Qualification of the ANET Code for Spallation Neutron Yield and Core Criticality in the KUCA ADS

Xenofontos Thalia¹, Panayiota Savva¹, Melpomeni Varvayanni¹, Jacques Maillard¹, Jorge Silva¹, Marc-Thierry Jaekel², Nicolas Catsaros¹

¹Institute of Nuclear and Radiological Sciences & Technology, Energy & Safety, National Centre for Scientific Research Demokritos, Aghia Paraskevi, Greece
²Laboratoire de Physique de l’Ecole Normale Supérieure, CNRS, Paris, France

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Abstract

Innovative nuclear reactor concepts such as the Accelerator Driven Systems (ADSs) have imposed extra requirements of simulation capabilities on the existing stochastic neutronics codes. The combination of an accelerator and a nuclear reactor in the ADS requires the simulation of both subsystems for an integrated system analysis. Therefore, a need arises for more advanced simulation tools, able to cover the broad neutron energy spectrum involved in these systems. ANET (Advanced Neutronics with Evolution and Thermal hydraulic feedback) is an under development stochastic code for simulating conventional and hybrid nuclear reactors. Successive testing applications performed throughout the ANET development have been utilized to verify and validate the new code capabilities. In this context, the ANET reliability in simulating the spallation reaction and the corresponding neutron yield as well as computing the multiplication factor of an operating ADS are here examined. More specifically, three cores of the Kyoto University Critical Assembly (KUCA) facility in Japan were analyzed focusing on the spallation neutron yield and the neutron multiplication factor. The ANET-produced results are compared with independent results obtained using the stochastic codes MCNP6.1 and MCNPX. Satisfactory agreement is found between the codes, confirming thus ANET’s capability to successfully estimate both the neutron yield of the spallation reaction and the $k_{eff}$ of a realistic ADS.

Keywords

Monte Carlo, Neutronics Analysis, Code Validation, Accelerator Driven Systems
1. Introduction

The Monte Carlo (MC) approach for reactor core analysis has steadily gained ground over the past decades due to the increased complexity of the reactor fuel and core configurations. Besides, new reactor concepts offering increased safety as well as solutions for waste management require detailed analysis with computational tools of enhanced capabilities. The Accelerator Driven System (ADS) constitutes an innovative reactor concept, since it is subcritical (i.e. safer) and can use fuel elements containing minor actinides as long-lived radioactive waste of conventional reactors, contributing thus to their optimum management via transmutation. The ADS simulation should comprise two combined parts, i.e. the one concerning the beam of deuterons or protons produced by an accelerator inducing the spallation reaction and the other concerning the nuclear reactor core. It arises that a code which can inherently deal with both ADS subsystems, i.e. a code comprising a high energy physics module and a neutronics component, would be required. The ANET development has been largely motivated by the above mentioned needs.

Until recently, the most common way to analyze ADSs was by simulating the spallation target and the sub-critical core using two different dedicated codes. Typical codes used for the spallation reaction simulation include FLUKA [1] [2] and MCNPX [3] [4] [5], while several neutronics codes are utilized for the neutronic/thermal-hydraulic subcritical core analysis, e.g. [6]. Only in a few cases [7] [8], effort has been made to analyze ADSs using a single code able to cover the broad energy neutrons spectrum involved in these systems.

The ANET development has been based on the open-source version of GEANT3.21 [9] which has been originally designed to analyze high energy physics (HEP) experiments. GEANT3.21 has been utilized as capable to simulate the passage of elementary particles through matter providing thus a tool for the analysis of the ADS accelerator/spallation target subsystem. At a first stage, the GEANT3.21 capability to be applied on nuclear reactor analysis was sought through the expansion of the treated energy spectrum to lower energies, so as to include the part involved in neutronics analysis and also through the incorporation of fission reactions [10] [11]. In the current ANET version, a bulk of subroutines has been incorporated so that the computation of the neutron multiplication factor, the neutron flux and the reaction rates are treated strictly with the stochastic approach using the standard MC estimators [12]. ANET code is continuously developing targeting at an enhanced MC code which will be also capable of performing core isotopic evolution calculations for conventional and innovative reactors, being at the same time prepared to be coupled with thermal-hydraulic solvers. The ANET code performance on dynamic reactor core analysis was preliminarily tested [13] and proved very promising indicating the code capability to inherently provide a reasonable prediction for the core inventory evolution. Moreover in [14], the ANET preliminary results are presented for an ADS concept that can operate as a breeder reactor. The present work fo-
cuses to the steady state ANET applicability to ADSs and in particular to its ability to inherently simulate the spallation process and compute the resulting neutron yield as well as the neutron multiplication factor of an operating ADS.

2. The ANET Code

ANET’s development efforts begun in the 1990s based on the open-source HEP code GEANT3.21, utilizing FORTRAN 90 as programming language. The main target for ANET’s development is the creation of an enhanced computational tool in the field of reactor analysis, capable of simulating both GEN II/III reactors and ADSs. ANET is structured with the inherent capability of a) performing core evolution and fuel burnup calculations and b) simulating the spallation process in the ADS analysis, in addition to the classical static stochastic neutronics analysis. ANET is developed based on the estimation that numerous advanced codes should exist, for intercomparison and cross checking purposes. ANET also aspires to respond to the Nuclear Community’s need for an advanced open source code.

The basis for ANET code was established following a fundamental GEANT3.21 modification, i.e. applicability extension for neutron energies below 20 MeV, which is the region of the neutron energy spectrum involved in fission nuclear reactors’ analysis. During the particle tracking, the energy of the particle is checked and the particle is accordingly treated either by FLUKA or INCL/ABLA [15] for energies above 20 MeV or by standard ANET procedures (energy below 20 MeV). As a result, particles of a wide range of energies can be inherently simulated in ANET.

Concerning neutrons interactions, at this stage ANET includes elastic collision, capture and fission. For elastic collision, the energy dependent angular distribution is used, taking also into account the effect of temperature. The treatment of the inelastic scattering will be implemented in the code in the near future.

Point by point cross sections are pre-tabulated, using available nuclear data libraries for each nuclide-energy pair while \( S(\alpha, \beta) \) and probability tables can be utilized when required. For the current version of ANET the JEFF neutron library is available.

The current version of ANET code utilizes the three standard MC estimators for the neutron multiplication factor (\( k_{eff} \)) calculation; that is the collision estimator, the absorption estimator and the track-length estimator are included. Regarding the simulation of neutron flux and reaction rates, the collision and the track-length estimators are implemented in ANET following the standard MC procedure. In addition, the ANET code has been successfully validated for its capability to reliably predict basic parameters of critical and subcritical reactor systems, namely the multiplication factor, neutron fluxes as well as neutron reaction rates, using international benchmarks and data from various installations [12].
3. Kyoto University Critical Assembly (KUCA)

The KUCA is located at the Kyoto University, Institute for Integrated Radiation and Nuclear Science (KURNS). The facility combines a subcritical assembly of solid- or water-moderated and reflected cores with the new fixed-field alternating gradient type accelerator installed in 2008. Thus pulsed protons of 100 MeV are injected onto the heavy metal target of Pb-Bi and the spallation neutrons produced are directed into the subcritical system. The latter is loaded with highly enriched uranium fuel while it is moderated and reflected with polyethylene or water [16]. At KUCA, cores A and B are moderated and reflected by polyethylene while core C is light water-moderated and reflected. At the normal operating state the three cores are operated at a very low power level (order of mW), while maximum power is 100 W.

For the present work, core A (Figure 1(a)) and particularly three variations of the main part of this core, i.e. Cases 1, 2 and 3 (Figure 1(b)-(d)) are selected. The normal fuel assembly in this core is represented as (F, 3/8"P36EU). It is composed of 36 fuel plates (unit cells) contained between two polyethylene blocks in an Al sheath. The Pb-Bi loaded fuel rod is consisted of 60 fuel plates, half of which contain Pb-Bi. At both rod boundaries polyethylene blocks exist. The aforementioned Al sheathing endues the above components. In the fuel area of the normal fuel assemblies a unit cell includes an enriched uranium fuel plate and two polyethylene plates. The Pb-Bi loaded fuel assemblies include two unit cells, both of them containing a highly-enriched uranium (HEU) fuel plate and a polyethylene or Pb-Bi plate. For the selected core configurations, all the control and safety rods are withdrawn. Precise descriptions of the fuel assemblies as well as the atom densities of the materials that compose the core elements, i.e. the HEU fuel plate, the polyethylene reflector, the polyethylene moderator, the aluminum sheath, the spallation target and the coating materials over Pb-Bi plate, are presented in detail in [16]. Regarding the accelerator, the main characteristics of the proton beam are 1 nA intensity, 20 Hz pulsed frequency, 100 ns pulsed width and 40 mm diameter spot size at the spallation target. A detailed description of the experiments that are conducted in the Kyoto University facility along with the relevant results can be found in [16].

4. Simulations

In the frame of the validation and verification of ANET’s capability to fully analyse an operating ADS, i.e. simulate the proton beam, the spallation reaction on the target, the spallation-generated neutrons (i.e. the neutron yield), and finally compute the neutron multiplication factor $k_{\text{eff}}$ of the subcritical core, the KUCA configurations 4, 5 and 6 were chosen. For this task, ANET results were compared to the results produced by the well-established stochastic neutronics codes MCNP6.1 [17] and MCNPX [18].

The core was modelled in a three-dimensional geometry by ANET and MCNP6.1 while the reference libraries for this task were JEFF3.1.2, ENDFBV-II
Figure 1. Top view of the KUCA A-core with 100 MeV protons. (b) Case 1. (c) Case 2. (d) Case 3.

and JENDL/HE-2007. MCNPX and the JENDL/HE-2007 library were employed for the simulation of the spallation procedure and the prediction of the neutron yield of the Pb-Bi target. ANET simulated the 100 MeV proton beam and the Pb-Bi target so as to produce the neutrons generated from spallation with the incorporated FLUKA module. The initial spatial and energetic distribution of the neutrons is the one derived from the spallation process. In ANET, $2 \times 10^4$ cycles of $3 \times 10^4$ particles were considered, which for the first cycle were protons while the neutrons generated from the spallation were stored and utilized for the second cycle. Subsequently, the standard MC treatment for the simulation cycles was applied. The neutron yield results for ANET are presented in Table 1 and are in very good agreement with the MCNPX results [19].
Table 1. Neutron yield computed by the ANET and MCNPX codes.

| Code/Neutron Library     | Neutron yield |
|-------------------------|---------------|
| ANET/JEFF3.1.2          | 0.39 ± 0.01   |
| MCNPX/JENDL/HE-2007     | 0.38 ± 0.01   |

Table 2. Comparison between the results of keff by ANET and MCNP6.1 codes.

| Code/Neutron Library     | Case 1       | Case 2       | Case 3       |
|-------------------------|--------------|--------------|--------------|
| ANET/JEFF3.1.2          | 0.95111 ± 4.0e−04 | 0.90667 ± 4.3e−04 | 0.89319 ± 4.2e−04 |
| MCNP6.1/ENDFBV-II       | 0.95784 ± 4.0e−04 | 0.91355 ± 4.0e−04 | 0.90006 ± 4.0e−04 |
| MCNP6.1/JENDL/HE-2007  | 0.95409 ± 1.1e−04 | 0.90996 ± 1.0e−04 | 0.89641 ± 1.0e−04 |

The results concerning the keff including the value obtained by MCNP6.1 simulations performed in the KUCA laboratory [16] [20], are presented in Table 2. ANET vs MCNP results’ discrepancies concerning keff are 673 pcm and 298 pcm for Case 1, 688 pcm and 329 pcm for Case 2, and 687 pcm and 322 pcm for Case 3 for MCNP/ENDFBV-II and MCNP/JENDL/HE-2007 respectively. In all cases, the ANET/MCNP discrepancies remain equivalent to, or lower than those found in typical benchmarks [21] and it is noticeable that ANET and MCNP6.1 results when using JENDL/HE-2007 are in better agreement compared to those obtained by MCNP6.1/ENDFBV-II. The intercomparison of MCNP6.1 keff computations with ENDFBV-II and JENDL/HE-2007 reveal variations ranging from 359 pcm to 375 pcm. The keff simulations point out that the influence of the neutron library on the results should be further studied.

5. Conclusions & Future Work

Three core configurations of the KUCA system were fully modelled by ANET in order to perform criticality tests in an operating ADS. FLUKA was employed as a high energy physics simulator in ANET to perform the spallation simulation and compute the neutron yield while the keff was computed by utilizing exclusively the relevant procedures for the standard stochastic estimators incorporated in ANET. The results were compared with independent simulations conducted at the KUCA facility using MCNP6.1 and MCNPX. The comparison showed that ANET successfully simulates the neutron yield of the spallation process as well as the criticality of an ADS indicating thus that the development of this advanced stochastic neutronics code, targeting to analyze not only conventional but innovative nuclear fission reactors as well, is proceeding satisfactorily. Further, a key point to ANET’s development has been the incorporation of new procedures that account for the assessment of the temporal changes in the fuel composition with very promising preliminary results [13]. This feature will also be validated by comparison with very recent measurement results of nuclear
transmutation of Minor Actinides (Np-237 and Am-241) obtained in KUCA [22].

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Conflicts of Interest

The authors of this manuscript wish to declare that there is not any conflict of interest regarding this work.

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