M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

MOTIVE - A New Modular Burn-up Code

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Abstract - *The new burn-up code MOTIVE, a successor to the established code KENOREST, is presented. It is a modular code written in C++ which couples external computational tools for neutron flux calculation and for inventory calculation in order to allow for nuclide inventory prediction of 3d fuel assembly models. The main goal in the development of the code is to provide flexible interfaces for easy exchange of external codes and of the data libraries used while providing an easy to use user interface. Currently, the latest versions of the Monte-Carlo neutron transport codes KENO-VI and OpenMC can be used as flux solvers in the code, and the in-house code VENTINA is used for the nuclide inventory determination. Four different nuclear data libraries are available in MOTIVE which are based on the evalutations ENDF/B-VII, ENDF/B-VII.1, JEFF-3.2, and JENDL-4.0. First verification and validation calculations have been performed using both experimental data from radio-chemical analyses of spent fuel samples and computational benchmarks for code-to-code comparisons. Examples of these calculations are presented and disussed.*

I. INTRODUCTION

The precise determination of the nuclide inventory of irradiated fuel assemblies plays an important role in a number of applications, e.g. in criticality safety or the determination of source terms for shielding calculations. For this purpose, so-called burn-up codes have been developed around the world. Modern 3d burn-up codes typically use an iterative scheme which involves solving the Boltzmann transport equation for determining the neutron flux which is then used as an input for a solver for the Bateman equation describing the time evolution of the nuclide densities in the fuel materials.

The Nuclear Fuel departement of GRS has a long standing history of developing tools for burn-up calculation cumulating in the development of the 3d burn-up code KENOREST [1]. While being among the first codes providing the possibility of calculating pinwise inventories taking into account the local neutron spectral properties of each pin KENOREST has become outdated in a number of aspects. This is mainly due to technical constraints imposed by the internal structure of the code. Amongst others, KENOREST is missing flexibility in the description of complex modern fuel assemblies and its cross-section libraries require a rather difficult updating procedure.

In order to overcome these constraints a new code dubbed MOTIVE (**MO**dular **T**ool for **In****VE**ntory Calculation) has been developed recently using modern programming techniques. This paper gives an overview over the concepts used in the developement of MOTIVE and presents the main goals and ideas in the implementation. A few details on special features are given. Finally, some aspects of verification and validation are presented together with exemplary results and an outlook on future development.

II. BASIC STRUCTURE

Like its predecessor KENOREST, MOTIVE couples external computational tools for neutron flux calculation and nuclide inventory calculation. The basic computational scheme applied is similar to that of most other contemporary burn-up codes and will therefore only shortly be described here.

The calculation starts by calculating the 3d neutron flux accross the region of interest, typically an axial slice of a fuel assembly. This is done by performing a criticality calculaiton using a continuous energy Monte-Carlo code. The flux data in the materials of interest are read out and processed to obtain reaction rates for the neutronic reactions. These are fed into a depletion code solving the Bateman equation over a predefined short time period. The resulting nuclide densities are read out and written back into the neutron transport code to update the critcality calculation. This process is iterated until the final burn-up is reached.

The coupling between the transport solver and the depletion solver is implemented using the approach of calculating reaction rates by collapsing a very fine energy group cross section library using corresponding flux spectra calculated in the Monte-Carlo transport calculation. This approach is significantly faster than directly determining the reaction rates via tallies [2]. Currently, a group structure of approximately 27000 energy groups is used in MOTIVE. The code is complemented with two independent python scripts which automatically generate the multi-group cross section data and the decay and fission yield data for the depletion calculation. These will be described in more detail later.

The main development goals for MOTIVE were modularity and a user-friendly, easy-to-use input. Modularity means in this context the ability to easily couple additional external tools used for neutron flux and inventory calculation and to be flexible in the use of the cross-section libraries. In order to achieve this goal, the code was written in C++ with usage of object-oriented programming techniques. The interfaces to the external codes are realized using general classes and functions which are not code specific. The coupling to the actual codes in use are achieved by derived classes using the concept of inheritence.

Currently, the flux calculation can be performed with the

Monte Carlo codes KENO-VI of the SCALE6.2.1 Package [3] and OpenMC [4], an open source Monte-Carlo code originally developed at MIT. For the depletion calculations the in-house code Ventina [5] is used, which is currently developed in cooperation with PSI, Switzerland.

Concerning the usability, the intention was to have a paramter-based input file with only very limited need for complex geometry specification. For example, the definition of a fuel assembly is done by stating the type of fuel assembly desired via a key word, the dimensions of the assembly as parameters and a list of numbers defining the pin array. The parameter values in the input are internally translated into Monte-Carlo code specific geometry definitions. Another advantage of this approach is the flexibility with regard to the coupling to a different flux solver. The input file itself is compatible to all flux solvers already coupled to the code without any changes. Therefore, if a new neutron transport code is integrated into MOTIVE all previously defined inputs can directly be used without modifications. The downside of this approach is a higher effort in the implementation of the internal geometry definitions. Also, the user can only simulate those assemblies that are already implemented. The object-oriented approach helps to keep this additional effort as small as possible. Currently, Pressurized Water Ractor (PWR) assemblies and most common Boiling Water Reactor (BWR) assembly types are implemented. Additionally, VVER-1000 assemblies can be simulated. An extension to other reactor types is planned.

III. CODE FEATURES

1. Material Property Calculation

MOTIVE has several options to calculate material properties internally, which is a unique feature of this code. From the moderator pressure and temperature provided in the input the moderator density is calculated by MOTIVE using the 1997 formulation of the IAPWS standard [6, 7]. For the direct comparisons with KENOREST an older VDI standard [8] is also implemented. Moreover, two different models for calculating the fuel and cladding temperatures are implemented into MOTIVE. These are both based on a solution of the heat transfer equation and need the fuel power and the moderator temperature as inputs as well as fuel pin dimensions. The first model uses an analytical approach as described in [9] the second model is an iterative solver similar to that implemented in the fuel code FRAPCON [10]. While the first approach is slightly faster the second approach is more flexible in terms of applicability to various complex fuel goemetries. In test calculations both methods have been shown to aggree very well for a typical PWR-type pin cell. Since computational benchmarks typically have defined values for moderator density (in terms of nuclide number densities) and material temperature it is also possible to fix these quantities in the input and switching of the calculational models described above.

2. Predictor-Corrector aproaches

In order to allow for larger time steps without comprimising the accuracy of the results, three different predictor-corrector methods have been implemented into MOTIVE which will be shortly described in the following:

1. In the predictor step the nuclide inventory is calculated with reaction rates obtained from a neutron flux calculation at the beginning of the time step. In the corrector step the nuclide inventory is recalculated using reaction rates calculated with the flux obtained the end of the time step, i.e. with a flux calculated with the nuclide inventory which resulted from the predictor step. Afterwards, the nuclide inventories obtained in the predictor and the corrector steps are averaged over to obtain the actual nuclide inventory of that time step. The predictor calculation of the next time step is done using the neutron flux already used for the previous corrector step. The process is repated for each time step.

2. This approach is basically identical to the one used in the TRITON burn-up code [3]: In a first start-up step the nuclide inventory is calculated up to the middle of the first time step. For this inventory a flux is calculated and used for a depletion calculation of the complete first time step. The calculation is continued to the middle of the next time step and the process described before is repeated.

3. For the third approach two start-up time steps are needed. With the reaction rates of these two steps, the reaction rates are linearly extrapolated up to the next time step and the depletion calculation for this step is done with the extrapolated rates. The advantage of this approach is that the time steps can be sub-devided into an arbitrary number of substeps at which extrapolated reaction rates can be used. Since the depletion calculation is computationally cheap compared to the neutron flux calculation, this approach doesn't result in much longer computation times. As long as the linear extrapolation process is a good approximation to the actual time development of the reaction rates, this apporach should lead to a significant improvement of the nuclide inventory calculation compared to using a single depletion step of the same length.

Note that in all three approaches the overall number of flux calculations in one burn-up calculation does not increase compared to the calculation without using a predictor-corrector approach. These approaches, as well as a number of other approaches, are described in more detail in [11].

3. Cross-section libraries

As mentioned earlier, a Python-based script environment has been developed in conjunction with MOTIVE with the purpose of making available an automated approach for generating consistent data libraries for all modules of MOTIVE. Currently, one Python script is used for the generation the

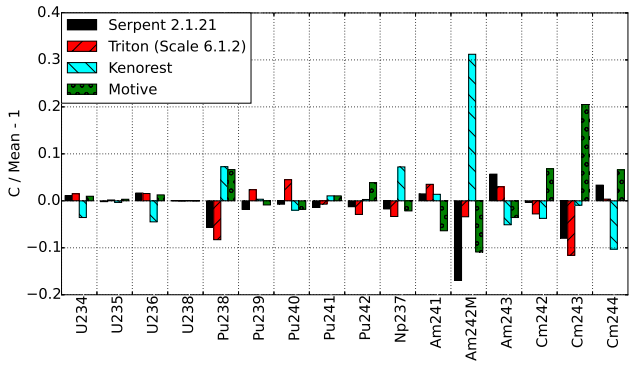

Fig. 1. Comparison of actinide number densities for different burn-up codes as computed/average -1.

multi-group library used for reaction-rate calculation in MOTIVE. This script automates calling the library processing code NJOY [12] for each nuclide and post-processing the resulting data into a library in HDF5 [13] format. A second script called ENDF2Graph directly parses nuclear data files in ENDF-format. It reads out and processes decay data, information on availble reaction channels, and fission yield data and stores them in a directed mathematical graph. From this graph the necessary information needed for the depletion code VENTINA is generated and processed into two files, one file containing decay data and reaction channel information and the other file containing the fission yield data. The Monte-Carlo codes KENO-VI and OpenMC each rely on their own continuous energy data libraries, in an AMPX-format and a HDF5 format respectively. Since SCALE6.2 [3] the AMPX-6 code package [14] for processing nuclear data libraries into the AMPX format is delivered together with the standard package. This makes it possible for the user to create his own custum nuclear data library to be used with e.g. KENO-VI (or other SCALE neutron transport codes). For MOTIVE this possibilty has been used to create libraries based on JEFF-3.2 and JENDL-4.0 evaluated data in addition to the existing ENDF/B-VII and ENDF/B-VII.1 libraries. OpenMC includes python scripts to process standard ACE format libraries into the native library format based on HDF5. With these tools existing libraries based on ENDF/B-VII, ENDF/B-VII.1, and

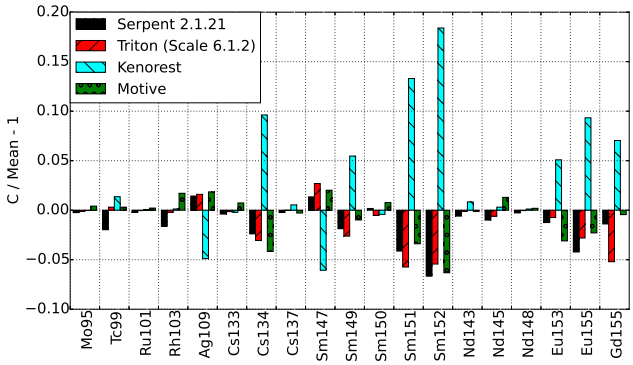

Fig. 2. Comparison of fission product number densities for different burn-up codes as computed/average -1.

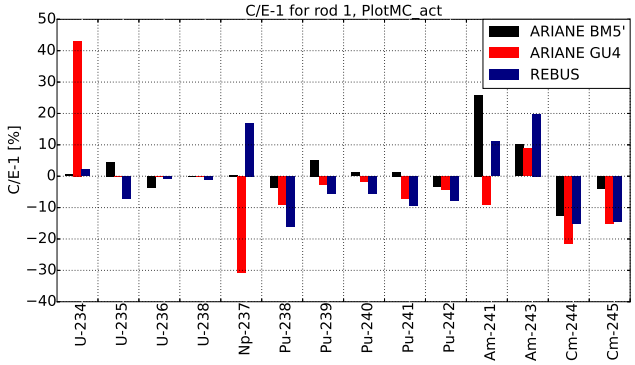

Fig. 3. Comparison of computed over experimental actinide inventory for three different samples from the ARIANE and REBUS experimental programms displayed as computed/experiment -1 in percent.

JEFF3.2 have been created to be used in conjunction with MOTIVE. The methods described above make it possible to provide consistent sets of nuclear data libraries, which allow to perform a MOTIVE calculation using data in the different calculation steps which is based consistently on a single data evaluation. Currently such data library sets for MOTIVE include ENDF/B-VII, ENDF/B-VII.1, JEFF-3.2 (KENO-VI and OpenMC), and JENDL-4.0 (KENO-VI only). These libraries are used consistently through the whole processing chain, i.e. for neutron flux calculation, reaction rate condensation, and nuclide inventory calculation.

IV. VERIFICATION & VALIDATION

First verification and validation calculations for MOTIVE have been performed using openly available post-irradiation examination data and code-to-code comparisons from a number of computational benchmarks. The first results look very promising. In order to give an overview over these verification efforts three examplary results are shown and shortly discussed in the following.

As an example for the code-to-code comparisons, Fig-

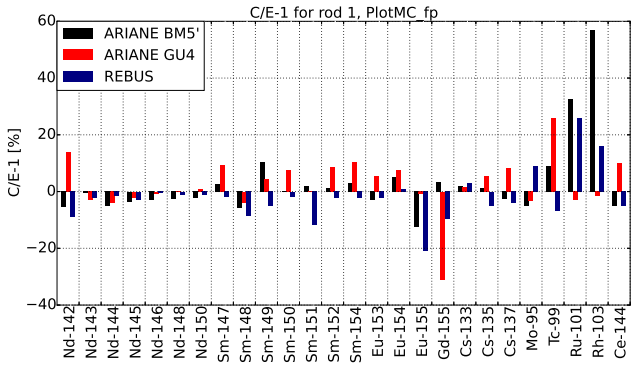

Fig. 4. Comparison of computed over experimental fission product inventory for three different samples from the ARIANE and REBUS experimental programms displayed as computed/experiment -1 in percent.

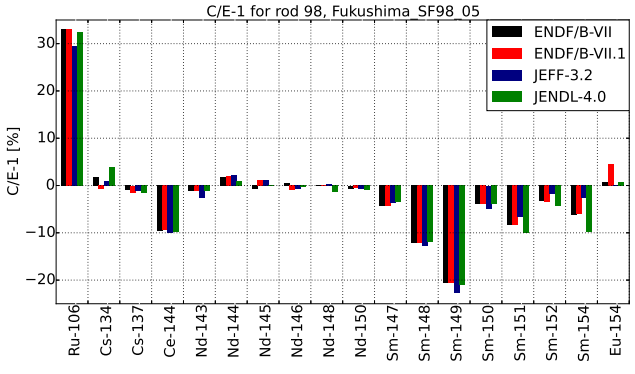

Fig. 5. Comparison of actinide inventoryof the Fukushima Daini 2 sample SF98-5 with MOTIVE calculations with different nuclear data libraries displayed as computed/experiment -1 in percent.

ures 1 and 2 show the results from an internal computational benchmark using a simple 18x18 PWR assembly. Four different codes were used, namely TRITON from SCALE6.1.2, Serpent 2.1.21 [15], KENOREST and MOTIVE. The Figures show assembly averaged nuclide inventory data plotted as relative deviation to the mean values of the four results.

The MOTIVE calculation was performed using KENO-VI from SCALE6.2 as flux solver and ENDF/B-VII.1 cross section data. In the Serpent calculation as well as the TRITON calculation ENDF/B-VII.0 data were used, whereas KENOREST uses JEF2.2 data. The MOTIVE results show good agreement with the results obtained with the other codes with the MOTIVE result beeing in the range of the variations of the other codes for most of the nuclides displayed. The aggreement is especially good with the more modern codes Serpent and TRITON. Somewhat larger deviations are seen for the Curium nuclides. However, comparisons with post-irradiation examination data have shown that MOTIVE typically reproduces these nuclides better than e.g. TRITON. Some of the differences might also be attributed to the different cross section libraries used. However, it is shown further below that the difference between ENDF/B-VII and ENDF/B-VII.1 is rather

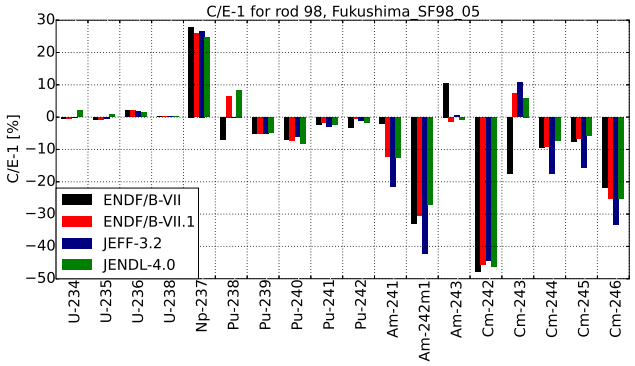

Fig. 6. Comparison of fission product inventory of the Fukushima Daini 2 sample SF98-5 with MOTIVE calculations with different nuclear data libraries displayed as computed/experiment -1 in percent.

small for many nuclides.

In addition to the code-to-code comparisons, calculations of various experimental isotopic composition data from post-irradiation examinations (PIE) have been performed. These were taken from the OECD/NEA PIE data base SFCOMPO [16]. From these analyses two exmaples are presented here two illustrate the current performance of MOTIVE with regard to isotopic compositions and to show the differences between the available data libraries. In Figsures 3 and 4 the computed value over experimental value ratios (C/E) for three samples from the experimental programs ARIANE [17] and REBUS [18, 19] are shown for actinides and fission products, respectively. Namely, these are the samples BM5 (Beznau MOX fuel assembly), GU1 (Gösgen PWR UO_2 fuel assembly), and M11 (GKN PWR UO_2 fuel assembly). The simulations have been performed with version v0.5 of MOTIVE using ENDF/B-VII.1 data. The conformance of the calculated results is very satisfactory and comparable to the results that have been obtained with other established codes [20]. The deviations for the uranium nuclides are mostly well below 5%, except for the ^{234}U value of the ARIANE GU4 sample. The deviations in the plutonium nuclides are only sligthly larger, americium and curium nuclides are around 10 to 20%, which quite small compared to previous calculations with other codes. Regarding the fission products neodynium and cesium nuclides are predicted very well as expected. Samarium and ^{153}Eu and ^{154}Eu are predicted almost as good. The other nuclides show somewhat larger deviations. However, one has to keep in mind that some of these nuclides are rather difficult be measured accurately. This is also reflected in the large variations in the predictions of the different samples. The Figures 5 and 6 show calculations of sample SF98-05 from the Fukushima Daini 2 BWR fuel assembly experimental data performed with MOTIVE v0.5 with KENO-VI as neutron flux solver using again the four different available libraries. Again the quality of the results is comparable to that of established codes [21]. Moreover, these plots show the possibilities that arise from beeing able to use a broad range of nuclear data. Comparing for each nuclide the results of the different libraries allows to assess differences in these libraries and also to estimate uncertainties resulting from the nuclear data. The largest deviations are seen for the Americium and Curium isotopes. These are mostly due to differences in som branching ratios for neutron reactions, e.g. the branching of neutron capture of ^{241}Am to ^{242}Am and ^{242m}Am, respecitvely. As mentioned above the differences between the calculations with ENDF/B-VII and ENDF/B-VII.1 are rather small except for ^{238}Pu, ^{241}Am, ^{243}Am, and ^{243}Cm. Overall, ENDF/B-VII, ENDF/B-VII.1, and JENDL-4.0 behave rather similarly. Larger differences are seen when comparing the JEFF-3.2 results to those of the other libraries.

V. CONCLUSIONS AND OUTLOOK

In this paper the newly deveoped burn-up code MOTIVE has been presented. It is written in C++ using modern programming techniques. It is easily extensible with respect to new functionality and allow for easy coupling to other external codes. First verification calculations show very promising results. It is planned to strongly increase the number of

verification calculations in the near future. One future developement goal is to provide the ability to cover larger systems, e.g. groups of fuel assemblies, as the computational power of available hardware increases.

VI. ACKNOWLEDGMENTS

This work is supported by the German Federal Ministry for Economic Affairs and Energy.

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