temperature (T_{fuel}), coolant temperature (T_{cool}) and density (ρ_{cool}), and boron concentration (C_b). This allows to account for all major TH reactivity effects including Doppler and coolant density feedbacks.

In SFRs, besides the TH feedbacks, thermal expansion reactivity effects play an important role and, therefore, should be properly treated. Currently, as a stand-alone code, DYN3D can model major thermal expansion effects at the reactor core level. The overview of the capabilities is presented in following.

In general, variations in temperature, density, and dimensions are modeled explicitly in the process of few-group XS generation. The application of these few-group XSs alone is sufficient to account for thermal expansion that *do not change* the nodal boundaries. For instance, this applies to radial expansion of fuel pins (Fig. 1a) and sub-assembly (SA) wrapper (Fig. 1b).

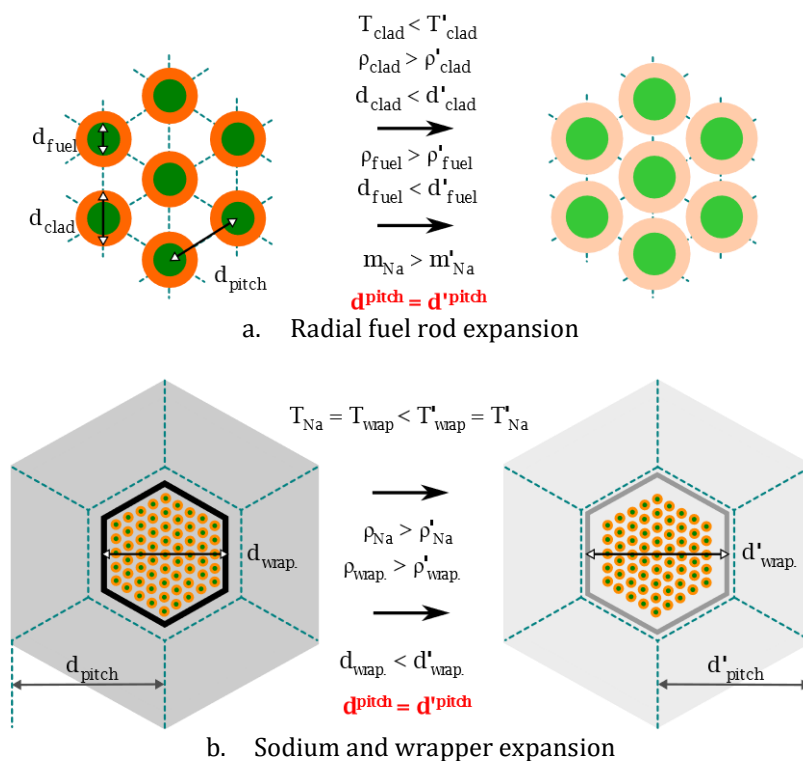


Fig. 1. Schematic overview of the thermal expansions that *do not change* the nodal boundaries and can be modeled with the help of the proper few-group XSs only.

When thermal expansions affect the nodal boundaries, the utilization of proper few-group XSs alone is not sufficient to treat the deformation of the nodal mesh. Therefore, two TM models were developed to model the radial diagrid expansion affecting the inter-assembly pitch size (Fig. 2a) and axial fuel rod expansion affecting its height (Fig. 2b). The radial diagrid expansion is modeled either using direct variation of the hexagonal SA pitch or application of the coordinate transformation method (Nikitin & Fridman, 2019a). It was found that both methods are equivalent when it comes to modeling uniform radial core expansions. However, since the latter method does not require modifications of the diffusion solver and has the potential to be extended to non-uniform expansions, it was selected as the standard method for DYN3D. The non-uniform axial fuel expansion is modeled based on the so called XS-mixing method (Nikitin & Fridman, 2018a).

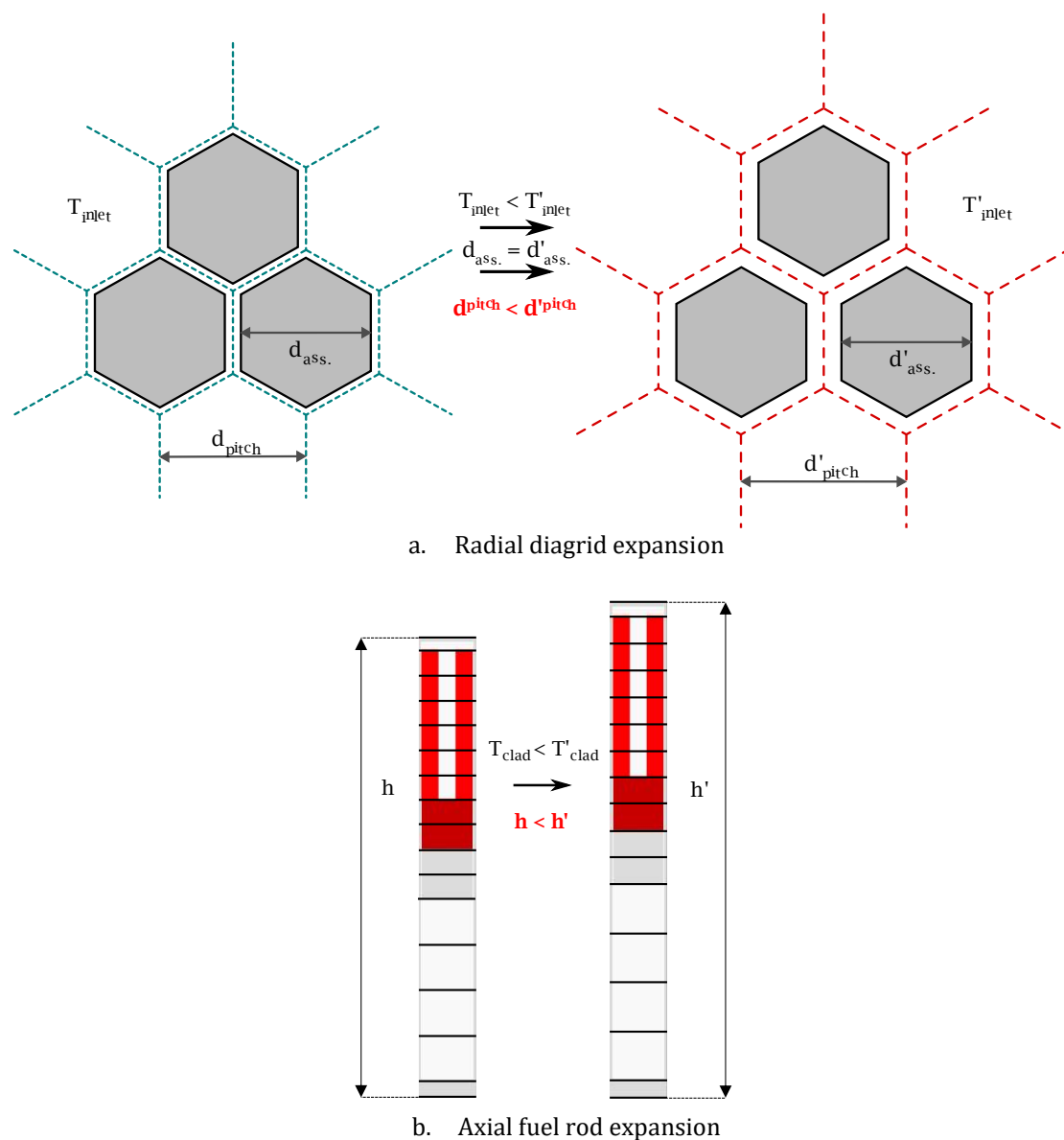


Fig. 2. Schematic overview of the thermal expansions requiring additional TM models in DYN3D

In order to cover the core level thermal expansion effects, the few-group XS parametrization scheme was also updated. Now, in addition to “standard” TH state variables such as fuel and coolant temperatures, the few-group XS are parametrized with respect to axial fuel rod expansion (ε_{rod}) and radial diagrid expansion ($\varepsilon_{\text{diag}}$) states. The expansion coefficient is calculated as shown in Eq. 1:

$$\varepsilon(T) = \frac{L(T)}{L(T_0)} = 1 + \alpha(T) \cdot (T - T_0) \quad (1)$$

where L is the linear dimension, α is the linear expansion coefficient corresponding to the temperature T , and T_0 is the reference temperature of the employed linear expansion correlation. The correlation can be arbitrary selected by a user prior to calculations. The final expansion-dependent few-group cross-section Σ is calculated from the library and the expansion coefficient by applying a linear interpolation (Eq. 2):

$$\Sigma = \Sigma_i + \frac{\varepsilon(T) - \varepsilon_i}{\varepsilon_{i+1} - \varepsilon_i} \cdot (\Sigma_{i+1} - \Sigma_i) \quad (2)$$

where $\varepsilon_i < \varepsilon < \varepsilon_{i+1}$ and $\Sigma = \Sigma(\varepsilon)$ are the pre-generated few-group XS in the library and i is an index of axial nodes.

The relevant local temperatures are provided by the TH module of DYN3D. In case of the radial core expansion, the driving temperature is the inlet sodium temperature (T_{inlet}). The axial expansion can rely on either closed gas-gap or open gas-gap hypothesis correspondingly driven by either clad or fuel temperatures. The thermal expansion of the assembly wrapper is assumed to be driven by the local sodium temperature.

2.2 Overview of the thermal expansions of OOC structures affecting CR position

In pool type SFRs, large and dimensional structures of the primary system such as reactor vessel, strongback, and CRDL can expand relatively to each other and by this affect the relative position of the CRs and the reactor core. A schematic overview of the expansions is presented in Fig. 3.

The CRDLs are fixed above the core and their thermal conditions are defined by the temperature of surrounding sodium in the hot pool, i.e. by the core outlet sodium temperature. When the latter increases, the CRDLs expand and push the CRs in the direction of the reactor core (Fig. 3a). Therefore, the CRDLs expansion leads to a negative reactivity insertion. The strongback, a large dimensional structure bearing the core, is located at the bottom of the reactor vessel. It hosts the diagrid plate with subassemblies inserted by their spikes. With increasing sodium temperature in the cold pool and, correspondingly, increasing core inlet sodium temperature, the strongback expands and lifts up the core towards the CRs (Fig. 3b).

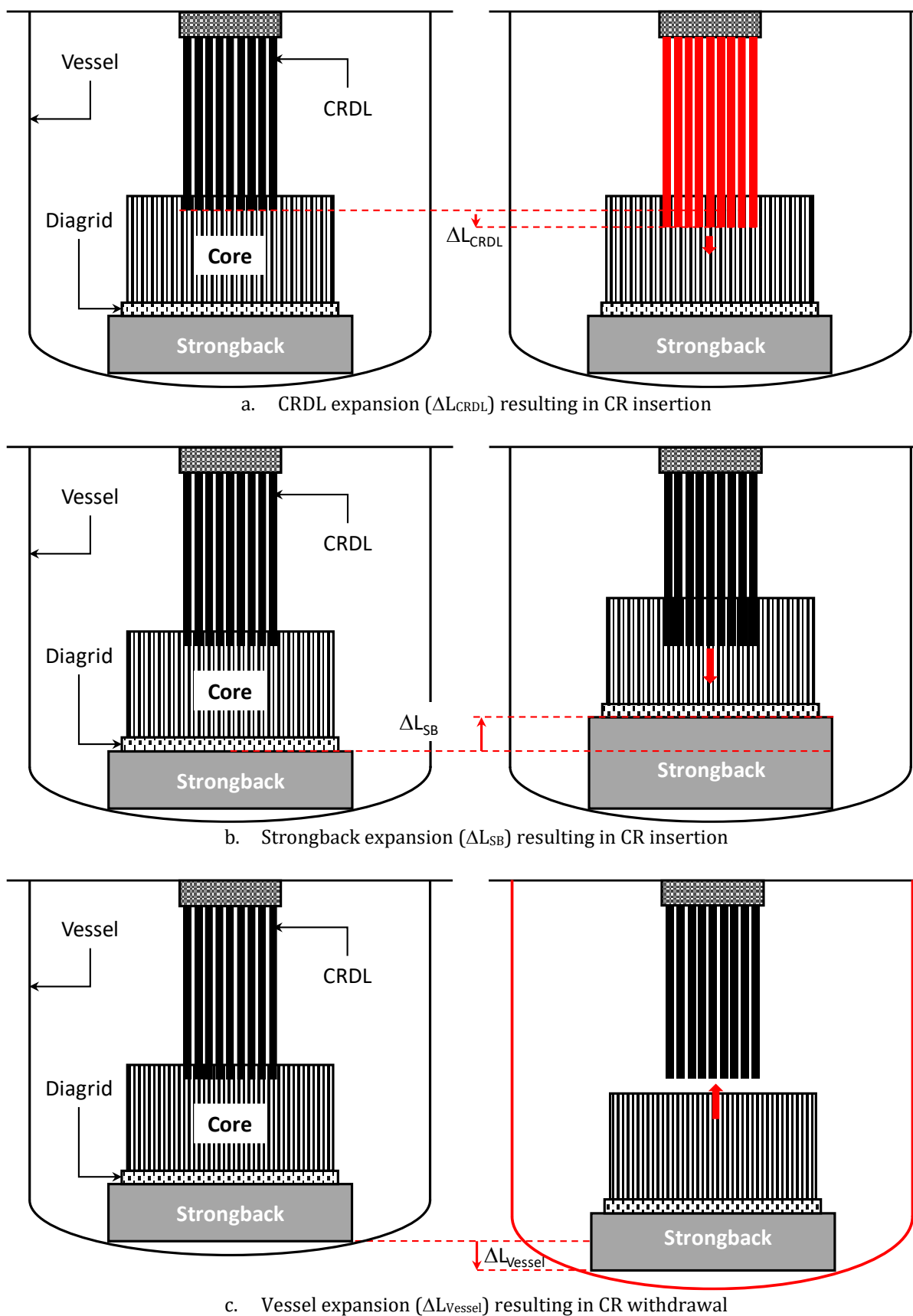


Fig. 3. Schematic overview of the thermal expansions of OOC structures affecting CR position.

Therefore, the strongback axial expansion introduces negative reactivity effect. The reactor vessel is typically free to expand downwards (Fig. 3c) as it is welded at its top to the slab structure bearing the whole reactor block. The vessel wall is cooled by sodium directed from the cold pool. It expands if the circumambient sodium temperature increases following the increase of the cold pool temperature. This expansion leads to withdrawing of the CRs from the reactor core, hence has a positive reactivity effect.

The overall reactivity effect is the outcome of the differential expansions of the CRDLs, strongback, and reactor vessel, which act on different time scales driven by sodium temperature variation at different locations of the primary system.

2.3 Adaptation of the existing DYN3D/ATHLET coupling for SFR analysis

In the LWR domain, the integration between DYN3D and ATHLET was realized via three alternative approaches, namely “internal”, “external”, and “parallel” couplings. In internal coupling, DYN3D acts as a 3D neutron kinetics solver, while ATHLET takes over both core and system TH by replacing the internal TH module of DYN3D. In external coupling, DYN3D simulates both core neutronics and TH, while ATHLET models the system TH only. The coupling between DYN3D and ATHLET is realized via the TH boundary conditions at the core inlet and outlet. The parallel coupling is a combination of internal and external methods. In this case, DYN3D and ATHLET run core TH calculations in parallel. ATHLET calculates the TH behavior of the reactor and provides the core TH boundary conditions to DYN3D. The latter performs core neutronics and TH calculations and transfers the core power distribution to ATHLET.

Among the three options, the internal coupling is considered as the most reliable approach mainly because it avoids potential inconsistencies between DYN3D and ATHLET TH models which may occur with the external and parallel methods. Due to this reason the existing internal coupling was selected as a starting point for extension of the DYN3D/ATHLET code system to SFR applications. Internal coupling option relies on an explicit coupling scheme and operator splitting technique. The neutron kinetics of DYN3D is called after the ATHLET step without any iteration between ATHLET and DYN3D.

The existing coupling allows to exchange the data relevant to LWR analysis. The data provided by DYN3D to ATHLET is the node-wise power distribution. The data transferred by ATHLET to DYN3D comprises node-wise distributions of TH properties such as fuel temperature (T_{fuel}), coolant temperature (T_{cool}) and density (ρ_{cool}), and boron concentration (C_b) as shown in Fig. 4a. DYN3D uses the provided TH distributions to update the node-wise few-group XSs and, consequently, to account for TH reactivity feedbacks.

In order to enable the modeling of the SFR relevant phenomena, the data exchange between DYN3D and ATHLET was updated as shown in Fig. 4b to include clad and diagrid temperatures.

In addition, ATHLET provides to DYN3D a new CR position (Z_{CR}) adjusted by expansion of the OOC structures. The dynamically adjusted Z_{CR} is calculated using the reference CR position (Z_0) and the relative shift in the CR position (ΔL_{CR}) (Eq. 3). ATHLET calculates ΔL_{CR} as an overall contribution from axial expansions of the CRDLs (ΔL_{CRDL}), strongback (ΔL_{SB}), and reactor vessel (ΔL_{Vessel}) using Eq. 4. It should be noted that all expansions are time-dependent and calculated relative to the reference steady-state conditions. The time-delays due to thermal inertia are also accounted for.

$$Z_{CR}(t) = Z_0(t) + \Delta L_{CR}(t) \quad (3)$$

$$\Delta L_{CR}(t) = \Delta L_{CRDL}(t) + \Delta L_{SB}(t) - \Delta L_{Vessel}(t) \quad (4)$$

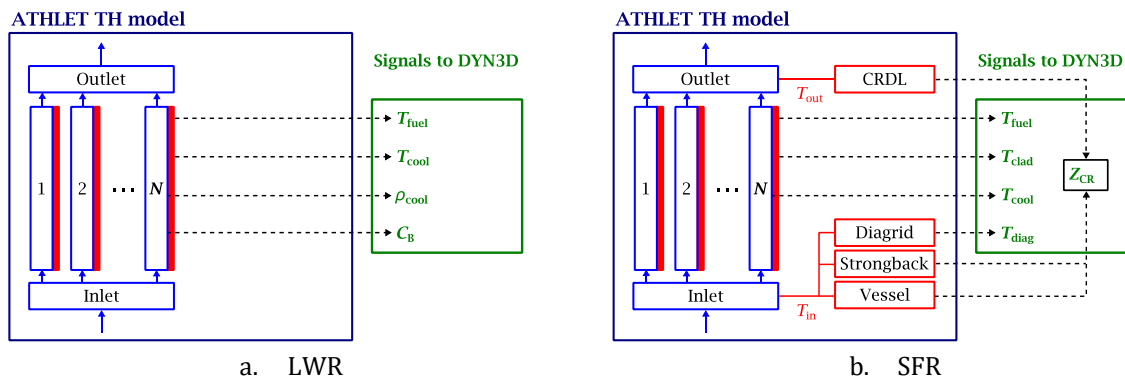


Fig. 4. ATHLET to DYN3D signals in the internal coupling scheme.

3. Verification and validation of the DYN3D/ATHLET code system

This section describes initial verification and validation (V&V) efforts related to the modified DYN3D/ATHLET code system. The V&V were carried out in two stages using the unprotected stage of the Phenix EOL natural convection experiment as a test case. First, the Phenix EOL test was modeled by DYN3D/ATHLET on the reactor core level only, without considering the thermal expansions of the OOC structures. The DYN3D/ATHLET results are verified against those obtained from the stand-alone DYN3D calculations. The purpose of this stage is to assess the consistency of the updated internal DYN3D/ATHLET coupling scheme. Second, the simulation of the Phenix EOL test was repeated by DYN3D/ATHLET, now including the modeling of the thermal expansions of the OOC structures. At this stage the DYN3D/ATHLET results are validated against the experimental data.

3.1 Description of the unprotected stage of the Phenix EOL natural circulation test

The Phenix EOL natural convection test (IAEA, 2013) was initialized with a manual dry out of the steam generators at reduced power output of 120 MWth. The unprotected stage of the transient lasted for 458 seconds until reactor SCRAM actuation. During this, the total primary mass flow rate remained constant, while the core inlet temperature has increased by around 40°C due to the loss of heat removal from the secondary circuit. The power evolution before SCRAM was defined by interplay of numerous reactivity feedback effects, such as the fuel Doppler, sodium density, the core axial and radial expansion, and the relative CR movement caused by expansions of the OOC structures. As a result, the power dropped to 50 MWth driven to large extent by the dominating negative reactivity feedback of the core radial expansion. On reactor core level, the following measurements were made available in (IAEA, 2013): average core inlet coolant temperature, region-wise averaged core outlet coolant temperatures, total power, and net reactivity.

The moderate change ($\sim 10^\circ\text{C}$) of the outlet coolant temperature has only a minor influence on the core inlet during the unprotected stage. Therefore, to a certain extent, the core TH behavior may be considered decoupled from the primary circuit, and can be modeled on core level by using the measured inlet temperature curve as time-dependent boundary condition (Fig. 5).

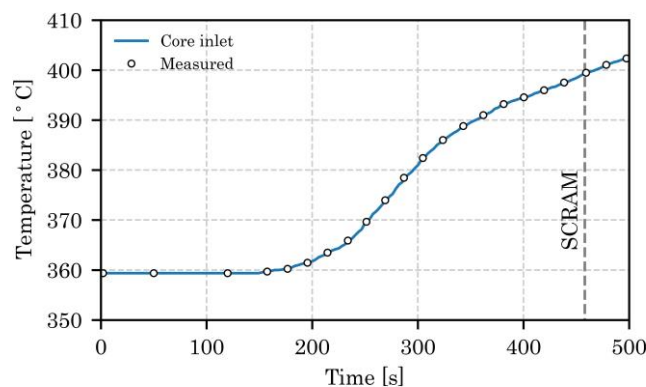


Fig. 5. Measured core inlet coolant temperature used as a TH boundary condition.

The reactor core itself consists of 54 inner and 56 outer MOX fuel assemblies surrounded, first, by 86 blanket assemblies and, secondly, by 252 reflector assemblies on the periphery (Fig. 6a). Furthermore, the core comprises 6 primary CRs, one secondary CR, and 14 reflector-type assemblies inside the core and blanket region as depicted in Fig. 6. The fuel assemblies contain 217 MOX fuel pins with stainless steel 316 as a structural material. The fuel rods are subdivided into six axial zones including lower reflector, lower blanket, fuel, sodium plenum, upper blanket and upper reflector periphery (Fig. 6b). The inner and outer fuels have different Pu content, which are rated at 22.4% and 27.4%, respectively. At room temperature, the core height is 264.95 cm, the fuel height is 85.0 cm and the assembly pitch size is 12.72 cm.

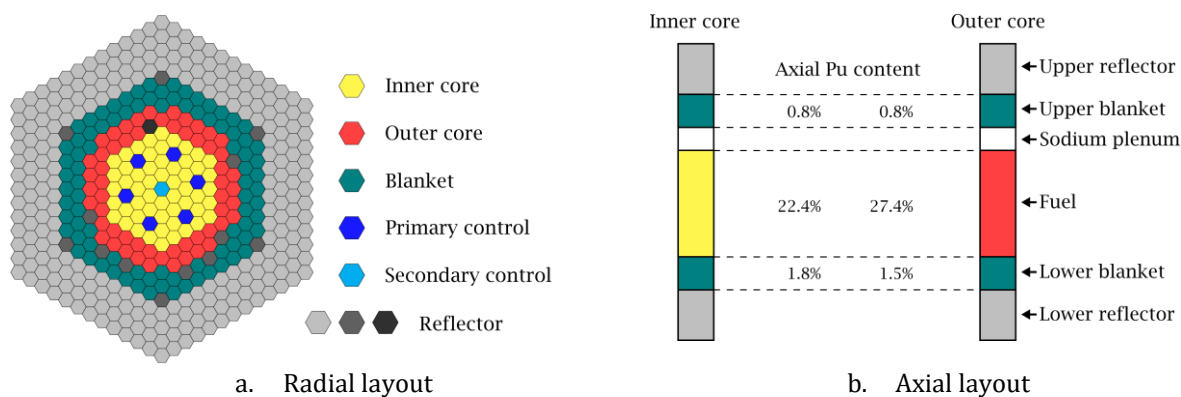


Fig. 6. Schematic overview of the Phenix EOL core.

3.2 *Neutronics and TH models (models and analysis methodology)*

3.2.1 *Generation of the few-group XS library*

The few-group XS library, required by DYN3D, was adopted from the previous studies on the Phenix EOL tests (Nikitin and Fridman, 2018a, 2018c). The few-group XSs were calculated with the Serpent MC code using a 24-energy-group structure (Fridman and Shwageraus, 2013) and detailed lattice level information on the core geometry and isotopic compositions. The relevant data was taken from the IAEA benchmark on the Phenix EOL control rod withdrawal tests (IAEA, 2014). The few-group XSs library was parametrized with respect to the fuel temperature, coolant temperature, axial fuel rod expansion and radial diagrid expansion. The span of the state parameters was selected to cover the full range of the reactor conditions relevant to the selected Phenix EOL test. The coolant density variation was implicitly accounted for in the coolant temperature variation. The axial fuel rod expansion was assumed to be driven by the clad temperature. A detailed description of the few-group XS generation process can be found elsewhere (Nikitin and Fridman, 2018a, 2018c).

3.2.2 *DYN3D neutronics/TH model of the Phenix EOL core*

As mentioned before, the unprotected stage of the Phenix EOL natural convection test was previously modeled with stand-alone DYN3D (Nikitin and Fridman, 2018c). The identical 3D Phenix core model was used in this study in order to make a consistent comparison between stand-alone DYN3D and the DYN3D/ATHLET code system. The model comprises all SAs presented in Fig. 6a including inner and outer fuel, blanket, reflector, CRs, and safety rods (SRs). In total, 469 full-size SAs are modeled. In axial direction, the SAs are subdivided in 38 axial layers. The identical radial and axial nodalization is used by both neutronics and TH solvers of DYN3D. This results in the 1:1 neutronics/TH mapping scheme where every SAs is represented by a separate TH channel. The inlet flow resistance coefficients of the assemblies are set to reproduce the mass flow rate distribution given by the test specification (IAEA, 2013). At the core inlet, a constant mass flow rate (\dot{m}_{in}) of 1254 kg/s and a time-dependent coolant temperature (T_{in}) shown in Fig. 5 are used as a boundary condition. Furthermore, it is assumed that the diagrid expansion in the Phenix reactor is directly driven by the average sodium inlet temperature without a delay, since the thermal inertia of the diagrid heat-structure is very limited (Chenu et al., 2012). The safety rods (SRs) are in fully withdrawn position, whereas the CRs are partially inserted to achieve a critical core state. To assure consistency between DYN3D and ATHLET, the heat transfer correlation used by ATHLET for bundle flow geometries (Mikityuk, 2009) was adopted by the internal TH module of DYN3D. The fixed value of fuel-cladding gap conductance was used during the whole simulation.

As recommended by the benchmark, the gap conductance values of 5000 W/(m²K) and 2500 W/(m²K) were used for the fissile and blanket fuels respectively.

3.2.3 ATHLET models of the Phenix EOL core

The TH model (Fig. 7a) of the Phenix core was created in ATHLET analogously to the internal TH model of DYN3D. One TH channel was assigned to each of the 196 fuel SAs, while other non-fuel SA types were represented by additional 4 individual SA type lump channels. In total, 200 TH channels are modelled ($N=200$ in Fig. 7). The axial discretization was kept identical to DYN3D. Each TH channel representing fuel SA includes a heat structure of the fuel rod bundle. The node-wise fuel (T_{fuel}), cladding (T_{clad}) and coolant (T_{cool}) temperatures are provided to DYN3D. Additionally, 0D plenums with perfect mixing assumption were added below and above the core for setting boundary conditions (T_{in} , \dot{m}_{in} and p_{out}). The diagrid temperature used for the modeling of the core radial expansion is linked to the core inlet temperature. The thermal inertia of the diagrid is neglected in the same way as it was modeled with stand-alone DYN3D.

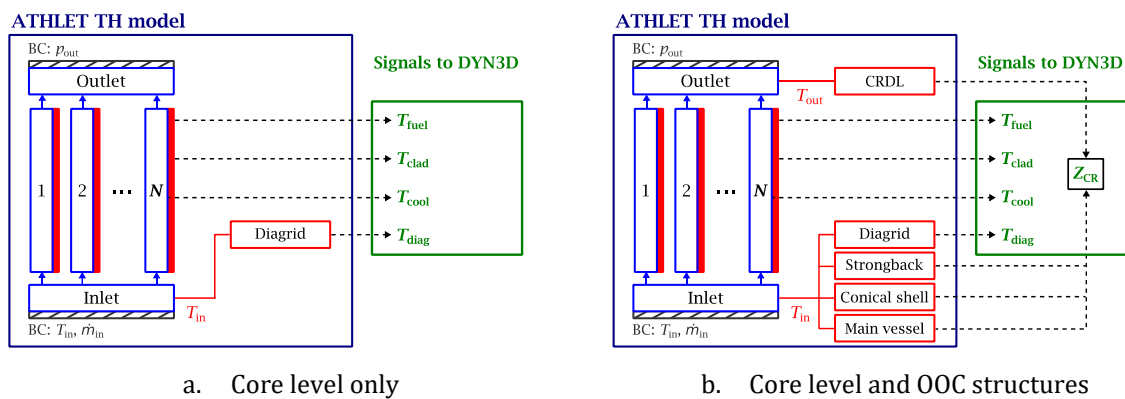


Fig. 7. TH ATHLET models with signals to DYN3D.

Later in the validation phase, this model is extended to reactor system level by adding different OOC heat structures connected to lower and upper plenums (see Fig. 7b). This enables the modeling of OOC thermal expansions by providing the modified CR positions (Z_{CR}) to DYN3D. For every structure, a simplified model was developed considering its location and surrounding sodium flow path, while realistic 3D sodium flow paths in the primary system were not modeled. The overall approach is similar to the one introduced in (Ponomarev et al., 2022a) for transient analysis of the Superphenix reactor. It aims to account for thermal expansions of primary system components using a relatively simple definition for individual contributors and avoiding TH modeling of the whole primary system.

The CRDL effect was modelled in a simplified way as the flow conditions around their whole length and the THs of the above core area is complicated and highly uncertain. The upper part of CRDL that resides within the control plug (Fig. 8) was excluded from the consideration, as its

temperature and length variations were considered to be negligible and would not influence the transient. This is attributed to the fact that the change of core outlet temperature is mild ($\sim 10^\circ\text{C}$), while only $\sim 1.5\%$ of the total mass flow passes through the control plug. The lower part of CRDL is modelled as a solid cylindrical structure with length of 1.418 m and outer diameter of 2 cm (IAEA, 2013). Its outer surface temperature is defined by the average outlet temperature of inner core SAs and its elongation is calculated as driven by the average structure temperature.

In contrast to the simplified description of OOC structures expansions given above, the peculiarity of the Phenix primary system design required a more specific approach to the modelling of the core support structures. The “in-compression” strongback structure lays on the “in-traction” conical shell which is in turn welded to the main vessel (Fig. 8). Thus, the modelling assumption considers three main components of the core support responsible for the relative core position change with respect to CR: 1) upper part of the main vessel from the reactor slab till the point of welding of the conical shell which expands downwards; 2) the conical shell expanding downwards; and 3) the strongback structure (together with diagrid) expanding upwards. With given assumption, the formulation (4) is transformed in the following one:

$$\Delta L_{CR}(t) = \Delta L_{CRDL}(t) + \Delta L_{SB}(t) - \Delta L_{MV}(t) - \Delta L_{CS}(t) \quad (5)$$

where ΔL_{MV} and ΔL_{CS} are the contributions of the main vessel and conical shell expansions, respectively.

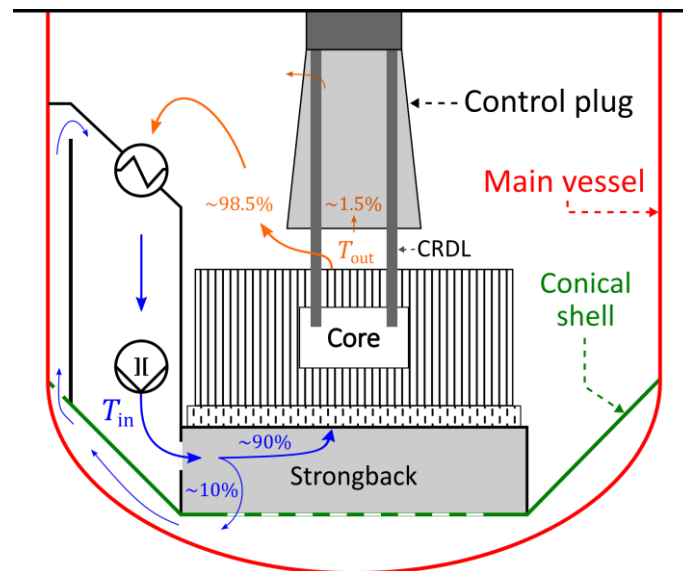


Fig. 8. Scheme of the primary coolant flow path. *Cold pool*: path around strongback, conical shell and main vessel. *Hot pool*: path around CRDL and control plug.

In ATHLET model the heat structures of strongback, conical shell and main vessel are linked to the cold plenum, while specific model features are also introduced in order to account for individual time delay in structure temperature change with respect to change of the cold pool temperature. These individual time delays were selected on the basis of engineering judgement of the specific flow path and corresponding temperature variation of the circumambient sodium for every component of the core support (Fig. 8).

The strongback is modelled as a cylindrical steel structure with the equivalent height of 1.5 m and wall thickness of 2 cm. Its outer surface temperature follows the core inlet temperature (T_{in}), while a specific time delay of 20 s with respect to the core inlet temperature variation is considered on its inner surface, thus accounting for sodium mixing inside this dimensional structure. The conical structure is modelled in a similar manner, as a structure with thickness of 2 cm and effective height of 2.5 m. It is also in contact with the cold pool sodium on one surface, while the other (lower) surface meets the cold pool sodium with delay of 60 s. This delay is caused by sodium flow path through the strongback direction vessel bottom, as about ~10% of nominal primary flow rate is directed to the vessel cooling. The temperature change will occur even later for the main vessel wall, as the sodium volumes below the strongback and conical shell are relatively large and the sodium path is much longer. The main vessel structure has thickness of 3 cm and effective length of 5 m, while the time delay of 160 s with respect to T_{in} was selected as an appropriate value.

It is acknowledged that the here defined system level TH model (Fig. 7b) is limited to the immediate surroundings of the core and does not include all flow paths and primary TH components (e.g., pumps, heat exchangers) of the primary circuit. However, the modelling of the thermal expansion of OOC structures with the attached TH volumes and heat structures extends the analysis beyond the core level, i.e., to the system level.

3.3 Verification of DYN3D/ATHLET vs. DYN3D at the reactor core level

At this stage, stand-alone DYN3D and the coupled DYN3D/ATHLET code system were applied to analyze the Phenix EOL test on the reactor core level only (Fig. 7a). The main goal of the verification phase is to test the consistency of the updated DYN3D/ATHLET coupling interface with the emphasis on the correct data exchange between the codes during transient calculation. With correct setting of ATHLET signals and with the identical neutronic model, the stand-alone and coupled approaches are expected to produce very close core-level solutions.

Fig. 9 presents the temporal evolution of the core power, the net reactivity and its components including Doppler, coolant temperature, axial expansion and diagrid expansion for two solutions. An appropriate agreement between the two approaches was clearly achieved indicating an accurate data exchange in the coupled case and general equivalency of two TH

models. The maximum difference in power is limited to 3 MW and maximum discrepancy in reactivity does not exceed 2 pcm. It was found that the transition from the core to system level analysis resulted in about 15% run time overhead.

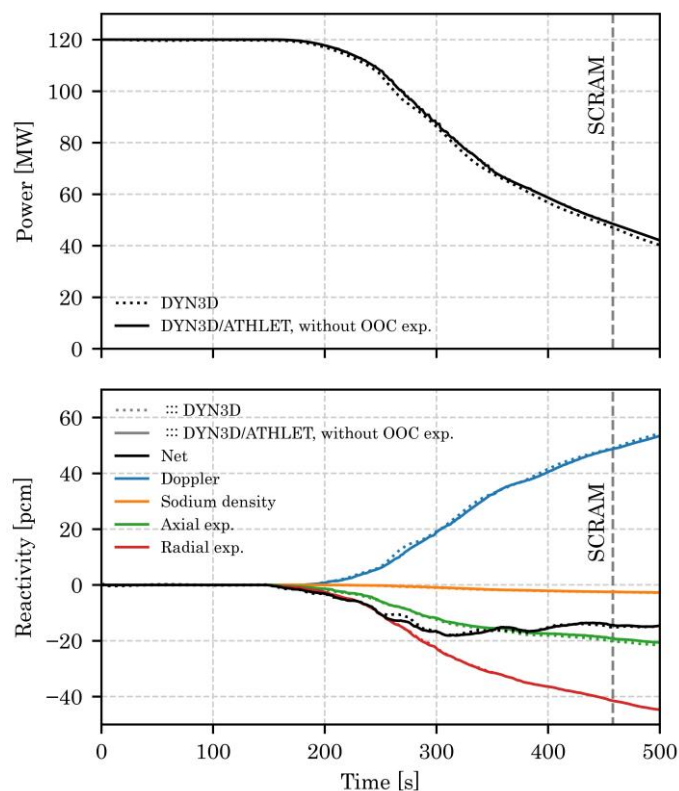


Fig. 9. DYN3D/ATHLET vs. DYN3D: transient power evolution and reactivity decomposition during the unprotected stage of the Phenix EOL natural circulation test.

It should be noted that in the previous study (Nikitin and Fridman, 2018c), the axial expansion component was noticeably weaker. This can be attributed to the different CR positions used. In the current analysis, an additional assumption was introduced that the CRs are partially inserted to critical position while in the former study the CRs were fully withdrawn. The axial expansion of the fuel changes the relative position of CRs in respect to the core and causes an indirect insertion of the absorbers. This secondary effect depends on the differential control rod worth, i.e. the slope of the so-called S-curve. The partially inserted CRs are in position of a stronger differential reactivity worth, which amplifies the axial expansion effect. On the other hand, the component of the diagram expansion was stronger in the preceding study due to inconsistent implementation of routines responsible for dynamic adjustment of the hexagonal pitch. The pitch size remained constant during the transient after it was expanded at steady state calculation. Therefore, the XS of the expanded state were fed into nodes with unchanged (and smaller than intended) pitch, resulting in an effective loss of fissile content, which added negative reactivity.

This was corrected later, and since (E. Nikitin and Fridman, 2019a) the reactivity effect of diagrid expansion is estimated weaker, exactly as presented in this paper. Although, corrections were made to both axial and radial expansion modelling, the elicited change in reactivity components resulted in nearly equal compensation and thus in an inconspicuous difference in net reactivity and transient power when comparing this study with the reference (Nikitin and Fridman, 2018c).

3.4 Validation of DYN3D/ATHLET vs. Phenix EOL natural circulation test at the reactor system level

At this stage, the DYN3D/ATHLET code system was validated against the measured data obtained during the unprotected stage of Phenix EOL natural convection test. Both, the core level (Fig. 7a) and the system level (Fig. 7b) DYN3D/ATHLET models were considered for analysis. The primary difference between the models is that the former neglects the OOC expansion effects while the latter considers them.

For both calculations, the experimental power (Fig. 10 upper panel) is predicted within the measurement uncertainty throughout the whole transient. However, the system level model starts overpredicting the power after about 320 sec while the difference to the measurement reaches up to 5 MW just before SCRAM. At the same time, the system level model improves the agreement in the net reactivity (Fig. 10 lower panel) and the outlet temperature of the inner core (Fig. 11).

With the core level DYN3D/ATHLET calculations, the net reactivity (Fig. 10 lower panel) is in a satisfactory agreement with the measured data until about 320 sec, while after it tends to deviate noticeably. The use of the expansion models for the OOC structures, especially those related to the core support structures, leads to a better prediction of the reactivity behavior and reduces the maximum discrepancy in the net reactivity from ~ 7 pcm to ~ 1 pcm at the time point of SCRAM (Fig. 10 lower panel). Similar conclusions were made elsewhere (Chenu et al., 2012).

Likewise, the inner core outlet temperature (Fig. 11) was also predicted well with both core and system level calculations. However, at the tail, the discrepancy with the measured data was reduced with the system level model, as the maximum temperature difference decreased from 4°C to below 1°C . Furthermore, the flattening of the temperature curve observed in experiment was reproduced with DYN3D/ATHLET when the thermal expansion of the OOC structures is modeled.

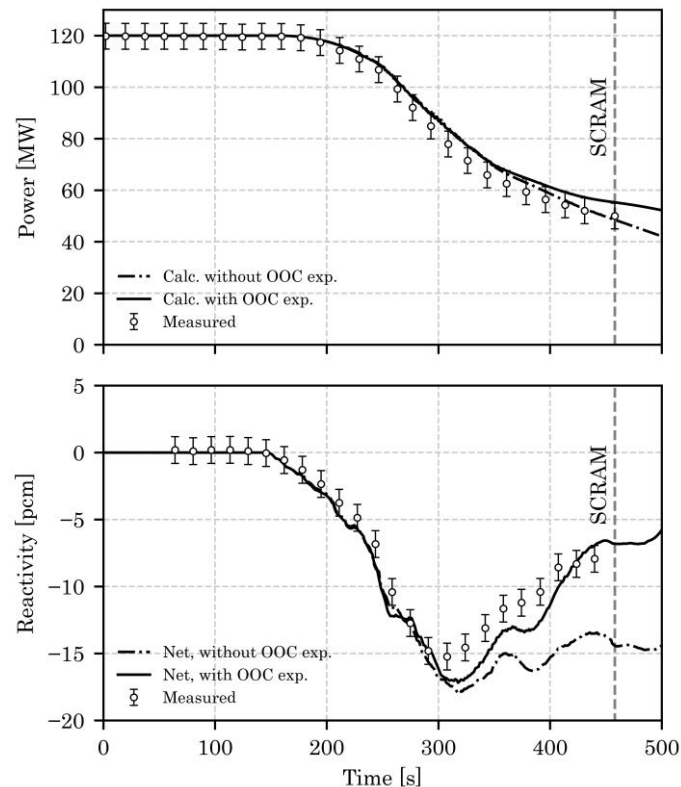


Fig. 10. DYN3D/ATHLET: Temporal evolution of the power and reactivity during the unprotected stage of the Phenix EOL natural circulation test.

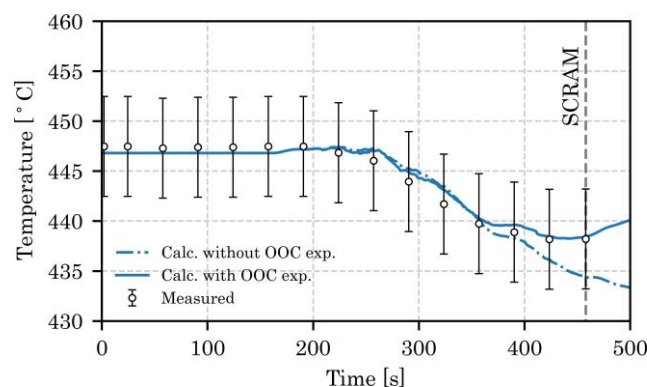


Fig. 11. DYN3D/ATHLET: Outlet sodium temperature in the inner core during the unprotected stage of the Phenix EOL natural circulation test.

The importance of the OOC expansions modeling is explained with the help of Fig. 12 presenting 1) temporal variation in the temperatures of the OOC structures; 2) corresponding variation in the CR position; and 3) the resulting contribution to the reactivity along with other reactivity components. As shown in Fig. 12 (top) the strongback, conical shell, and main vessel are heated up with a certain delay with respect to the variation in the core inlet temperature. The

variation in the CRDL temperature, also given in Fig. 12, nearly follows the core outlet temperature. Axial expansions of these four components result in individual contributions to the shift of the CR position as presented in Fig. 12 (middle). Initially, the strongback and conical shell expansions mostly compensate each other, but after about 350 s the net CR shift becomes noticeable due to the expansion of the main vessel. This delayed effect inserts up to 18 pcm of positive reactivity (Fig. 12, bottom). This is not negligible contribution as compared to the major positive reactivity component (Doppler) introducing up to 40 pcm and major negative reactivity component (radial diagrid expansion) introducing up to -40 pcm.

As demonstrated in Fig. 12, the CRDL expansion effect was found to be minor. Within the applied model assumptions, the main reasons for the small CRDL effect are 1) the design of the control plug that hides a significant length of CRDL from the dominant fraction of outlet mass flow, and 2) a moderate variation of the core outlet temperature affecting the lower part of the CRDL (Fig. 11). While the CRDL effect in this Phenix test case was minor, it may be of much higher importance in other SFR designs such as Superphenix or ESFR, where the dominant flow rate passes through the above core structure hosting the CRDLs.

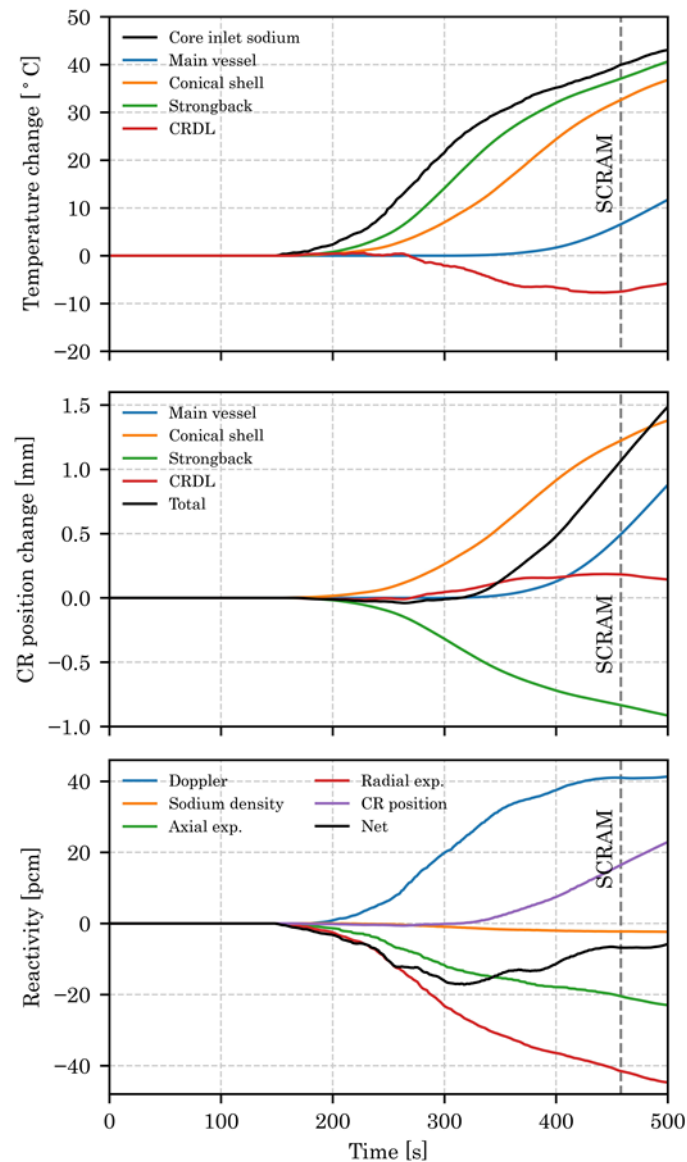


Fig. 12. Unprotected stage of the Phenix EOL natural circulation test modeled with DYN3D/ATHLET: (top) variation in the temperatures of the coolant and OOC structures; (middle) corresponding components of the CR position change; and (bottom) resulting contribution to the reactivity along with other reactivity components.

4. Summary and conclusions

The existing LWR-oriented DYN3D/ATHLET coupling was adapted and extended to perform coupled 3D neutron kinetics/TH analysis of SFRs at the reactor system level. The coupling techniques used to integrate DYN3D with ATHLET were described in the paper. The modifications required to enable the modeling of SFR specific phenomena were summarized. The approach to the modeling of thermal expansions of the out-of-core structures affecting the position CRs such as reactor vessel, strongback, and CRDL was presented.

The paper also includes the summary of the initial verification and validation efforts related to the modified DYN3D/ATHLET code system. The unprotected stage of the Phenix EOL natural convection experiment was used as a test case. The verification and validation were carried out in two stages. First, the consistency of the updated DYN3D/ATHLET coupling was demonstrated by analyzing the Phenix EOL on the *reactor core level* and verifying the results against the stand-alone DYN3D calculations.

Second, the initial validation of the DYN3D/ATHLET code system was carried out by simulating the Phenix EOL test on the *reactor system level* and comparing the DYN3D/ATHLET results to the experimental data. The importance of the out-of-core expansion modeling was discussed and demonstrated.

The near future research activities will be focused on the further validation of the DYN3D/ATHLET code system. The available experimental SFR data will be used for this purpose including Superphenix start-up test (Ponomarev et al., 2022a) and the benchmark of the Fast Flux Test Facility (FFTF) loss of flow without scram test (IAEA, 2019).

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