Development of the darwin3-sfr fuel cycle toolfor decay heat calculations in new generation fast reactors

C. Vaglio-Gaudard, P. Bellier, L. Buiron, S. Lahaye, J.-F. Lebrat, P. Miranda, B. Roque, A. Tsilanizara

DEVELOPMENT OF THE DARWIN3-SFR FUEL CYCLE TOOL FOR DECAY HEAT CALCULATIONS IN NEW GENERATION FAST REACTORS

C. Vaglio-Gaudard*[1], P. Bellier[2], L. Buiron[1], S. Lahaye[2], JF. Lebrat[1], Ph. Miranda[1], B. Roque[1], A. Tsilanizara[2]
Commissariat à l'Energie Atomique et aux Energies Alternatives
[1] CEA, DEN, DER, SPRC, Cadarache, F-13108 Saint-Paul-Lez-Durance, France
[2] CEA, DEN, DM2S, SERMA, Saclay, F-91191 Gif-sur-Yvette, France
* claire.vaglio-gaudard@cea.fr

ABSTRACT

The DARWIN3-SFR tool is the new calculation tool dedicated to the estimation of fuel cycle parameters (material balance, activity, radiotoxicity, etc), decay heat and material activation for GEN-IV reactors. The tool will be industrialized by the end of 2017; it will be used to perform cycle/decay heat calculations needed by the ASTRID preliminary safety report, foreseen at the end of the ASTRID Basic Design Phase in 2019.

It integrates two calculation routes: the APOLLO3®-MENDEL route and the TRIPOLI4®-MENDEL route. The APOLLO3®-MENDEL route is operational. It integrates today the same functionalities as the previous tool used for SFR calculation, DARWIN2.3. It is more easily implemented, more flexible in use, than the previous DARWIN2-SFR tool, based on the ERANOS2 and DARWIN/PEPIN2 codes. The TRIPOLI4®-MENDEL route will operational by 2017.

The V&V-UQ process will be followed in the next DARWIN3-SFR version (V1). The numerical validation (it only concerns the neutron flux calculation step) will mainly consist in comparison between APOLLO3® calculations and reference Monte Carlo calculations at step 0. The experimental validation will be performed for the DARWIN3-SFR calculations concerning actinide material balance, decay heat and secondary sodium activation. The final quantification of calculation biases and uncertainties for the ASTRID cycle parameters will rely on both the experimental validation and a priori nuclear data uncertainty propagation (by deterministic approach).

The DARWIN3-SFR first implementation was performed on the numerical benchmark described in this paper, which corresponds to a homogeneous sodium reactor core. It was the first demonstration of the APOLLO3®-MENDEL chaining feasibility.

Key Words: **DARWIN3, MENDEL, ASTRID, FUEL CYCLE, DEPLETION, DECAY HEAT.**

1. INTRODUCTION

The ASTRID (acronym for Advanced Sodium Technological Reactor for Industrial Demonstration) demonstrator is an innovative Sodium Fast Reactor (SFR) core representative of technological options and performances of the future SFR industrial cores. It integrates improvements concerning safety, performances and resource economy. It will also have a capability for minor actinides transmutation and will contain experimental irradiations (in support to the SFR development). It will be put into operation in the 2020's.

The ASTRID design exhibits rather unusual features compared to past designs and requires improved tools [1] with accuracies meeting the design team requirements. In parallel, CEA and its industrial partners have launched a large program for developing a new generation of simulation codes facing the challenges of multiphysics coupling and high-performance computing on massively parallel computers. These codes belong to the new CEA simulation neutron platform.

The ASTRID neutron parameters for design and safety studies will be determined with 3 different neutron tools relying on the new CEA simulation neutron platform:

- the core physics tool, based on the APOLLO3® [2] [3] new deterministic transport code;
- the shielding tool, based on the TRIPOLI4® [4] stochastic code:
- the fuel cycle and depletion tool, based on the APOLLO3® and TRIPOLI4® neutron transport codes, and the MENDEL [5] depletion code. Note that these three codes share the same depletion solver.

The fuel cycle and depletion tool is called DARWIN3-SFR and is under development. It makes it possible to determine the physical parameters characterizing the fuel cycle, the material activation and the core decay heat. They are calculated since the reactor shutdown until at least 1000 years, for all the core constituents, containing actinides, fission and activation products (respectively noted FPs and APs).

The objectives of the DARWIN3-SFR tool are:

- To be consistent (in terms of codes, calculation schemes, nuclear data libraries) with the other neutron tools (in particular the core physics tool, APOLLO3-SFR) used for the ASTRID design and safety calculations,
- To be more easily implemented, more flexible in use, than the previous DARWIN2-SFR [6] tool (based on the ERANOS2 [7] and DARWIN/PEPIN2 [8] codes),
- To have an extended validation domain,
- To determine uncertainties associated with physical calculated parameters by propagation of nuclear data covariances,
- To improve the input data consistency between fuel cycle and activation calculations,
- To improve the post-processing of the calculation results and the accessibility to input data (visualization of nuclear data for example),
- To benefit from the new functionalities introduced in the MENDEL depletion code,
- To benefit from the performances of the new APOLLO3® SFR flux calculation scheme.

The tool will have to be industrialized by the end of 2017, during the ASTRID Basic Design Phase (2016-2019) to perform the studies required by the ASTRID preliminary safety report foreseen in 2019. The preliminary safety report will integrate the feedback of the Verification&Validation-Uncertainty Quantification (V&V-UQ) process on the tool application domain.

This paper describes the new DARWIN3-SFR tool and gives elements of the V&V-UQ process implemented for the next DARWIN3-SFR version. It also shows the first implementation of DARWIN3-SFR on a numerical benchmark to get verification elements versus the previous tool based on the DARWIN2-SFR tool.

2. DESCRIPTION OF THE DARWIN3-SFR TOOL

The DARWIN3-SFR tool makes it possible to estimate the following physical parameters, at all times of the cycle, consisting of phases under irradiation or out of neutron flux: isotopic concentrations (for actinides, fission and activation products), weights, activities, radiotoxicities, partial (α,β,γ) and total decay heat, emitted particle (α,β,γ) spectra, total neutron sources and associated spectra (induced by (α,n) reactions, spontaneous fissions and delayed neutrons).

The DARWIN3-SFR tool is a consistent set of components relying on neutron simulation codes (APOLLO3®, TRIPOLI4®, MENDEL), nuclear data libraries for neutron transport (JEFF3/GP), depletion chains, decay data (JEFF3/RDD) and activation (JEFF3/A or EAF). It contains calculation recommendations /or calculation schemes for APOLLO3®, TRIPOLI4® and MENDEL. The V&V-UQ report collecting the physical parameter calculation biases and uncertainties is associated with the tool.

The DARWIN3-SFR tool integrates two calculation routes. The first one, the “standard” one, is based on the chaining between APOLLO3® and MENDEL; it will be used for calculations concerning the ASTRID core. The second one, less “standard”, is based on the chaining between TRIPOLI4® and MENDEL; it will be used mainly for the estimation of other parameters calculated “far” from the code, such as the secondary sodium activation and the tritium production in the primary circuit.

DARWIN3-SFR version V0 is today operational. The code chaining relative to the APOLLO3®-MENDEL route in DARWIN3-SFR is described in Figure 1. The TRIPOLI4®-MENDEL route of DARWIN3-SFR will be operational by 2017.

The APOLLO3® calculation step solves the Boltzmann and the Bateman equations, with a simplified depletion chain, at each core depletion step. At the end of the APOLLO3® calculation, a unique library, called MPO (Multi-Parameter Output) is generated. It contains for each fuel zones in the reactor core:

- the initial material balance;
- the fuel microscopic self-shielded cross-sections, spatially homogenized and collapsed from 1968 energy groups into 33 energy groups, with the neutron flux calculated with the Method Of Characteristics solver on an assembly 2D-exact geometry in infinite lattice. Due to the low impact of the self-shielding iteration and of the neutron spectrum modification during depletion for a Fast Neutron Reactor (SFR), the APOLLO3® assembly calculations for the different core fuel zones are performed only at time 0;
- the 3D scalar neutron flux in the 33-energy group mesh on the core elements (full core, assemblies, etc), for which the calculations of the fuel cycle parameters are expected. The flux is tabulated in the MPO versus burnup. It relies on a full 3D core calculation with the transport theory (SN MINARET solver) in depletion.

The options detailed in the previous paragraph are relative to the first version (V0) of the DARWIN3-SFR tool. The APOLLO3® calculation scheme of the DARWIN3-SFR next versions will be developed consistently with the APOLLO3® recommendations [9] issued in the framework of the APOLLO3-SFR tool development. The APOLLO3-SFR tool is dedicated to the ASTRID neutron core physics.

The MENDEL calculation step solves the fuel Bateman equation, under irradiation or under cooling (with no neutron flux), with a reference depletion chain. The equation solved under neutron flux (with the 4th order Runge Kutta method) uses the self-shielded cross-sections and the 33-energy group neutron flux transmitted by the APOLLO3® code thanks to the MPO structure. It makes it possible to calculate the depleted fuel inventory. The convolution of the fuel inventory with nuclear data leads to physical quantities such as decay heat, activity and radiotoxicity.

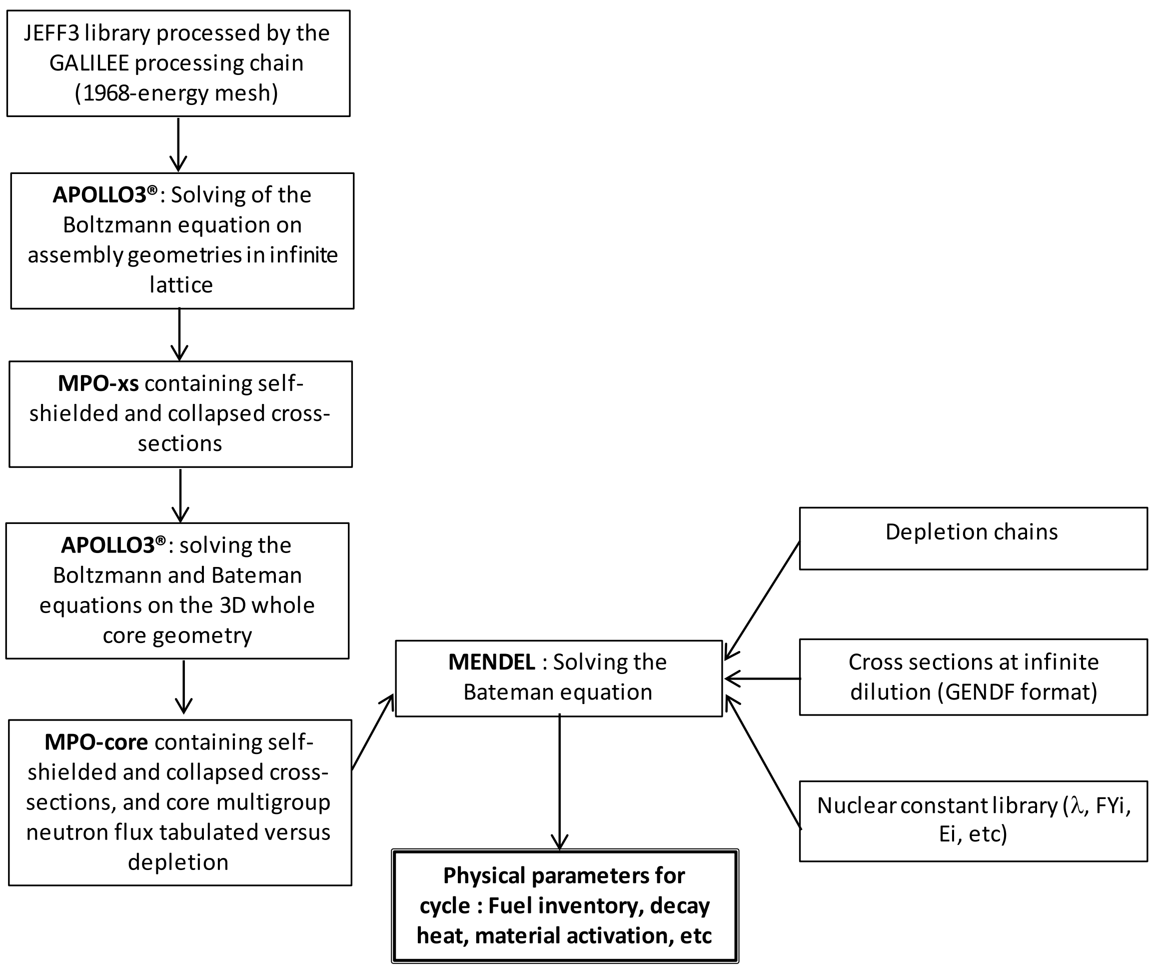

Figure 1. Description of the code chaining relative to the APOLLO3®-MENDEL route of DARWIN3-SFR

The DARWIN3-SFR tool will have to make it clear its ability to reach the accuracy levels requested by the ASTRID selected design criteria. The target-uncertainties defined for the cycle physical parameters in the ASTRID Basic Design Phase are given in Table 1.

Table 1. Target uncertainties associated with the calculation of cycle physical parameters with DARWIN3-SFR

Physical parameters calculated by DARWIN3-SFR	**Relative target uncertainty (1σ)**
Actinide and FP material balance at the end of an irradiation cycle	2% for main isotopes U and Pu 10% on other actinides 10% on main FPs
Decay heat	10% ($t_{cooling}$ < 10 s) 5% ($t_{cooling}$ > 10 s)
Spent fuel radiation dose (neutrons/g)	15%/30%
Secondary sodium activation	50%
Tritium production in the primary circuit	10%

3. V&V-UQ PROCESS IMPLEMENTED DURING THE DEVELOPMENT

The DARWIN3-SFR calculations are used to predict the ASTRID cycle parameters with quantifiable confidence and across the ASTRID application domain. The rigorous V&V-UQ process, classically used in many disciplines of science and engineering is implemented in parallel of the DARWIN3-SFR development, to calibrate the biases and uncertainties associated with the calculation tool. These biases and uncertainties will be put in perspective using the target uncertainties defined in Table 1.

The DARWIN3-SFR V&V work includes both the generic V&V work performed separately for each code APOLLO3® and MENDEL, as well as the specific V&V work performed for the tool and the application (ASTRID), consistently with the tool validation domain. Elements concerning the APOLLO3® V&V are given at this conference in reference [10]. The MENDEL V&V work began in 2012, with the calculation of several Light Water Reactor UOX and MOX cells. It made it possible to check MENDEL by comparison versus the current industrial codes APOLLO2 [11] and DARWIN/PEPIN2 and to get first validation element with the analysis of an OECD benchmark [5]. It brought into relief the MENDEL robustness and accuracy. MENDEL V&V elements for fast reactor calculations were shown in 2015; the MENDEL V&V work will de dedicated to activation calculations in 2016.

The DARWIN3-SFR specific validation will begin in 2016 and will be implemented for the next DARWIN3-SFR version V1. It can be split into 2 steps: the numerical validation step and the experimental validation step. The numerical validation step allows for the calibration of the biases due to the models, and more generally, all the approximations used in the whole tool calculation scheme or in parts of the calculation scheme. The numerical validation will rely on comparisons between APOLLO3® calculations (used in DARWIN3-SFR to estimate the neutron flux) and reference Monte Carlo calculations, at time 0.

Some complementary studies will be performed to get numerical validation elements in depletion, by comparisons between the DARWIN3-SFR calculations, TRIPOLI4®-D and APOLLO3®-MENDEL calculations with a refined energy mesh (1968 groups).

The DARWIN3-SFR experimental validation will rely on the analysis of following experiments:

1. destructive post-irradiated experiments (PIE), concerning only measurements of actinide inventory, on fuel samples irradiated in the French PHENIX experimental reactor [6]: the TRAPU experiment for SFR fissile assemblies and the DOUBLON experiment for SFR fertile assemblies,
2. measurements of SFR whole assembly dissolution campaigns in reprocessing plants,
3. measurements of fission pulses [12] [13] in fast neutron spectrum,
4. decay heat measurements in the PHENIX [14] and SUPERPHENIX reactors,
5. measurements of the secondary sodium activation [15] in the SUPERPHENIX reactor.

These experiment analyses will allow for the validation of the ASTRID fuel inventory calculation (actinides and fission products) with points 1 and 2, the ASTRID decay heat calculation with points 3 and 4, and the secondary sodium activation with point 5.

In order to get the calculation bias and uncertainty quantification on the DARWIN3-SFR application domain for the parameter set defined in Table 1, the experimental validation studies will be completed with studies of a priori nuclear data (ND) uncertainty propagation. It will be implemented for the following parameters:

- *FP material balance*: no PIE concerning measurements on FPs (except Nd isotopes which are used as burnup indicators) is available. The ND uncertainty propagation will rely on the ND covariance matrix database developed by CEA [16] and on the specific ND experimental validation works for the FP capture cross sections in a fast neutron spectrum with the analysis of the PROFIL [17], STEK and SEG [18] experiments;
- *Decay heat*: since the experimental validation will give elements on a restricted range of cooling times (a few days after the irradiation shutdown), ND uncertainty propagation [19] will be performed to estimate calculation uncertainties for the cooling times ranging from 0. s to 1000 years;
- *Spent fuel neutron radiation dose*: since no experimental data are available, ND uncertainty propagation studies will have to be done;
- *Tritium production*: tritium measurements have been performed in the PHENIX core. However, they will not be analysed: indeed, measurements are difficult to exploit due to the phenomenon complexity linked to the fuel tritium release and tritium migration through cladding. Thus, ND uncertainty propagation studies will have to be done.

4. FIRST IMPLEMENTATION OF DARWIN3-SFR ON A NUMERICAL BENCHMARK

The first implementation of DARWIN3-SFR, and thus the first chaining APOLLO3®-MENDEL were performed on a SFR-type numerical benchmark in 2015. The core (Figure 2) is composed of 6 hexagonal fuel assembly rings (a total of 91 assemblies). Only one fissile type of assembly is considered; it contains 37 (U-Pu)O_2 fuel pins. A continuous irradiation (with no operation parameter modification, no shutdowns) is modelled for 5 cycles. Each cycle lasts 200 days. The core power is 100 MW.

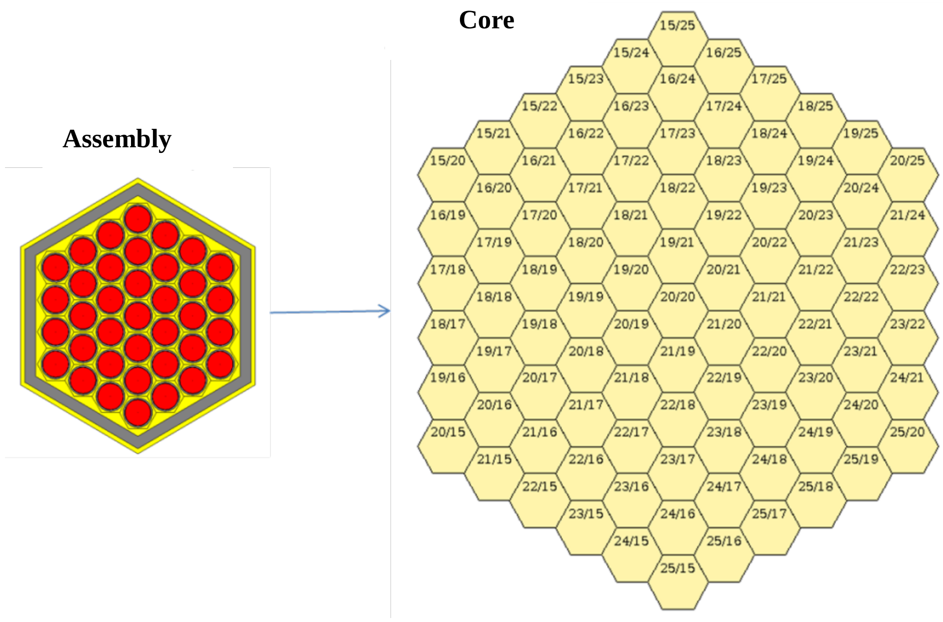

Figure 2. Description of the SFR-type numerical benchmark

The fuel inventory and the decay heat of the numerical benchmark were calculated with the DARWIN3-SFR tool, from the irradiation end to a 30-year cooling time, on the whole core and on the central and peripheral assemblies (Figure 3 and Figure 4).

Comparison elements between DARWIN3-SFR and DARWIN2-SFR were obtained on the fuel inventory (main actinides, burnup indicator nuclides, decay heat nuclides) and the decay heat. It showed the good consistency between both tools; the controlled discrepancy which were brought into relief are explained by discrepancies in the transport calculation schemes APOLLO3®-ERANOS2 and discrepancies in modelling choices between the depletion codes DARWIN/PEPIN2 and MENDEL.

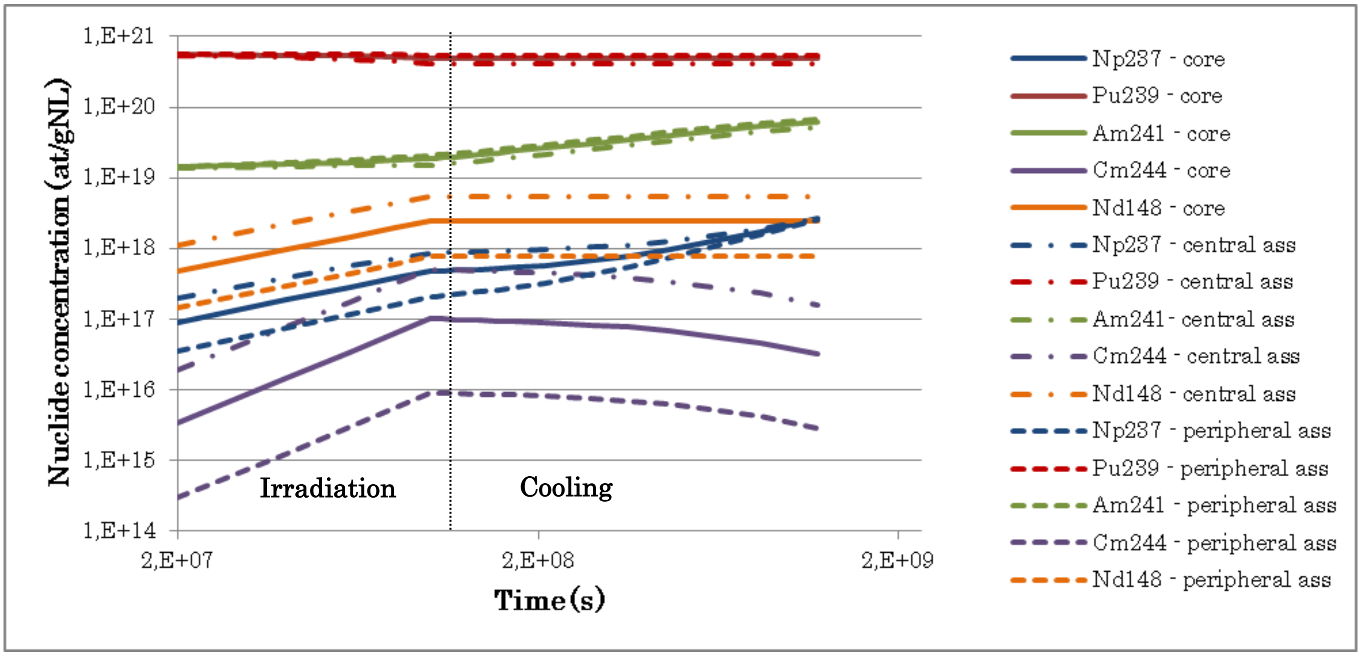

Figure 3. Nuclide concentrations calculated with DARWIN3-SFR on the SFR-type numerical benchmark for the average core, the central assembly and a peripheral assembly

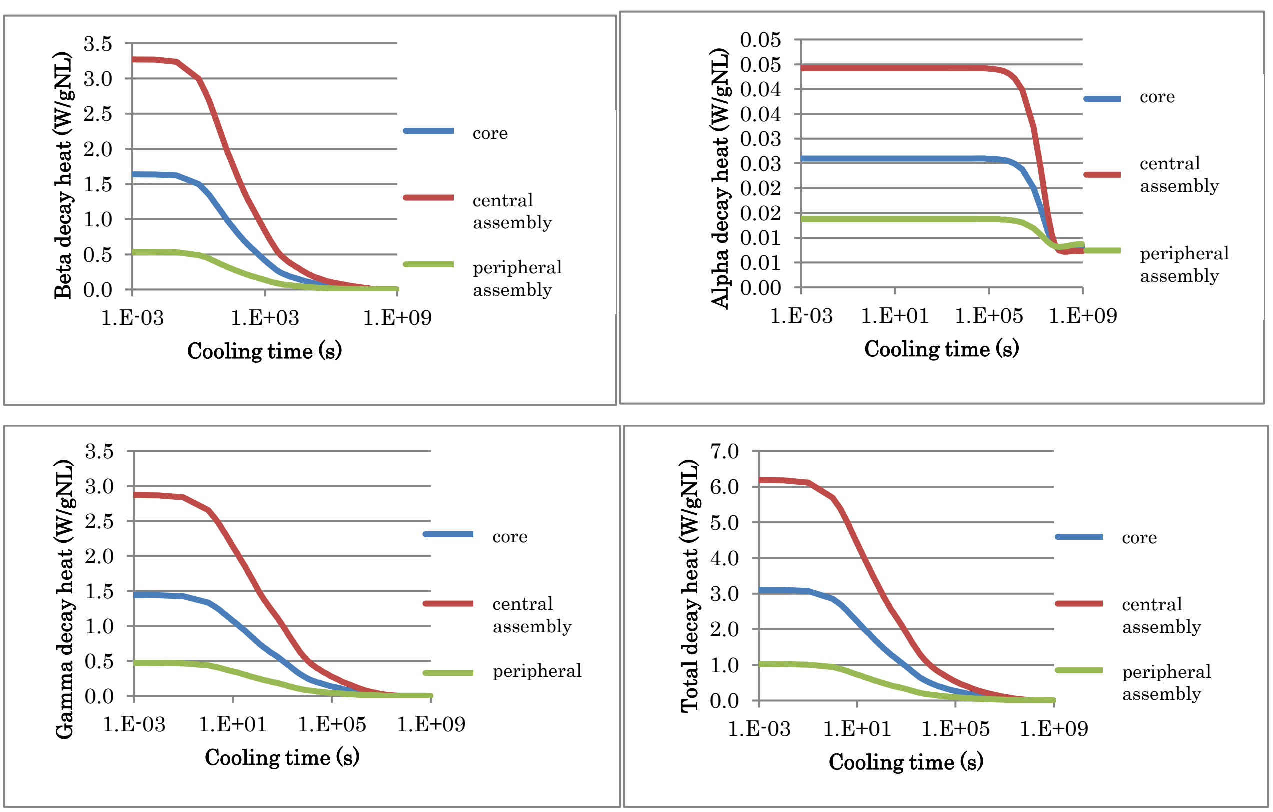

Figure 4. Decay heat calculated with DARWIN3-SFR on the SFR-type numerical benchmark for the average core, the central assembly and a peripheral assembly

5. CONCLUSION

The DARWIN3-SFR tool integrates two calculation routes: the APOLLO3®-MENDEL route and the TRIPOLI4®-MENDEL route. The APOLLO3®-MENDEL route is today operational. It makes it possible to determine the physical parameters characterizing the fuel cycle, the material activation and the core decay heat: these parameters are needed for the design and the safety demonstration of the ASTRID reactor. It integrates today the same functionalities as the previous tool used for SFR calculation, DARWIN2.3.

The V&V-UQ process is implemented in parallel of the DARWIN3-SFR development, to calibrate the biases and uncertainties associated with the calculation tool. The DARWIN3-SFR specific validation will begin in 2016 and will be implemented in the next DARWIN3-SFR version V1. The V&V-UQ report associated with DARWIN3-SFR will collect the whole bias and uncertainty set needed for the calculation of cycle physical parameters; these elements are essential for the writing of the ASTRID preliminary safety report.

The DARWIN3-SFR first implementation was performed on the numerical benchmark described in this paper, which corresponds to a homogeneous sodium core. It was the first demonstration of the APOLLO3®-MENDEL chaining feasibility. The next test step foreseen is to implement DARWIN3-SFR on a heterogeneous core, containing several fissile and fertile fuel zones, like the ASTRID core.

ACKNOWLEDGMENTS

The authors would like to thank EDF and AREVA-NP for their collaborative work and financial support concerning APOLLO3® and MENDEL code developments.

REFERENCES

[1] G. Gaillard-Groleas, “New simulation tools to be developed for the ASTRID program”, Technical meeting on Priorities in Modelling and Simulation for Fast Neutron Systems, IAEA, April 2014

[2] H. Golfier, R. Lenain, C. Calvin, JJ. Lautard, AM. Baudron, Ph. Fougeras, Ph. Magat, E. Martinolli, Y. Dutheillet, “APOLLO3: a common project of CEA, AREVA and EDF for the development of a new deterministic multi-purpose code physics analysis”, Proc. Int. Conf. M&C2009, Saratoga Springs, New York, USA, May 2009

[3] B. Roque, P. Archier, P. Bourdot, C. De Saint Jean, F. Gabriel, JM. Palau, V. Pascal, D. Schneider, G. Rimpault, JF. Vidal, “APOLLO3 roadmap for a new generation of simulation tools devoted to the neutronic core calculation of the ASTRID prototype”, Proc. Int. Conf. on Fast reactors and related fuel cycles, FR13, Paris, France, May 2013

[4] E. Brun, F. Damian, CM. Diop, E. Dumonteil, FX. Hugot, C. Jouanne, YK. Lee, F. Malvagi, A. Mazzolo, O. Petit, JC. Trama, T. Visonneau, A. Zoia, , “TRIPOLI-4, CEA, EDF and AREVA Reference Monte Carlo Code”, Proc. Int. Conf. SNA+MC 2013, Paris, France, October 2013

[5] S. Lahaye, P. Bellier, H. Mao, A. Tsilanizara, Y. Kawamoto, “First verification and validation

steps of MENDEL release 1.0 cycle code system", Proc. Int. Conf. PHYSOR2014, Kyoto, Japan, October 2014

[6] JF. Lebrat, J. Tommasi, V. Pascal, R. Eschbach, "Analysis of the TRAPU and DOUBLON irradiations in PHENIX for the experimental validation of the DARWIN package for fast reactors", Proc. Int. Conf. GLOBAL2015, Paris, September 2015

[7] JM. Ruggieri, J. Tommasi, JF. Lebrat, C. Suteau, D. Plisson-Rieunier, C. De Saint Jean, G. Rimpault, JC. Sublet, "ERANOS 2.1 : The international code system for GEN IV fast reactor analysis", Proc. Int. Conf. ICAPP'06, Reno, Nevada, USA, June 2006

[8] A. Tsilanizara, CM. Diop, B. Nimal, M. Detoc, L. Luneville, M. Chiron, TD. Huynh, I. Bresard, M. Eid, JC. Klein, B. Roque, P. Marimbeau, "DARWIN: an evolution code system for a large range applications", Journal of Nuclear Science and Technology, Supplement 1, 845-849, 2000

[9] P. Archier, J.-M. Palau, J.-F. Vidal, V. Pascal, G. Rimpault, B. Roque, S. Santandrea "New reference APOLLO3 calculation scheme for sodium cooled fast reactors: from sub-assembly to full-core calculations", at this conference

[10] JM. Palau, P. Archier, JF. Vidal, B. Roque, V. Pascal, G. Rimpault, "Recent progress in the V&V process of the new CEA APOLLO3® code: advanced FBR assembly and core calculations", at this conference

[11] R. Sanchez, I. Zmijarevic, M. Coste-Delclaux, E. Masiello, S. Santandrea, E. Martinolli, L. Villatte, N. Schwartz, N. Guler, "APOLLO2 Year 2010," Nucl. Eng. Tech., **42**, No. 5, pp. 474-499, 2010

[12] M. Akiyama, K. Furuta, T. Ida, K. Sakata, S. An, "Measurements of gamma-ray decay heat of fission products for fast neutron fission of ^{235}U, ^{239}Pu, and ^{233}U", Journal of the atomic energy society of Japan, **24**, 709, 1982

[13] M. Akiyama, S. An, "Measurement of fission-product decay heat for fast reactors", Proc. Int. Conf. on nuclear data for science and technology, Antwerp, Belgium, 1982

[14] JC. Benoit, P. Bourdot, R. Eschbach, L. Boucher, V. Pascal, B. Fontaine, L. Martin, O. Serot, "Decay heat of sodium fast reactor : comparaison of experimental measurements on the PHENIX reactor with calculations performed with the French DARWIN package", Proc. Int. Conf. PHYSOR2012, Knoxville, Tennessee, USA, 2012

[15] N. Chapoutier, A. Janet, G. Nolin, MC. Ricol, AC. Scholer, D. Verrier, C. Venard, ASTRID Core Shielding – Design Studies and Benchmark Analysis, Proc. Int. Conf. ICAPP 2015, Nice, France, 2015

[16] P. Archier, C. De Saint Jean, G. Noguere, O. Litaize, P. Leconte, C. Bouret, "COMAC: nuclear data covariance matrices library for reactor applications", Proc. Int. Conf. PHYSOR2014, Kyoto, Japan, 2014

[17] J. Tommasi, G. Noguere, "Analysis of the PROFIL and PROFIL-2 sample irradiation experiments in Phenix for JEFF-3.1 nuclear data validation", Nuclear Science and Engineering, **160**, 232-241, 2008

[18] K. Dietze, M. Ishikawa, G. Rimpault, "Integral test of neutron data and comparisons of codes by re-analysis of the SEG and STEK experiments", JEFF meeting, JEF/DOC-861, NEA, Issy-les-Moulineaux, France, 2001

[19] V. Vallet, S. Lahaye, A. Tsilanizara, L. San Felice, R. Eschbach, "Deterministic approach of the decay heat uncertainty due to JEFF-3.1.1 nuclear data uncertainties with the CYRUS tool and the DARWIN2.3 depletion code", Proc. Int. Conf. PHYSOR2014, Kyoto, Japan, 2014