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New Multi-group Transport Neutronics (PHISICS) Capabilities for RELAP5-3D and its Application to Phase I of the OECD/NEA MHTGR-350 MW Benchmark

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Abstract – *PHISICS is a neutronics code system currently under development at the Idaho National Laboratory (INL). Its goal is to provide state of the art simulation capability to reactor designers. The different modules for PHISICS currently under development are a nodal and semi-structured transport core solver (INSTANT), a depletion module (MRTAU) and a cross section interpolation (MIXER) module. The INSTANT module is the most developed of the mentioned above. Basic functionalities are ready to use, but the code is still in continuous development to extend its capabilities.*
This paper reports on the effort of coupling the nodal kinetics code package PHISICS (INSTANT/MRTAU/MIXER) to the thermal hydraulics system code RELAP5-3D, to enable full core and system modeling. This will enable the possibility to model coupled (thermal-hydraulics and neutronics) problems with more options for 3D neutron kinetics, compared to the existing diffusion theory neutron kinetics module in RELAP5-3D (NESTLE).
In the second part of the paper, an overview of the OECD/NEA MHTGR-350 MW benchmark is given. This benchmark has been approved by the OECD, and is based on the General Atomics 350 MW Modular High Temperature Gas Reactor (MHTGR) design. The benchmark includes coupled neutronics thermal hydraulics exercises that require more capabilities than RELAP5-3D with NESTLE offers. Therefore, the MHTGR benchmark makes extensive use of the new PHISICS/RELAP5-3D coupling capabilities. The paper presents the preliminary results of the three steady state exercises specified in Phase I of the benchmark using PHISICS/RELAP5-3D.

I. INTRODUCTION

The simulation of complex transients for advanced reactors such as Generation IV systems poses a challenge to existing code systems like RELAP5-3D. In particular, to model the General Atomics prismatic Modular High Temperature Gas Reactor (MHTGR) design [1], more neutronic capabilities are desirable compared to the available NESTLE package in RELAP5-3D.

The RELAP5-3D code was developed for best-estimate transient simulation of light water reactors [2]. The code is able to model coupled behavior of the reactor core and the thermal-hydraulics of the power plant. Applications of the code include simulations of transients such as loss of coolant, anticipated transients without scram, and operational transients such as loss of feed water, etc. The multi-dimensional neutron kinetics model in RELAP5-3D is based on the NESTLE [3] code, which solves the two or four group neutron diffusion equations in either Cartesian or hexagonal geometry using the nodal expansion method.

A diffusion solution of the flux in 4 energy groups may not be sufficient to get an accurate representation of the power distribution for the MHTGR. In addition, linear cross section feedbacks on thermal hydraulic state parameters (such as fuel/moderator temperature) as supported by NESTLE/RELAP5-3D are not detailed enough to capture the complex MTHGR cross section behavior.

PHISICS (Parallel and Highly Innovative Simulation for INL Code System) is a neutronics code system currently under development at INL [4]. The different modules for PHISICS are a nodal and semi-structured spherical harmonics based transport core solver (INSTANT) for steady state and time dependent problems, a depletion module (MRTAU) and a cross section mixer-interpolator (MIXER) module. This package provides the functionality to cope with the neutronic challenges of the MHTGR design on core simulation level.

The Very High Temperature Reactor (VHTR) Methods Development group at the Idaho National Laboratory (INL) has recently focused on improving modeling capability of prismatic VHTR designs, as part of the larger New Generation Nuclear Project (NGNP). One effort of this project is to couple the neutronic code package PHISICS to RELAP5-3D.

The verification and validation of new reactor analysis tools is a crucial element in the life cycle of software development and assessment. The validation data from current or past prismatic VHTR experimental facilities or reactors are however severely limited. Therefore, in cooperation with General Atomics (GA), a code-to-code benchmark specification based on the MHTGR 350 MW design was recently developed [5]. The new coupled code system PHISICS/RELAP5-3D will be part of the ongoing MHTGR benchmark effort.

In addition to a discussion of the PHISICS/RELAP5-3D coupling and an introduction to the MHTGR benchmark, first results of the Phase I of the MHTGR benchmark computed with PHISICS/RELAP5-3D are presented in this paper.

II. THE PHISICS CODE PACKAGE

As mentioned in the introduction, PHISICS is a neutronic code system currently under development at INL. Its goal is to provide state of the art core simulation capability to reactor designers. It follows a modular approach to simplify development and long term maintenance of the code. Each different module of PHISICS contains a kernel (module) that solves a basic problem. A local driver is assigned to each kernel which is able to run it in standalone mode. For example, the INSTANT kernel driver is able to read data from an input file and run a standalone INSTANT calculation. Communication between the kernels is managed by the use of global data types that hold global information (cross section data, mesh, fluxes, etc.) that are needed by more than one kernel to perform complex calculations involving different kernels. Global drivers solving a complex problem calling different kernels can be developed easily with this flexible software structure.

Table 1 shows a comparison of the NESTLE/RELAP5-3D and PHISICS/RELAP5-3D capabilities so far. The PHISICS code is still in development to extend its capabilities.

Table 1: NESTLE/RELAP5-3D and PHISICS/RELAP5-3D capabilities

Feature	NESTLE/ RELAP5-3D	PHISICS/ RELAP5-3D
Energy groups	2 or 4	Not bounded
Diffusion	Yes	Yes
Transport	No	Yes
Triangular Mesh	No	Yes
Unstructured Mesh	No	Yes
Adjoint	No	Yes
Depletion	No	Yes
Multi-Dim Cross Section Tables	No	Yes
Speed (single proc.)	Fast	Slow
Multiprocessor	No	Yes
Discontinuity Factors	Yes	Future
Cylindrical Geometry	No	Future
Perturbation Theory	No	Future
Localized refinement	No	Future

The following sections give a short description of the different modules of PHISICS currently under development, namely:

- INSTANT: nodal and semi-structured spherical harmonics based transport core solver (steady state and transient)
- MRTAU: depletion module
- MIXER: cross section mixer-interpolator module.

II.A INSTANT

The transport core solver INSTANT [6] (Intelligent Nodal and Semi-structured Treatment for Advanced Neutron Transport) is the most developed kernel of the PHISICS framework. INSTANT is parallelized and is designed to take full advantage of medium to large clusters (10 to 1000 processors). INSTANT is based on the second order formulation of the transport equation discretized in angle by spherical harmonics while in space it uses orthonormal polynomials of an arbitrary order [7]. Its key features are:

- 2D/3D Cartesian geometry
- 2D triangular, Z extruded
- 2D hexagonal, Z extruded
- Unlimited number of energy groups
- Unlimited number of up-scattering groups
- Up to P33 anisotropy
- Reflective, vacuum and periodic boundary conditions
- Computation of fundamental mode and source problems: forward and adjoint
- Chebyshev acceleration for power iterations
- Diffusion partitioning for inner iterations

In order to be able to solve transient problems, a time dependent scheme has recently been implemented as a new module for the PHISICS suite. The chosen scheme is based on a second order backward Euler scheme with explicit delayed neutron treatment [8, 9].

II.B MRTAU

MRTAU (Multi-Reactor Transmutation Analysis Utility) is a generic depletion/decay/burn-up code developed at INL [10]. The code tracks the time evolution of the isotopic concentration of a given material accounting for nuclear reaction happening in presence of neutron flux and also due to natural decay (Bateman equation). Moreover the code can provide, as additional output, information regarding integral quantities associated with different nuclear reactions like helium production and energy released (pseudo isotopes are used to simulate decay heat). The calculation flow could be controlled in such a way that in-core and out-core periods could be alternated freely. The main features of MRTAU are:

- Use of Taylor series expansion based algorithm at arbitrary order and CRAM methodology [11] for computation of the exponential matrix
- Criticality search option, i.e. the isotopic densities are changed in a material to preserve core criticality. Typically, the boron concentration is changed in a region to simulate control rod movement
- Multi transmutation and partitioning loops
- Possibility for the user to deplete only the actinides or actinides and fission products
- Power history specification
- Separation efficiency specification for each isotope

II.C MIXER

A MIXER module is also part of the PHISICS suite. This module does all the cross section handling for the different kernels. The MIXER can handle macroscopic, microscopic and “mixed” cross sections.

A macroscopic cross section library contains macroscopic cross sections for each type of material used in the calculation (fuel, reflector, etc.) tabulated for the state parameters (temperature, burn-up, control rod position, etc.). The mixer just interpolates these cross sections at the requested state parameters. No limits in tabulation dimensions or neutron energy groups exist.

A microscopic or “mixed” cross section library contains the tabulated cross sections for each isotope considered in the calculation. The mixer reads a description containing a list of isotopes and corresponding densities for each material. Microscopic cross sections are interpolated at the requested state parameters and macroscopic cross sections for each material are generated with the corresponding densities. With this capability, “mixed” macroscopic and microscopic cross sections are also possible. For example, it is possible to provide macroscopic absorption cross sections without xenon for a material and the microscopic xenon absorption cross section together with a xenon density. The mixer will calculate the xenon contribution for the absorption and add it to the macroscopic cross section.

Micro, macro or “mixed” cross section libraries can be specified in different ways:

- A simple XML structure is available if cross sections are available in text format from any source.
- The MIXER also reads the AMPX and ISOTXS library formats if cross section libraries are prepared with SCALE, ERANOS [12] or MC2 [13].

More library types are planned to be supported in the future.

III. THE COUPLING OF PHISICS TO RELAP5-3D

There are two considerations by coupling the PHISICS suite to RELAP5-3D. First, on the RELAP5-3D side a low user impact is strived for, i.e. it should be possible to run existing RELAP5-3D input decks with INSTANT instead of NESTLE. Second, on the PHISICS side, it is desirable to have lean software interdependency, for further maintenance of the coupling. It was decided to couple the different modules of PHISICS directly to RELAP5-3D, i.e. PHISICS is integrated in RELAP5-3D as a set of subroutines. This gives the user access to the full capability of PHISICS from within RELAP5-3D. The PHISICS part of coupled calculations can be parallelized on multiple processors.

The calculation is always driven by RELAP5-3D. The RELAP5-3D input reader decides if parts of PHISICS are needed and calls the PHISICS/RELAP5-3D driver accordingly. The driver collects the available input data from RELAP5-3D (geometry, calculation options) and adds, if needed, data from special PHISICS input files to complete the needed information for the required calculation. Once all the inputs are collected, the PHISICS/RELAP5-3D driver calls the required modules like INSTANT, MRTAU or the MIXER and feeds back the results (power distribution) to RELAP5-3D for the next iteration. Fig. 1 shows the general input data flows between the two packages.

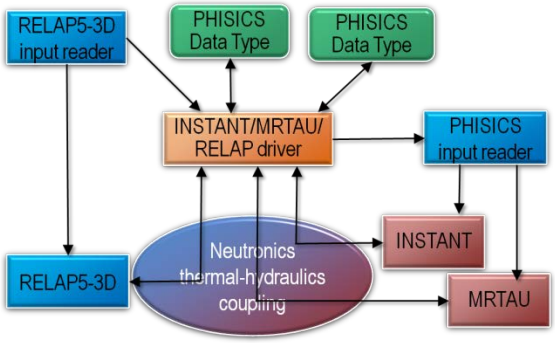

Fig 1: PHISICS/RELAP5-3D coupling structure

This “direct” coupling allows the user to run existing RELAP5-3D input decks with INSTANT as the core solver (this option is made accessible from within RELAP5-3D through a new keyword). The coupling is compatible with the existing RELAP5-3D cross section and feedback options. Existing cross section inputs and mappings from kinetic nodes to thermal hydraulic zones can be used with the INSTANT option. The RELAP5-3D control rod model can also be used. In addition, the coupling supports a new cross section option which lifts the RELAP5-3D limitation of four energy groups. The number of neutron energy groups is only limited by the available computer memory. Multi-group cross sections for this new option support an unlimited number of tabulation dimensions (fuel temperature, moderator temperature, control rod position, xenon density, etc.) and an unlimited number of tabulation points per dimension. This new cross section option is compatible with existing mappings from kinetic nodes to thermal hydraulic zones in RELAP5-3D. In addition, the new cross section option is also compatible with the RELAP5-3D control rod model.

The depletion code MRTAU is also coupled to RELAP5-3D as part of the PHISICS suite. It can be used to perform core depletion calculations with coupled thermal hydraulic feedbacks. In addition, MRTAU is able to burn the core to a desired depletion level, or to perform cooling (decay), before a transient is initiated. MRTAU can also be used for decay heat calculation and poison tracking during transients. The possible calculation paths resulting by combining INSTANT, MRTAU and RELAP5-3D are manifold. The calculation paths utilized so far in a variety of calculations are presented in detail in [8]. The next section focuses on a summary of the calculation path used for Phase I of the OECD/NEA MHTGR-350 MW benchmark.

The calculation path can be split into two main classes, namely the “depletion time evolution” and the “time dependent” calculation path.

III.A Depletion time evolution calculation

The “depletion time evolution” scheme is used to compute core depletion with the correct temperature field in the core. The user can choose at which time pints during the depletion he wants to update the temperature field using RELAP5-3D. Fig 2 shows the calculation path for the “depletion time evolution”. First (shown on the left in the figure), the MIXER evaluates the microscopic cross sections at the initial state parameter conditions (temperatures, densities, control rod positions, etc) from RELAP5-3D. It then creates the macroscopic cross sections for each material with the initial isotopic densities from MRTAU. INSTANT calculates the power distribution for this interpolated macroscopic cross section set and sends it to RELAP5-3D, where the corresponding temperature field for this power distribution is calculated (one iteration in steady state mode). The MIXER then re-evaluates the cross sections for the new state parameters keeping the isotopic densities constant. INSTANT re-computes the power distribution and sends it to RELAP5-3D.

This loop is iterated until convergence for the temperature field is reached. The calculation then goes into the depletion loop (shown on the right in the figure). Here, the MIXER keeps the thermal hydraulic state parameters constant, but updates the isotopic densities from the depletion calculation. The evaluated macroscopic cross sections for each material in the core are sent to INSTANT which computes the flux distribution and sends it to MRTAU, where the core is depleted for a time step (Δt) specified by the user. This loop is repeated until a temperature field update is requested by the user ($t=T_n$). The depletion loop can also adjust control rods or boron concentration to maintain criticality during the depletion (not shown in the figure since this option was not used in the MHTGR benchmark analysis).

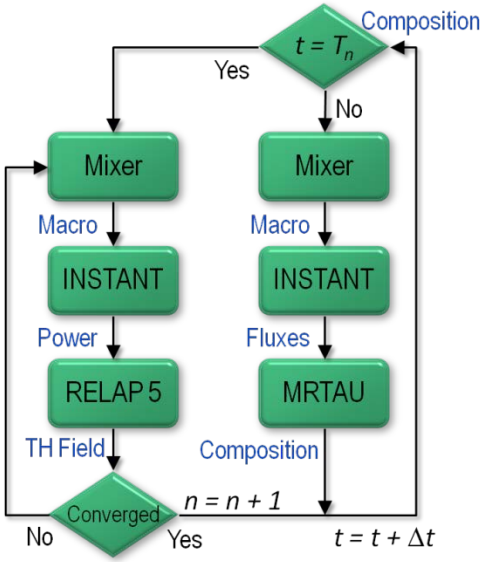

Fig 2: Depletion time evolution scheme

This "depletion time evolution" scheme is used in the MHTGR benchmark analysis to find the steady state temperature distribution in the core with xenon at its equilibrium value (see Phase I Exercise 3, Section V.C).

III.B Time dependent calculation

The "time dependent" calculation scheme with MRTAU is used to track isotopic densities during a coupled thermal hydraulic transient (i.e. RELAP-3D in transient mode). This scheme is utilized to track poison densities (xenon, samarium, etc.) and to compute the decay heat during a coupled transient. It is worth mentioning that MRTAU needs to track enough isotopes contributing to the decay heat generation to get an accurate estimate of the core decay heat.

Fig. 3 shows the calculation scheme for the "time dependent" mode. In this mode, MRATU depletes the core for one time step given by RELAP5-3D. The new isotopic composition and burn-up level are then sent to the MIXER which interpolates the microscopic cross sections and generates the macroscopic cross sections keeping the thermal hydraulic state parameters constant (as for the "depletion time evolution" mode). The time driver then evaluates the delayed neutron concentration and corresponding delayed neutron source. In addition, the time driver evaluates the "time source" and adds the "time absorption" to the cross sections (as explained in [8]). These new sources and cross sections are then sent to INSTANT which computes the new core power and power distribution for the current time step. During the next time step RELAP5-3D calculates the new temperature distribution. The MIXER finally updates the cross sections for the new thermal hydraulic state variables and sends it to MRTAU for the next depletion.

In this mode, control rod movements during the transient can also be introduced by RELAP5-3D, if required.

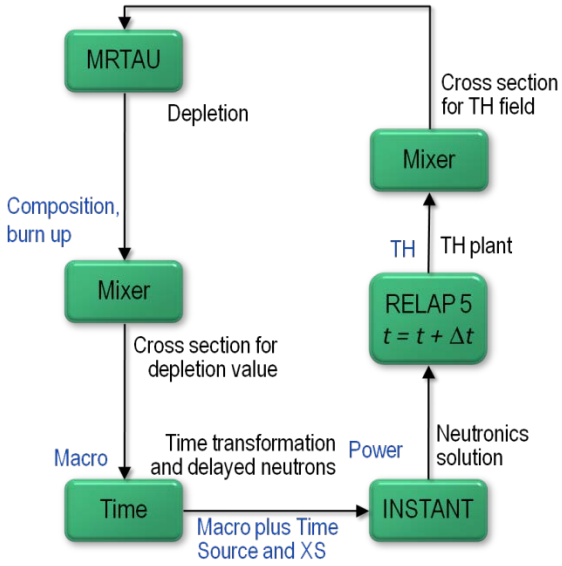

Fig 3: Time dependent calculation scheme

IV. THE OECD/NEA MHTGR-350 MW BENCHMARK

As already explained in the introduction of the paper, the VHTR Methods Development group at INL has recently focused on improving modeling capability of prismatic VHTR designs. As part of this effort, a benchmark specification [5] based on the MHTGR 350 MW design was developed in cooperation with General Atomics to compare different codes and methods, since validation data from current or past prismatic VHTR experimental facilities or reactors are severely limited.

The benchmark was launched on March 1, 2012 for international participation after formal approval was received from the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD)

The scope of the benchmark is to establish a well-defined problem based on a common given data set, and to compare methods and tools in core simulation and thermal hydraulic analysis with a specific focus on transient events through a set of multi-dimensional computational test problems. As a secondary goal, the depletion capabilities of various lattice physics codes available for prismatic reactors will also be compared.

The MHTGR-350 MW benchmark is based on the approach followed for the OECD/NEA PBMR-400 MW benchmark [14, 15]. The benchmark consist of three Phase I steady state exercises, four Phase II transient exercises, and a single Phase III depletion exercise, as summarized below

- **Phase I**
  - **Exercise 1:** Neutronics only steady-state solution for a 350 MW End of Equilibrium Cycle (EOEC) MHTGR core, using the provided geometry, material descriptions, and detailed cross-section libraries.
  - **Exercice 2:** Thermal hydraulics only steady state core solution. Four sub-cases are defined, depending on the core bypass flow type and the use of fixed or variable thermo-physical material properties. Participants are expected to provide steady-state solutions for each of these sub-cases according to their codes' capabilities. A defined core power map must be used, since no neutronics are involved in this exercise.
  - **Exercice 3:** Coupled neutronics-thermal hydraulic core steady state. This exercise is a combination the first two exercises and the coupled steady-state solution must be calculated using the provided temperature dependent cross-section library, burn-up and fluency distributions. The participants are expected to compute the xenon equilibrium for their steady state solution as well.
- **Phase II**
  - **Exercise 1:** Depressurized Conduction Cooldown (DCC) transient, with and without reactor trip to allow for re-criticality to occur. Initial conditions for the transients are obtained from the steady state solution of Phase I Ex. 3.
  - **Exercise 2:** Pressurized Conduction Cooldown (PCC) with a reactor trip.
  - **Exercise 3:** Water ingress with reactor trip. Two variations of multiple steam generator tube rupture accidents are defined. In both, 125.4 kg steam is injected into the primary system. In the two sub-cases, the steam is injected over 22 and 2 seconds, respectively. The latter case is included in the benchmark set as a Beyond Design Basis (BDB) example of a prompt critical transient event.
  - **Exercise 4:** Xenon stability test. Power 100-80-100 load follow that tracks the build-up and decay of xenon and the subsequent core reactivity behavior over 72 hours.
- **Phase III**
  - **Exercise 1:** "Assembly-level" depletion calculation, consisting of a fresh fuel block surrounded by a "super-cell" of depleted fuel blocks on the left boundary and reflector blocks on the right boundary. Two sub-cases are defined, one with and without burnable poison compact in the corner nodes of the fresh fuel block.

The radial and axial core layouts of the MHTGR-350 MW are shown in Fig. 4 and Fig. 5, respectively, and the major core characteristics are summarized in Table 2.

Table 2: MHTGR-350 main characteristics

Description	
Power	350 MW(t)/165 MW(e)
Core and fuel design	Graphite moderated 660 prismatic hex-blocks with 15.5 wt% enriched UCO TRISO fuel compacts
Coolant	Helium @ 6.39 MPa
Core in/out gas temp.	259^{o}C / 687^{o}C

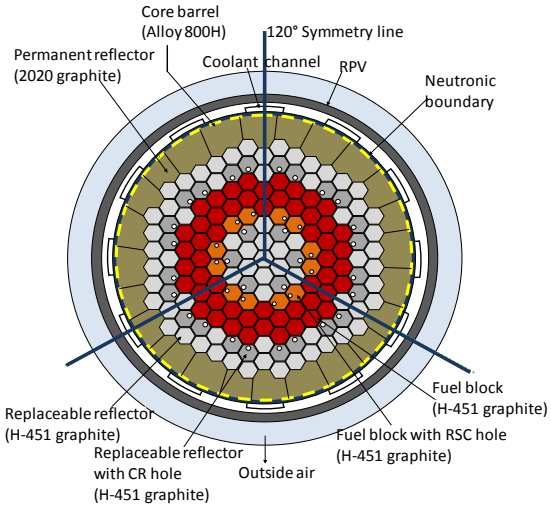

Fig. 4. MHTGR-350 core radial layout.

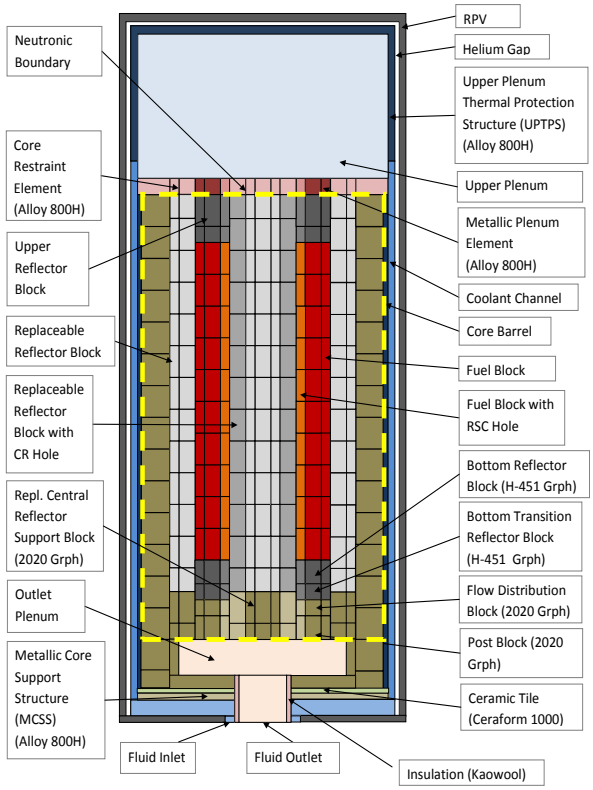

Fig. 5. MHTGR-350 core axial layout.

V. MHTGR-350 BENCHMARK: PHASE I RESULTS USING PHISICS/RELAP5-3D

V.A PHISICS/RELAP5-3D model

A PHISICS/RELAP5-3D model has been set up for the benchmark. The main elements of the model are given here, whereas more details on the PHISICS/RELAP5-3D model can be found in [1]. The thermal hydraulic core nodalisation for RELAP5-3D is shown in Fig. 6. The core consists of 9 parallel flow channels representing each a ring in the core, i.e., there are three channels representing the inner reflector, three channels representing the three fuel rings, two channels representing the replaceable outer reflector and one channel representing the permanent outer reflector. Each channel is attached to its own heat structure representing the fuel or graphite blocks in the corresponding core ring. Additional pipe components are used to model the core bypass flow.

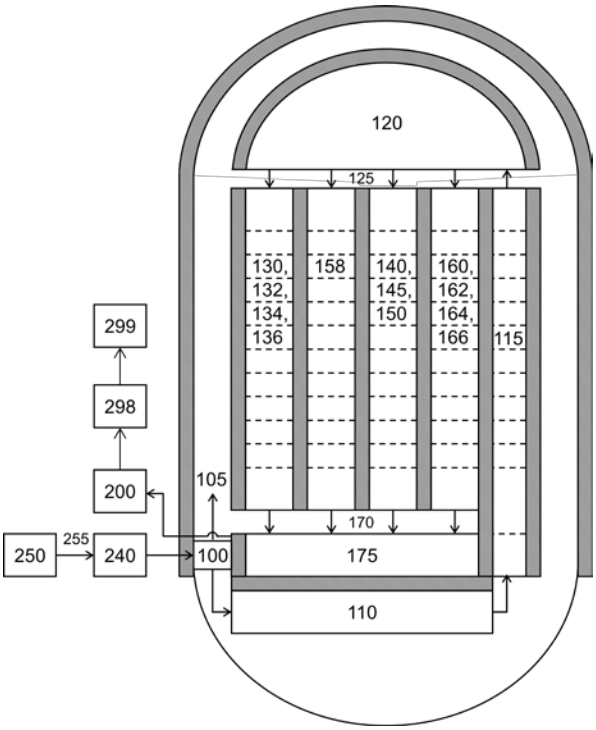

Fig. 6. RELAP5-3D nodalisation.

As shown in Fig. 6, in addition to the core region (component numbers 130-166), the model includes an inlet boundary condition on mass flow (250), lower plenum (110), coolant riser (115), upper plenum (120), outlet plenum (175) and outlet boundary condition on pressure (299). The vessel gap (105) and the vessel structures are included in the model as well.

A number of conduction and radiation sets are included in the model to account for radial conduction and axial radiation between the graphite structures in the inner, outer, top and bottom reflectors. Radial radiation heat transfer is also modeled between the outer reflector surface and the core barrel, and from the outer surface of the reactor vessel to the boundary air layer. Adiabatic boundary conditions are applied at the top and bottom model boundaries, and the outer radial air layer is defined to be at a constant temperature of 30°C.

PHISICS uses a hexagonal mesh for the neutronics solution corresponding to a fuel or reflector block. One third of the core is modeled (see 120^{o} symmetry line in Fig. 4). The core is divided into 14 axial levels, two each for the upper and lower reflector and 10 for the core region. The 26 energy group cross-section library is read as separate data structures, and updates are performed on these base cross-section sets during the steady state convergence process in the mixer module of PHISICS. Cross section updates are performed for four state parameters: moderator and fuel temperature, xenon-135 concentration and the hydrogen concentration (for the water ingress transient).

V.B Phase I: Exercise 1 results

Benchmark Exercise 1 of Phase I is a neutronics only steady state for the MTHGR core. Different macroscopic cross sections for each of the 22 fuel assemblies on each of the 10 core axial levels are provided in 26 groups as part of the benchmark specifications. In addition, reflector cross section sets are provided together with a load map for the core. INSTANT in stand-alone mode has been used to solve this problem. A full spatial and angular convergence study is still in progress, but first scoping results for k_{eff} are presented in Table 3. The table presents k_{eff} for three different cases, one where the control rod bank is at its nominal position, one where the control rod bank is fully inserted and one where it is fully extracted. All cases use PN 1 with first order surface and 3^{rd} order source expansion, and the flux convergence criteria where set to 1E-6 for the outer iterations and 1E-4 for the inner iterations. The number of up-scattering iterations was limited to 5 to improve the balance between fidelity and run-time performance.

To check the spatial convergence, the initial 10 axial nodes where subdivided in 6 nodes each (for the triangular (TRI) cases), and 3 nodes each for the hexagonal (HEX) cases. The hexagonal blocks were also decomposed into 6 triangles for the TRI cases. Table 3 compares results for hexagonal geometry using 6^{th} order polynomial expansion for the flux, and two triangular geometry cases, one using 3^{rd} and one 6^{th} order polynomial flux expansion.

Table 3: Phase I, Exercise 1: k_{eff}

Description	CR @ nominal	CR out	CR in
HEX 6^{th}	1.06688	1.06761	1.05816
TRI 3^{rd}	1.06632	1.06729	1.05491
TRI 6^{th}	1.06631	1.06728	1.05490

As one can see from the above table, all results are within 50 pcm except the hexagonal case where the control rod is fully inserted. This larger difference for the CRI cases can be expected from the basic cross section definition, since the control rods data for the TRI cases were only defined in a single triangle ($1/6^{th}$ of a full block, e.g region 234 in Fig. 7), whereas the control rods in the HEX cases were homogenized over the entire block volume (e.g. region 232 in Fig. 7).

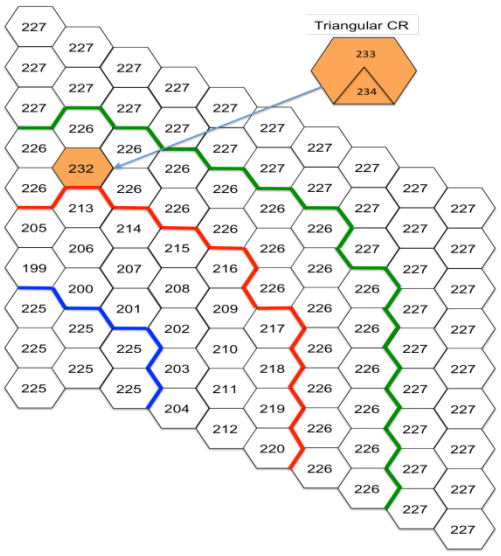

Fig. 7. Cross section map of core axial level 2, with control rod bank regions 232 (HEX) and 234 (TRI) indicated.

V.C Phase I: Exercise 2 results

Benchmark Exercise 2 of Phase I is a thermal hydraulics only steady state core solution. RELAP5-3D in stand-alone mode has been used to solve one of the four sub-cases defined, Exercise 2c. Fluence-dependent fuel and graphite thermophysical properties have been used, as specified in the benchmark definition. The flow resistance factors at the channel inlets have also been determined for the

7 core bypass flows to match a total of 11% core bypass flow, and the power density distribution, based on data from General Atomics, was implemented. Since this power density data is supplied for each of the hexagonal blocks in the fuelled area of the core, an equivalent volume averaged power density has been determined for each of the 3 fuel rings in the RELAP5-3D model. Fig. 8 shows the axial power density distribution for the three fuel rings.

The primary parameters of interest are the gas and solid temperatures and global parameters such as the pressure drop over the core and the inflow mass flow rate. The benchmark does however require participants to also report secondary parameters such as the calculated thermal conductivities, mass flow rate or velocities in bypass channels and heat transfer factors, since this data can be utilized to trace the source of possible differences in the primary parameters.

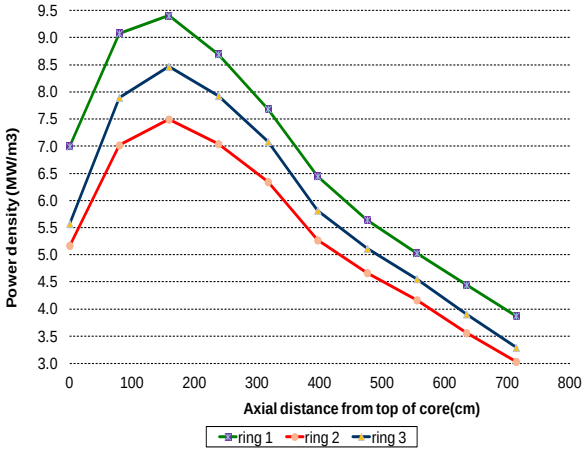

Fig. 8. Ring averaged axial power density distribution for the three fuel rings (ring 1: inner fuel ring, ring 2: center fuel ring, ring 3: outer fuel ring).

The global parameters of interest for Ex. 2c are presented in Table 4. The core inlet coolant temperature and outlet pressure have been used as boundary conditions to obtain the outlet gas temperature, total mass flow rate, inlet pressure and therefore core pressure drop, maximum fuel temperature and the average core barrel temperature from the RELAP5-3D steady state calculation. The maximum fuel temperature (1062°C) is reached in the inner fuel ring at the bottom of the core.

Fig. 9 shows the volume-averaged axial temperature profiles for the 3 inner and 3 outer reflector rings (IR/OR), as well as the 3 fuel rings (CR1-3). The average inner fuel ring temperature is significantly higher than the center and outer fuel rings, caused by the combined effect of the higher power density specified (Fig. 8) and the smaller volume of the inner fuel ring. The inner reflector is on average hotter than the outer reflector, but since both these structures are cooled by the bypass flows defined for Ex. 2c, a smaller increase in the graphite temperatures is observed from the top to the bottom of the core.

Table 4: Exercise 2c: Global results

Description	Value and unit
Core inlet/outlet gas temperature	259°C / 687°C
Inlet mass flow rate	154.3 kg/s
Inlet pressure	6.39 MPa
Core pressure drop	19.9 kPa
Maximum fuel temperature	1062°C
Average core barrel temperature	322°C

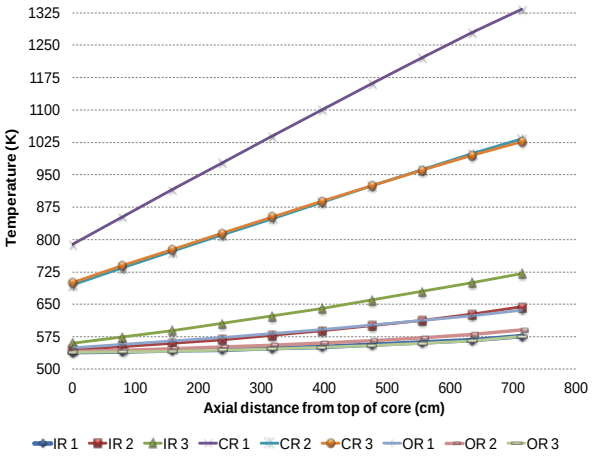

Fig. 9. Exercise 2c: Axial average temperature profile for the 9 core channels. (IR: inner reflector, CR: core ring, OR: outer reflector).

As mentioned in the description of Exercise 2 (Section IV), four sub-cases are defined with and without consideration of the core bypass flow. Fig. 10 shows a comparison of the inner fuel ring and inner reflector ring graphite temperatures with and without core bypass flow considered. The difference in the inner fuel ring temperature is insignificant, since the forced heat removal difference between full flow (154 kg/s) and 11% less (137 kg/s) through the core region is very similar. The presence of a bypass flow channel connected to the inner reflector structure does however lead to a much higher heat removal along the axial height of the core; at the

bottom of the inner reflector the difference between the two cases is almost 450 K. The importance of including these bypass flow path in the MHTGR core model is illustrated by the temperature difference shown in Fig. 10: the inner reflector becomes a much more effective heat sink when bypass flows are present, and this has a strong influence on the timing and amplitude of the heat flow from the center of the core to the final radial boundary during a Loss of Forced Cooling (LOFC) transient [15].

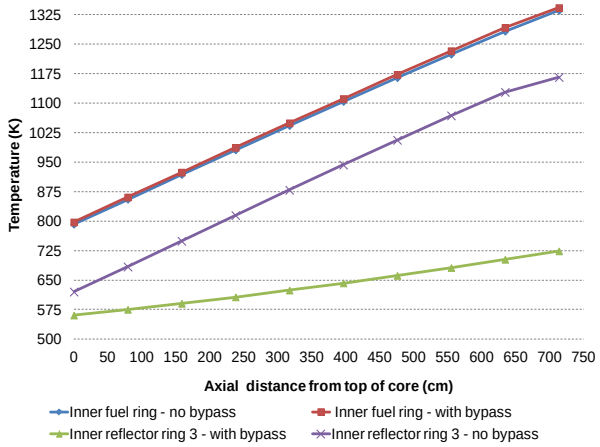

Fig. 10. Exercise 2: Comparison of axial average temperature for the inner fuel ring and the inner reflector ring with and without core bypass flow.

V.C Phase I, Exercise 3 results

Exercise 3 of Phase I is a coupled neutronic thermal hydraulic steady state with xenon equilibrium. The coupled PHISICS/RELAP5-3D package using the "depletion time evolution" mode has been used to solve this problem.

The same boundary conditions and assumptions as in Exercise 2c have been used for the RELAP5-3D model. A one third hexagonal core model has been used for PHISICS (as shown for core level 2 in Fig. 7). The core solver parameters for INSTANT are: PN 1, a 1^{st} order surface and 6^{th} order flux expansion, and a 3^{rd} order source expansion.

The Ex. 3 cross section library contains a tabulated 26 group cross section set for each of the 22 fuel nodes on the 10 axial core layers, and 14 cross section sets for all the reflector nodes (i.e. a total of 234 cross section sets). Each cross section set is tabulated as a function of fuel and moderator temperature, as well as for the xenon concentration. All cross sections are macroscopic cross sections except the xenon absorption. The absorption contribution from xenon has to be calculated from the provided tabulated microscopic xenon absorption ant the xenon density computed by MRTAU.

The mapping from the RELAP5-3D heat structure channels to the kinetic mesh for temperature feedbacks has been constructed as follows: The three inner reflector and the three outer reflector channels feed the graphite temperature back to the corresponding meshes in each plane of the neutronic mesh, i.e. all kinetic meshes in one axial level corresponding to a reflector ring are assigned the same graphite temperature to evaluate their cross sections. Similarly, the three fuel heat structure channels feed fuel and moderator temperatures back to the corresponding neutronic meshes.

As a first step, the xenon equilibrium is obtained by using MRTAU to "burn" the core in 8 time steps of 2.5 days each, i.e. for a total of 20 days. This process involves 8 recalculations of the flux with INSTANT after every 2.5 days. During the burning, the fuel and reflector temperatures for the cross section evaluation are kept constant. For each flux recalculation with INSTANT, the macroscopic cross section sets are first interpolated for the new xenon density. The new xenon absorption contribution for each node is then calculated with the updated xenon density and added to the macroscopic cross section sets. (Note that since the core is only burnt for a very small duration, the assumption that all the material number densities apart from xenon remain constant is acceptable).

Once the xenon equilibrium is reached, RELAP5-3D iterates with INSTANT to obtain a converged temperature field for this xenon distribution. After this initial MRTAU-INSTANT-RELAP5-3D iteration, MRTAU burns the core again for 5 days to find the new xenon equilibrium corresponding to the new temperature distribution. This scheme (see Section II.A) is iterated until converged temperature, flux and xenon distributions are found.

Fig. 11 shows k_{eff} during the steady state search. The top figure shows the evolution of k_{eff} during the xenon build-up with MRTAU. The red lines indicate points in time when the temperature field is updated. K_{eff} during the INSTANT-RELAP5-3D iterations are shown in the bottom figure for each temperature field update. First, the core is burned with the initial temperature distribution for 2.5 days (top figure). One can see that k_{eff} stabilizes around 2 days of burning, which indicated that the xenon reached its equilibrium. At 2.5 days, a thermal hydraulic solution for this xenon distribution is searched (blue line in bottom plot). K_{eff} decreases from ~1.062 to ~1.050 due to the temperature rise in the core from

initial conditions to operating conditions. Once the temperature field is converged, the core is burned again for 2.5 days. One can see that after 2 iterations (5 days burning), k_{eff} does not change anymore, neither during the burning, nor during the thermal hydraulic iterations (shown in the bottom figure as 4 overlapping "flat" lines); a converged steady state with xenon at equilibrium has been found.

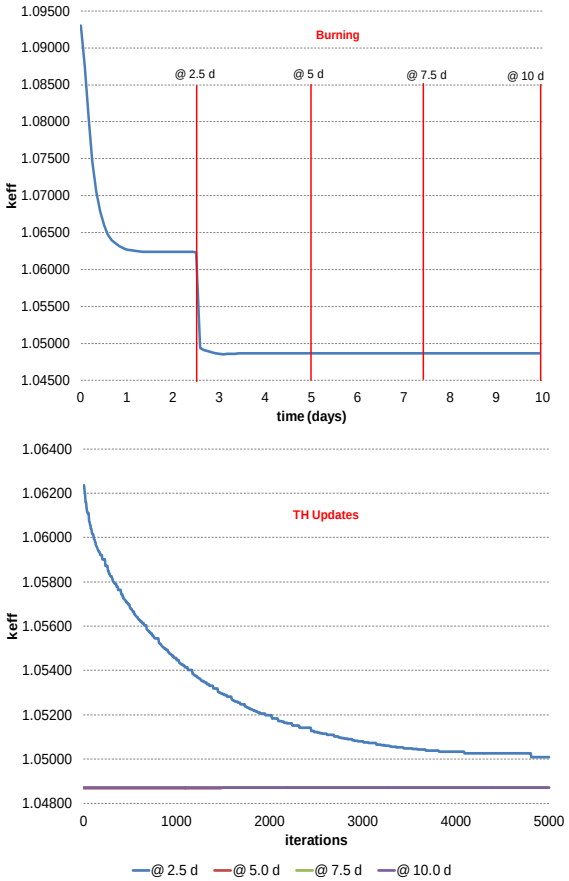

Fig. 11. Exercise 3: Convergence of k_{eff} during coupled neutronic thermal-hydraulic steady state with xenon equilibrium search.

The final converged k_{eff} value of 1.04230 is obtained after the RELAP5-3D model has reached temperature and flow stability (approximately 20000 iterations are required – only the first 5000 are shown in Fig. 11). Fig. 12 shows the converged power and xenon distributions for core axial level 5 (mid core), and the group 1 flux distribution for the full core model at the same axial level is presented in Fig. 13. The effect of the control rod bank located in the outer reflector (node 232 in Fig. 7) can be seen in both figures as a depression of the flux in the outer fuel ring and a coupled increase in the power density and fluxes in the inner fuel ring.

The maximum fuel temperature obtained for Exercise 3 is 967°C, i.e. only 21°C lower than the value obtained for Exercise 2c (Table 4). These PHISICS/RELAP5-3D results will be compared in future publications with the results from other participants in the OECD/NEA MHTGR-350 MW benchmark, as the data becomes available.

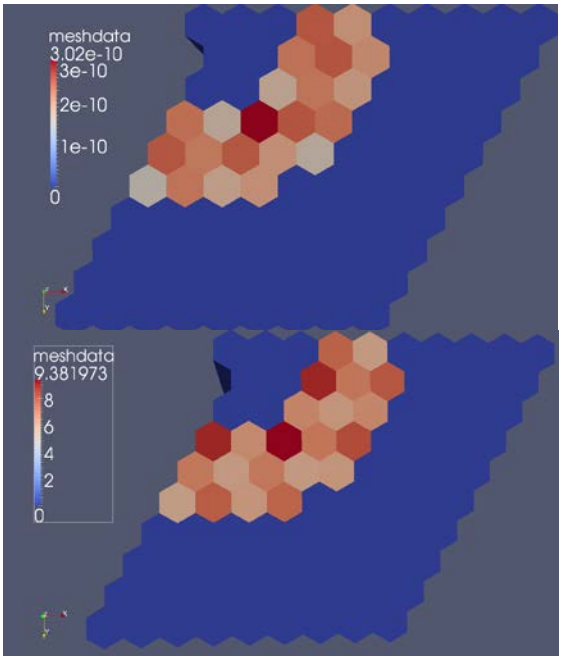

Fig. 12. Exercise 3 one third core; mid core axial level: (top) xenon distribution (1/(barn*cm)), (bottom) power density distribution (MW/m^3).

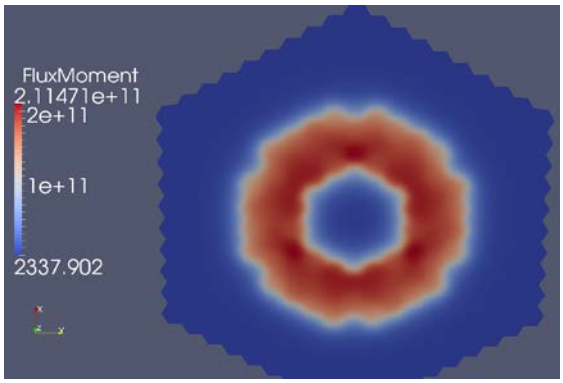

Fig. 13. Exercise 3 full core; mid core axial level: group 1 flux distribution (1/cm^3).

VI. CONCLUSIONS

This paper presents the status of the coupling of PHISICS to RELAP5-3D and presents preliminary results from Phase I of the OECD/NEA MHTGR-350 MW Benchmark. First, the different modules of the PHISICS code package have been described. It

has been shown that PHISICS is highly modular, which makes it easy to develop new capabilities and maintain existing code. PHISICS has been coupled to the thermal-hydraulic code RELAP5-3D for steady state and transient calculations.

The coupling is compatible with existing RELAP5-3D input decks, and adds the following features to the RELAP5-3D neutronic capabilities:

- Transport calculation up to 33rd order
- Spatial and angular mesh refinement
- Unlimited number of neutron energy groups
- Cross section tabulation
- Microscopic cross section handling

For depletion calculations with temperature feedback, poison tracking and decay heat calculation during transients, MRTAU has been coupled to RELAP5-3D. It has been shown that calculation possibilities with INSTANT, the MIXER, MRTAU and RELAP5-3D are manifold. It is worth mentioning that the coupling benefits directly from further developments made in the PHISICS framework. The mentioned coupling capabilities are currently being further tested and validated.

For verification purposes, a well-defined and challenging OECD/NEA code-to-code benchmark was developed by the INL, in cooperation with General Atomics, based on the MHTGR 350 MW prismatic design.

The paper provided an overview of the OECD/NEA MHTGR-350 MW Benchmark and presented selected PHISICS/RELAP5-3D steady state results for Phase I. It is currently planned to publish the PHISICS/RELAP5-3D results of the four transient exercises defined for Phase II by the end of 2012. OECD/NEA comparison reports for all participant submissions will be created for both Phases I and II by the end of 2013.

ACKNOWLEDGEMENTS

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