First Results for Fluid Dynamics, Neutronics and Fission Product Behaviour in HTR applying the HTR Code Package (HCP) Prototype

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Abstract - To simulate the different aspects of High Temperature Reactor (HTR) cores, a variety of specialized computer codes have been developed at Forschungszentrum Jülich (IEK–6) and Aachen University (LRST) in the last decades. In order to preserve knowledge, to overcome present limitations and to make these codes applicable to modern computer clusters, these individual programs are being integrated into a consistent code package. The so-called HTR code package (HCP) couples the related and recently applied physics models in a highly integrated manner and therefore allows to simulate phenomena with higher precision in space and time while at the same time applying state-of-the-art programming techniques and standards. This paper provides an overview of the status of the HCP and reports about first benchmark results for an HCP prototype which couples the fluid dynamics and time dependent neutronics code MGT-3D, the burn up code TNT and the fission product release code STACY. Due to the coupling of MGT-3D and TNT, a first step towards a new reactor operation and accident simulation code was made, where nuclide concentrations calculated by TNT are fed back into a new spectrum code of the HCP. Selected operation scenarios of the HTR Module 200 concept plant and the HTTR were chosen to be simulated with the HCP prototype. The fission product release during normal operation conditions will be calculated with STACY based on a core status derived from SERPENT and MGT-3D. Comparisons will be shown against data generated by the legacy codes VSOP99/11, NAKURE and FRESCO-II.

I. INTRODUCTION

The history of gas cooled high-temperature reactor research in Germany is closely related to Forschungszentrum Jülich and its Institute for nuclear waste management and reactor safety (IEK–6). While HTR research at IEK-6 was formerly focused on the development of pebble bed reactor designs, the key task today is the evaluation and improvement of safety aspects during both normal operation and accident conditions.

A variety of individual computer codes have been developed, validated and optimized to simulate the different aspects of HTRs, which allow conducting the previously mentioned safety analysis. These codes are widely used today and are applied in recent licensing procedures. These codes cover different aspects of an HTR. Among these codes the two system codes VSOP [1] and MGT-3D [2,3,4] are applied to simulate the reactor core/primary loop of an HTR. VSOP is mainly used for core design, fuel cycle and reactor operation simulation on a long time scale. This allows for studying safety aspects under normal operating conditions, e.g. establish a
core status as input for an accident analysis. For some accident scenarios where neutronics is not involved, the analysis can be performed with VSOP. VSOP establishes the basis for more in-depth safety studies.

MGT-3D is applied to study the dynamical behavior of an HTR on a short time scale. Together all codes offer a wide range of physics modules including 2D/3D coupled neutronics and fluid dynamics, fuel shuffling, burn up, forced flow and natural convection, gas mixture and gas diffusion as well as graphite corrosion chemistry. The calculation of the power and temperature history with correlated burnup and isotope compositions can then be used to run decay heat calculation codes such as NAKURE [5] on one hand and fission product release and fuel performance codes such as FRESCO-II [6] and PANAMA [7] on the other hand. These fission product release and fuel performance codes use calculated temperatures from VSOP and MGT-3D as input to determine the release rates of isotopes of radiologic importance.

In order to document and conserve the know-how gained during decades in the field of HTR safety studies, to overcome the limitations of the before mentioned codes and to exploit the advantages of modern computer clusters, these individual programs developed at Aachen University and Forschungszentrum Jülich are being integrated into a consistent code package applying state-of-the-art programming techniques and standards. For some HTR specific issues new modeling approaches are used, which document the knowledge in contemporary fashion. The HTR code package (HCP) couples the related and recently applied physics models in a highly integrated manner (see Fig. 1). This will allow the simulation of steady state and transient operating conditions of a full 3D reactor model including physical aspects such as fission product release calculations for each core zone or dust production and transport simulation which allow for more in-depth safety analysis. The architecture of the final HCP is displayed in figure 1.

The HCP includes the backbone software (driver) which is a new code written in C++. The backbone performs all I/O operations, the data management and the main program control. Several modules are coupled to this backbone. Each of the modules deals with a different physical aspect of an HTR reactor core / primary circuit. The neutronics (MGT-N) as well as the fluid dynamics module (MGT-FD) are derived from the code MGT-3D. As a first step towards the separate modules MGT-N and MGT-FD, the MGT-3D code was refactored and rewritten in Fortran 90. The algorithms for the calculation of burnup (TNT) and fuel management (SHUFLE) are partly derived from the VSOP code system, but have been extended by new features and are being rewritten in C++. The system code VSOP itself is not part of the HCP, although it will be the reference code for the validation of the code package. STACY is a code module replacing and extending the legacy codes FRESCO-II, FRESCO-I and PANAMA. Its task is to simulate the fuel performance as well as the fission product release and transport through the core.

II. RECENT DEVELOPMENTS

In the following, a detailed overview of the status of each module as well as first benchmark results are presented which show the applicability of the selected approach.

II.A. HCP Backbone

Integrating all modules into one code package requires the handling of a huge amount of data which used to be scattered over the different legacy codes. Due to the fact that the way of data handling within the individual legacy codes has reached its limits, a new contemporary data model was developed for the HCP. It manages all data of all modules in an object-oriented way using features of C++ and its libraries. Physical entities are abstracted and modelled by data objects with specific properties and functions.

Within the data model, two different types of data classes are distinguished. First, there are classes describing the lower level basic physical quantities like Energy and Temperature. Based on these classes, more complex and reactor specific classes are defined in order to describe higher level data objects. The implementation of these higher level classes is ongoing. Step by step, both classes which contain input values and other classes which contain output values are implemented. Meanwhile, tests are being performed to demonstrate that former results can be reproduced.

Fig. 1: Final architecture of the HTR Code Package
Eventually, all modules will use the same set of input data, and data can be shared between the different code modules. This reduces the effort needed to perform the analysis of an accident scenario. In addition, this solution is less error prone because a consistent input data set is used for the evaluation of the different physics aspects. In case of the former codes, different aspects were treated by several stand-alone codes, for which individual input files have to be created. An adaptation in one of them can require an adaptation of others.

The VSOP module DATA-2 has also been rewritten. This module converts a user defined fuel element into a homogenized nuclide vector. A fuel element is e.g. being defined by the coated particles radii, the material being used for the different layers and the composition of the matrix.

II.B. Fluid dynamics and neutronics module

Some extensions have been made to physics aspects within the fluid dynamics (MGT-FD) and neutronics module (MGT-N). An excerpt of these extensions will be discussed within this paragraph. All extensions being discussed are available within the stand-alone version of MGT (MGT-3D) as well, because the HCP modules MGT-FD / MGT-N and MGT-3D share the same Fortran code.

An important aspect of MGT-3D is the coupling between the fluid dynamics and the neutronics part with respect to the fuel and moderator temperature. Due to the high power density in the fuel kernel, its temperature is significantly higher than the surrounding graphite. So far, a so-called overheating model determined the maximum fuel kernel temperature. Here an effective heat flux resistance is defined in the heat conduction equation. The different coated particle layers are homogenized and a temperature difference between the fuel kernel and the matrix based on a parameter called “PUEBH” is calculated. So an adequate value for this parameter for different reactor and fuel designs is needed.

In order to get a more accurate fuel temperature feedback, an explicit model has been developed which solves the heat conduction equation with mixed boundary conditions. The model takes the spatial deposition of local and non-local power within the different coated particle layers and its different thermal properties into account. The new explicit model can treat both the equilibrium case and all kinds of transient cases. The effect of this kernel model in comparison to different choices of “PUEBH” for a fast control rod ejection accident is shown in figure 2. It can be seen that a wrong value of “PUEBH” can lead to huge differences e.g. in the reactor power. On the other hand “PUEBH” can now be derived by making use of the new kernel model.

In addition, MGT-3D has been extended to calculations of prismatic block HTRs. Originally, the code was developed for pebble bed HTRs only, where the heterogeneous temperature calculation could only be performed for spherical fuel elements. The extension allows the treatment of prismatic block HTRs for both the American design (GT-MHR) and Japanese design (HTTR). For prismatic block HTRs, the unit cell which is the smallest geometrical volume representing the symmetrical structure within the fuel block, can be used to analyze the heterogeneous temperature distribution of moderator and fuel rods. The calculation of the heterogeneous temperature distribution is needed for a correct feedback of the temperatures to the neutronics calculation.

The new model has been verified by a CFX simulation within an IEK-6 internal benchmark (see Fig. 3). The 2D result of the CFX calculation is displayed in Fig. 4.

As the figure shows, the radial temperature profiles obtained by CFX and MGT-3D calculations are in
good agreement. In addition, the equation to calculate the thermal conductivity of the medium, which is composed of several materials, is applied to calculate the homogeneous anisotropic thermal conductivity of the reflector and reactor core of prismatic block HTRs.

![Fig. 4: Steady state power profile within a unit cell of the GT-MHR fuel element calculated by CFX [8]](image)

Within the HCP, fluid dynamics data is not only used in the neutronics code part (as it was in MGT), but also in the fuel performance code module STACY. At the same time, the heat source calculation in HCP is now mainly being performed by TNT based on the actual nuclide inventory. Therefore a more sophisticated decoupling of the fluid dynamics and neutronics calculation within MGT is needed to be able to couple the other modules to MGT-FD an MGT-N. The decoupling opens the possibility to perform a more complex calculation of the heat transfer to outside of the fuel element reducing significantly the number of its iterations with the fluid dynamic calculation. More details and results with respect to the decoupling of both will be presented in a dedicated paper later on.

### II.C. Spectrum code

A completely new spectrum code has been written in C++ taking full advantage of the HCP data library. The code was written with the aim of replacing the MUPO library currently used in MGT-3D, with its simplifications. It also allows the usage of the ENDF/B-VII library and the NJOY code.

The new spectrum code contains several modules with the purpose of providing the necessary spatial details in order to treat each region of the reactor adequately (reflector/core interfaces, control rod and burnable poison regions). In particular, the 0-D module is implemented with two different methods, a diffusion method (comparable to MUPO) and a transport method, while the 1-D and the 2-D subroutines use the neutron collision probability method. The MCNP dependency of MGT, used in the kappa factor evaluations, has been replaced by Dancoff factors calculated with an analytical approach. This finally replaces the “kappa factors” in MGT-3D, which take into account the double heterogeneity of the fuel.

Within the HCP framework, the new spectrum code will allow the choice of different methods for different regions and scenarios (for example normal operating conditions/transient conditions) according to the needed accuracy and calculation time.

The 0-D spectrum code module is implemented within the HCP prototype and currently being compared to MUPO results. First verification efforts have shown good agreement. Further results with respect to this new spectrum code will be presented in a dedicated paper.

### II.D. Depletion module

The HCP depletion module named TNT (Topological Nuclide Transmutation) has been parallelized and a graphical user interface (GUI) has been implemented. Besides time-dependent nuclide inventories under irradiation, TNT calculates the thermal power being generated by neutron induced reactions and decay by using the nuclide vector itself and the Q-values of all possible reaction types.

In the past, a less time consuming solution for the calculation of the decay power has been established. The resulting German standard DIN-25485 [9] contains a set of equations describing the decay heat as a function of time and other variables like the final burn up. These equations are based on a large set of individual ORIGEN calculations. Concerning the decay power of the fission products, the standard is valid for all kinds of thermal reactors. The rules concerning additional sources of decay power (for example activation products) are exclusively valid for non-recycled fuel of pebble bed HTRs. The DIN standard evaluates the total decay power of the reactor as well as the decay power of discharged fuel for a decay time of up to 30 years [9]. The FZJ code NAKURE-99 [5] is a code that calculates the decay power based on the DIN-25485. The calculation deals with the reactor operation history in terms of power histograms (see Fig. 5). NAKURE, which is available both as a stand-alone version and as an integral part of the system code VSOP, has been rewritten in C++ and benchmarked against the original code version for many cases. A comparison is shown in Figure 6. It can be seen that results of the old and new version of NAKURE are in perfect agreement. The same holds for the other contributions to the decay heat and for other scenarios being simulated.
In comparison to TNT, which is universally applicable, the DIN standard can only be applied to HTRs as long as the boundary conditions are met, for which the equations have been derived. Boundary conditions are defined for example for the average power density within the core and the final burn up of the fuel. Due to the fact that no time consuming depletion calculation is involved in NAKURE, the execution time is much less in comparison to TNT. Due to this and the goal of preserving existing legacy codes, it has been decided to integrate the capabilities of NAKURE as an additional option for the calculation of the decay power in TNT.

Another aspect is the execution time of TNT. By using the ENDF/B-VII library, far more nuclides are considered within the burn up calculation in comparison to the burn up calculation in VSOP. In addition, a higher number of batches will be considered in the HCP. For this reason, the execution time of TNT was optimized by studying the run time effects in detail [11]. The runtime of a calculation comprises the time needed to read the data library (e.g. ENDF/B-VII), to perform the depletion calculation and to save the results and code status messages. About 80% of the time is needed for the calculation itself in case of an HTR-Modul-200 fuel element [11]. During the analysis, time consuming routines and algorithms have been identified. Some of the routines could be optimized with respect to execution time.

In the second step, the effect of semi-implicit parallelization with OpenMP has been studied. The study showed that the effect of parallelization of the calculation itself is rather limited. For this reason, the parallel execution of depletion calculation of different nuclide vectors on a multi-CPU machine has been investigated. It could be shown that in case of 4 CPUs, the speed up effect with respect to the execution time was equal to 1.6 [11]. In case of eight CPUs, the speed-up is equal to 2.8 [11]. In case of a complete HTR core, this can contribute effectively to a reduction of the execution time. The effect of parallelization of Open MPI has not been studied, because this would require extensive adaptations of the source code and would lead to an additional independent version of TNT.

Another aspect studied is the usability of the input. Usability has become a more and more important measure for the quality of software. Attributes to be considered with respect to a good usability are for example a rapid learnability, high efficiency, easy memorability, a low error-rate and a high user satisfaction [12]. The corresponding engineering discipline, which takes these aspects into account, is called Usability Engineering.

Regarding the HCP, a new human-machine-interface (HMI) is in development in order to improve the usability of the system and raise the level of acceptance. TNT is the first module for which this new HMI has been developed.

In the development process, selected Usability Engineering methods have been applied [12]. First, an observation of users while working with the previous command-line interface of TNT has been conducted. Mainly, problems handling the XML input files due to limited XML experience were revealed. In addition, entering the input of file paths manually via the command-line turned out to be error-prone. Therefore, as a first step, the development of a new XML-independent interface for the creation of the TNT input files has been initiated.

An iterative development approach has been used for the development of the interface. Scenarios paper-prototypes and wireframes have been used to
create blueprints of the interface. These have been evaluated based on a defined set of usability heuristics (Heuristic Evaluation [12]) before they have been implemented as a first running prototype of the system. A screenshot of the implemented prototypic interface is depicted in figure 7. The user defines the weighting spectrum and enables the reactions that should be taken into account during the depletion calculation within this part of the interface.

Fig. 7: Excerpt of the HCP graphical user interface for TNT [13]

In order to ensure the usability, a formal heuristic evaluation and a user test have been conducted based on this prototype. A chosen group of test users was asked to express their thoughts aloud while creating a given TNT input using the new interface. Their remarks have been recorded by an observer. This helped to identify the needs for improvements which can be realized in the subsequent iterations of the interface.

II.E. Fuel management module

The fuel management module named SHUFLE (Software for Handling Universal Fuel Elements) has been extended and optimized. Especially the code structure has been optimized which allows for even more flexibility. A generic fuel container called FuelCollection was created. This fuel collection can be a cask, containing fresh or (partly) depleted fuel elements, or the active core. These generic structures allow a high level of flexibility with respect to fuel shuffling.

II.F. Fission product release module

The fission product release module STACY was extended in a way that it can be applied to different kinds of (accident) scenarios and prismatic block HTR. This paragraph discusses this extension towards prismatic HTR cores and the treatment of running-in phases.

In case of prismatic reactor cores, such as the Japanese HTTR, the coated particles are formed to cylindrical compacts instead of spheres. The compacts are encapsulated within cylindrical fuel rods, which are filled with stagnant helium. The fuel rods are surrounded by the coolant flow.

Legacy codes such as FRESCO-II were limited to spherical fuel elements. As a further extension of STACY, the diffusion calculation has been extended to other geometrical bodies, which allows for calculating Fickian diffusion of fission products in e.g. spheres and cylinders of infinite length. The implementation has been benchmarked to several cases which can be solved analytically. These cases cover the full scope of the code. The numerical results calculated by STACY are in perfect agreement with the analytical results (see Fig. 8). The initial radial fission product is depicted in blue. With increasing time, fission products diffuse outwards due to the concentration gradient. The numerical solution being used in STACY is in good agreement with the analytical solution for the different time steps. Other benchmark cases resulted in equally good results.

Fig. 8: Relative FP product concentration along the radius of a hollow cylinder (red: analytical solution, green: STACY) [14]

The new calculation method allows for fission product release calculations of both pebble bed and prismatic block HTR.

In case of a pebble bed reactor, the fission product release from a large number of so-called tracer fuel elements is calculated. In equal way, the fission product release of a user-defined number of compacts per block is calculated in case of a prismatic block type reactor. As a part of the extension towards a prismatic block HTR, the compacts to be calculated are determined by a random number generator. By using a spatially resolved distribution for the nuclide inventories and fuel temperatures, this approach allows for a spatially resolved fission product release calculation for prismatic HTRs.

The legacy code system VSOP does not allow a detailed calculation of the HTTR, due to the fact that
the prismatic fuel elements contain sticks with burnable poison which cannot be modeled with the needed accuracy. The content of the sticks is smeared out over larger areas. The neutron flux depression in these areas cannot be taken into account. For this reason, the Monte Carlo neutronics and depletion code Serpent [15] has been used to calculate the time depending distribution of the nuclide inventories. An interface has been created which enables the usage of these nuclide inventories in the fission product release calculation. Based on this calculation, the temperature distribution can be determined by performing a MGT-3D calculation.

In comparison to the former version, which could only calculate the fission product release of an equilibrium core or transients starting from such a core status, the code can now handle running-in phases as well. The extended model allows for calculating the fission product release rate during the actual running-in phase of the HTR-10 reactor core. Details with respect to this specific extension of STACY and its application to the HTR-10 can be found in [16].

III. Benchmark calculations

The development of the HCP is ongoing. The rework or replacement of existing code modules and the coupling some code modules to the HCP backbone has been finished. For these modules, first benchmark calculations can be performed. An excerpt of these calculations will be presented.

III.A. Fission product release calculations with STACY

Formerly, the code FRESCO-I or FRESCO-II was used for a full core fission product release calculation. FRESCO-I is designed to calculate the fission product release rates of reactors with a single core pass fuel strategy. In case of the HTR-Module with a nominal core pass number of 15, the approach does not fulfill the before mentioned fuelling strategy. By using FRESCO-II, results from a few fuel elements were extrapolated to derive the fission product release for the whole core. Results for the newly developed fission product release code STACY with respect to pebble bed reactors can be found in [18].

One of the benchmark calculations with respect to fission product release is the simulation of the High Temperature Engineering Test Reactor (HTTR). In [17] a predictive fission product release calculation was performed for the HTTR for some nuclides with high radiologic relevance. Within this study, the anticipated operation plan was considered to be 660 equivalent fuel power days. During this “standard operation plan”, a high temperature phase was foreseen, at which the HTTR is operated at coolant outlet temperature of 950°C. The hollow fuel compacts were approximated within the calculation by spheres of equal volume. The calculation was only resolved in axial direction. That means that the fuel blocks within one layer were lumped together. Data of layer averaged fuel temperatures and coated particle failure fractions were provided by JAEA.

Due to the extension of STACY, which now allows for describing the Fickean diffusion in cylindrical (annular) bodies, the real geometry of the HTTR compacts can be taken into account. In addition, a resolved fission product release calculation can be performed based on the fission product inventories being calculated by performing a coupled Monte-Carlo and depletion calculation with Serpent. Within a first step, the FRESCO-II calculation has been repeated with STACY by using the same input parameters. Results from former FRESCO-II calculations could be repeated with STACY for all cases. In the next step, the hollow cylinder was modeled in detail. Within these calculations, the core was still subdivided in five fuel layers as in the FRESCO-II calculation. Release results are only adapted for several percent (see Fig. 11).

Fig. 11: Comparison of the Cs-137 fractional release calculated by FRESCO-II and STACY [14]

In the third set of calculations, each of the 150 fuel blocks is treated individually (see Fig. 12). Due to this, the distributions of burn up values, nuclide inventories, neutron fluxes and fuel temperatures are considered in more detail. This calculation series resulted in release values which are about 18 % for Sr-90, 14 % for Cs-137 and 23 % lower for I-131
comparison to the FRESCO-II calculation in case of
design values [14]. In case of expected values,
releases are about 29% for Sr-90, 44% for Cs-137
and 48% lower for I-131 [14].

Fig. 12: Spatial distribution of burn up within the
third fuel layer from the top of the HTTR after 660
EFPD [14]

The code module STACY allows performing a
spatially resolved fission product release calculation
for both pebble bed and prismatic block HTRs.
These results and a comparison to former results
determined by Siemens Interatom have been
published in [18].

III.B. Decay heat calculations with TNT

As part of VSOP, the NAKURE module
calculates the spatial distribution of the decay power
as a function of time. Within the HCP, the depletion
module TNT offers the possibility to determine the
decay power based on the nuclide vector and the Q-
values of the single reactors for both normal
operating conditions and accidents. A benchmark
calculation between the NAKURE approach and
TNT has been performed, whose results are

The figure shows that results of the re-
implemented NAKURE do reproduce results of the
original NAKURE. The decay power after the TNT
approach is slightly lower at the beginning of the
accident. This can be explained by the fact that the
curves of the DIN standard have been derived by a
set of ORIGEN calculations in a conservative way.
That means that the DIN standard overpredicts the
actual decay power to be on the conservative side
with respect to fuel temperatures.

Fig. 13: Comparison of the decay power according
to the NAKURE and TNT approach [10]

III.C. The HCP Prototype

As a first step towards a fully integrated code
package, a prototype of the HCP coupling MGT-3D,
SPEC, TNT and STACY is now available. Therefore
parts of the MGT-3D main control program were re-
implemented and are now located within the
backbone, so no I/O coupling is involved. The data
flow for this HCP prototype is depicted in Figure 9.
The data library was extended towards multiple
temperatures and background cross sections.

Fig. 9: Architecture of the HCP prototype

The prototype can perform a sequence of
consecutively steady-state calculations for a given
reactor model. Starting from an XML input file,
which includes data for the different code modules, a
first spectrum calculation is performed. The
spectrum code then provides mesh-wise broad group
cross sections, weighting spectra and diffusion
constants to MGT and TNT. In a next step
MGT-3D calculates the steady-state condition with
respect to e.g. broad neutron fluxes, fuel and
moderator temperatures. Afterwards a batch-wise
burn up calculation is performed using the depletion
code TNT based on output data from MGT and the
spectrum code.
IV. CONCLUSIONS

The development of the HTR Code Package is ongoing. Code modules such as MGT-3D and STACY have been extended towards prismatic block calculations. The depletion module TNT has been optimized with respect to execution time and full core calculation can be performed in parallel. On top of this, a graphical user interface has been developed for TNT. A new spectrum code has been developed which is replacing MUPO in MGT-3D and allows a more precise treatment of the different zones. The decoupling of the neutronics and fluid dynamics within MGT-3D is work in progress. First results of benchmark calculations like for example fission product release calculations or coupled neutronics and depletion calculations look very promising. In most cases, like for example the fission product release calculation, new functionalities could be demonstrated.

V. OUTLOOK

The coupling of other modules to the HCP backbone and the development of the HCP is work in progress. By coupling the remaining code modules to the backbone, the benefits of the approach can be fully exploited and will allow for performing more detailed safety studies. Replacing modules with more advanced modules, such as the new 1D and 2D spectrum code, allows for taking more detailed physics aspects into account. On top of this, an extensive verification and validation process will be performed to demonstrate the predictive quality of the HCP.

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