# Development and Benchmark calculations of Monte Carlo Transport Program MATS for R&D of Accelerator-Driven System

**Authors:** Wei, Xiao-Qiang, Cai, Hanjie, Mr. Xunchao Zhang, Pu, Dr. Neng, Fang, Mr. Peng, Jia, Huan, Prof. Yuan He (何源), Yongwei Yang, Prof. Rong Wang, Yan, Prof. Mingfei, Zhu, Xiao-Chong, Mr. Peng Hui, Luo, Xinyuan, He, Prof. Yuan 何源

**Date:** 2024-12-23T22:50:41+00:00

## Abstract

Accelerator-driven System (ADS) is widely regarded as the most effective transmutation solution for nuclear waste. The Monte Carlo transport simulation of full-energy-range particles, which are involved in both the spallation target and the sub-critical blanket, forms the foundation of ADS simulation studies. A Monte Carlo program named MATS has been developed in conjunction with ADS research activities and development projects in China, aiming to achieve key technology breakthroughs as well as facility construction. This paper introduces the development background of the program, the transport framework and functional modules developed for full-energy-range transport, along with validations and conclusions. Benchmark calculations of the OECD-ADS model demonstrate that MATS can be used to perform ADS physical studies with reasonable deviations for both the spallation target and the sub-critical reactor.

## Full Text

## Development and Benchmark Calculations of Monte Carlo Transport Program MATS for R&D of Accelerator-Driven Systems

Xiao-Qiang Wei,[1,2] Han-Jie Cai,[1,2,†] Xun-Chao Zhang,[1,2] Neng Pu,[1,2] Peng Fang,[1,2] Huan Jia,[1,2] Yuan He,[1,2,‡] Yong-Wei Yang,[1,2] Rong Wang,[1,2] Mingfei Yan,[3,4] Xiao-Chong Zhu,[1,2] Peng Hui,[1,2] and Xin-Yuan Luo[1,2]

[1]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China

[2]School of Nuclear Science and Technology, University of the Chinese Academy of Sciences, Beijing 100049, China
[3]School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China
[4]RIKEN Center for Advanced Photonics, RIKEN, Wako 351-0198, Japan

Accelerator-driven systems (ADS) are widely regarded as the most effective solution for nuclear waste transmutation. Monte Carlo transport simulation of full-energy-range particles, which are involved in both the spallation target and the sub-critical blanket, forms the foundation of ADS simulation studies. A Monte Carlo program named MATS has been developed for this purpose.

Deterministic codes have traditionally served as the primary tools for reactor physics analysis [22–25]. With advancing computational capabilities, the number of Monte Carlo programs applied to nuclear reactor research and development has grown steadily. Typical Monte Carlo programs such as MC21 [26], Serpent [27], JMCT [28], RMC [29,30], SuperMC [31], NECP-MCX [32], and OpenMC [33] can simulate the transport and reactions of low-energy neutrons in ADS reactors. Compared to deterministic neutron transport programs, Monte Carlo methods can provide more accurate and spatially dependent neutronics characteristics in realistic three-dimensional geometries of arbitrary complexity. However, like deterministic programs, these Monte Carlo codes rely on external neutron information provided by a first-step simulation when applied to ADS analysis.

In the sub-critical reactor of an ADS, a certain fraction of neutrons exceeds 20 MeV. Although relatively small in proportion, these high-energy neutrons play a pivotal role in defining the neutronics characteristics of the system. The Monte Carlo programs mentioned above are primarily designed for critical reactors and are based on nuclear data libraries. The completeness and accuracy of nuclear data, particularly the scarcity of experimental data involving high-energy neutron interactions with actinides, impose significant limitations on data-driven Monte Carlo programs for ADS simulations. At Los Alamos National Laboratory, the MCNPX program [34] and its enhanced version MCNP6 [35] have been developed to perform both reactor calculations and full-energy-range Monte Carlo simulations of ADS. MCNPX/MCNP6 integrates several functional modules and physical models, enabling the simulation of transport and reactions of high-energy particles in both the spallation target and the sub-critical blanket. This capability is essential, as two-step methods tend to underestimate neutron fluence in the sub-critical reactor, resulting in an overestimation of beam requirements by 20%–30% [20]. Along with the development of ADS facilities in China, a Monte Carlo program named MATS has been developed, enabling users to simulate the transport processes of protons, neutrons, pions, and main light nuclei across the full energy range of ADS target-reactor systems.

MATS is based on the GMT program [36,37], which was developed by the Institute of Modern Physics, Chinese Academy of Sciences, for ADS target simulation. It also incorporates elements from OpenMC, an open-source reactor-oriented program developed by MIT. MATS implements the transport and physics codes from GMT within the framework of OpenMC, enabling comprehensive simulation of transport processes in an ADS, from high-energy protons hitting the target to neutronics characteristics in the sub-critical blanket.

[Figure 1: see original paper] (Color online) The modules and framework of MATS.

## II. Framework and Functional Modules Developed for Full-Energy-Range Transport

### A. Bases and Framework of MATS

The Monte Carlo programs GMT and OpenMC each have distinct features dedicated to transport simulations of high-energy charged particles and neutrons, respectively. OpenMC features comprehensive modules for reactor calculations and tally functions [38]. MATS integrates these two programs by incorporating GMT's functional modules for charged particles and high-energy neutrons—including the electromagnetic calculation module, hadronic interaction simulation module, and high-energy cross-section module [36]—into OpenMC's framework. As depicted in Fig. 1, the newly integrated modules for MATS are highlighted in red. Furthermore, the particle definition module, particle advance function, and tally module have been extended, as illustrated in Fig. 2 [Figure 2: see original paper].

The basic particle definitions in OpenMC have been extended to include particles necessary for ADS computations, such as protons, high-energy neutrons (>20 MeV), pions, and light nuclei from deuteron to carbon. During program initialization, MATS incorporates the ionization energy loss calculation module from GMT. This process involves establishing energy loss-range relationships for each charged particle (excluding general ions) and each nuclide, storing the data in memory as a hash table for direct retrieval during subsequent particle transport.

Once cross-section calculations are completed, particles proceed to move forward. Since the transport processes of charged particles differ significantly from those of neutrons, MATS adopts the charged particle transport method from GMT. Charged particles are advanced step by step using the same ray-tracing technique as GMT until a collision event occurs. The loop terminates only when the particle reaches a collision point or when its energy falls below the low-energy cutoff. If a particle survives after a track without interaction, it will traverse the current geometric entity. Before that, the particle is positioned at the surface of the next geometric entity. In this scenario, the particle has reached the boundary, so its spatial position remains unchanged; only the geometric entity it is associated with is updated.

When a particle reaches a collision position, for neutrons and photons with energies below 20 MeV, MATS employs the original processing code from OpenMC. For particles in other scenarios, the hadronic interaction module is utilized. In the case of ordinary elastic scattering, the program directly computes the scattering angle, with the particle changing direction and losing energy accordingly. In the case of electron knock-out scattering, the program first calculates the energy of the knocked-out electron and samples its direction. Then it calculates the scattering angle for the incident particle. Ultimately, this process results in the production of an electron, with the energy and direction of the incident particle being altered.

In MATS, the original post-processing functions of OpenMC have been modified to accommodate new transport and reaction modules. This includes statistical analysis of heat production, flux, reaction rates of high-energy interactions, and time-dependent phenomena. As depicted in Fig. 2, through the combination of functions from the two programs, MATS has gained the capability to simulate the entire physical process, from proton-target interactions to the subsequent transport of secondary particles in both the spallation target and the sub-critical blanket. This is particularly relevant in the simulation of an ADS subcritical system.

### B. High-Energy Cross Section Module

OpenMC is typically capable of calculating reaction cross-sections for neutrons and photons at energies below 20 MeV, depending on the nuclide cross-section database used. When neutron energies exceed 20 MeV or when dealing with new particle types, MATS directly derives high-energy cross-sections for elastic scattering, inelastic scattering, and electron knock-out processes, utilizing the cross-section module from GMT.

Within MATS, the Glauber calculation method [39] in combination with a data-based approach is employed to calculate strong interaction cross-sections. This includes calculations of both elastic and non-elastic reaction cross-sections between hadrons and atomic nuclei, as well as between nuclei themselves. For proton and pion elastic and non-elastic reactions with atomic nuclei where abundant experimental or evaluated data exist (representative elements such as aluminum, copper, and lead), the cross-section data are listed and stored. When calculating proton and pion reaction cross-sections, empirical fitting and interpolation based on the listed data can be applied to obtain better accuracy.

### C. Electromagnetic and Tracking Modules

The electromagnetic module calculates ionization/excitation energy loss based on the Bethe-Bloch formula, as shown in Eq. (1):

$$\frac{dE}{dx} = 4\pi N_A r_e^2 m_e c^2 \frac{z^2 Z}{\beta^2}\left[\ln\left(\frac{2m_e c^2\beta^2\gamma^2}{I}\right) - \beta^2 - \delta\right]$$

In the equation, $z$ represents the charge of the incident particle; $Z$ and $A$ denote the atomic number and mass number of the material's atoms, respectively; $m_e$ stands for the electron mass; $r_e$ signifies the classical electron radius; $N_A$ denotes Avogadro's constant; $I$ represents the average excitation energy; and $\delta$ signifies the density effect correction.

During program initialization, the energy deposition rate $dE/dx$ is precalculated for materials specified in the model, thereby determining the ranges of charged particles at various energies in different materials. This computed data is then stored in tabular format for efficient and direct retrieval during subsequent particle transport simulations.

For the electromagnetic process of Coulomb scattering, the program employs the multiple scattering method, which is grounded in Molière theory. This method is used for the distribution of Coulomb scattering angles [40] and is applicable to charged particles across a wide energy range.

For charged particles, the electromagnetic process is continuous, making it impossible to calculate the collision distance directly as done in neutron transport. Our program uses the ray-tracking method to determine the physical collision points of charged particles. This method is combined with step limits of the particles to determine their transport distances.

This method uses the concept of $n\lambda$ in the particle transport process, converting the collision distance into a specific coefficient of the mean free path: $n\lambda = \Sigma_t \cdot l$, where $\Sigma_t$ is the total macroscopic cross-section and $l$ is the distance. The randomized value $n\lambda$ follows the probability distribution:

$$P(n_r < n\lambda) = 1 - e^{-n\lambda}$$

Therefore, the sampling formula for $n\lambda$ is derived as follows:

$$n\lambda = -\log(\eta)$$

where $\eta$ represents a random variable uniformly distributed in the interval $(0, 1)$. Once $n\lambda$ is determined through sampling, it is then updated at each step of the particle's track, which is expressed as:

$$n\lambda' = n\lambda - \Delta x$$

When $n\lambda'$ is sufficiently small, it indicates that the particle has reached the collision point, thus ending its current advancement.

### D. Hadronic Interaction Modules

In the process of hadronic interaction during particle transport, the most crucial aspect is the spallation reactions of high-energy particles. Spallation is a type of nuclear reaction where a relativistic hadron or light nucleus bombards a high mass number nucleus, triggering a cascade of intranuclear hadronic interactions and de-excitation processes. This reaction results in the emission of numerous hadrons (primarily neutrons, protons, and pions) and light-nucleus particles. Typically, the de-excitation process is accompanied by the production of fission fragments.

As previously mentioned, the spallation reaction can generally be divided into two stages: the Intra-Nuclear Cascade (INC) process and the de-excitation process of the residual nucleus [41,42]. Several INC models and evaporation/fission models have been developed over the past three decades. INC models such as CEM, BERTINI, ISABEL, and INCL have been widely adopted in Monte Carlo programs.

In the domain of evaporation/fission models, eminent contenders such as ABLA [43] and DRENSER [44] are prominent. Beyond the INC and de-excitation processes, it is generally accepted that a pre-equilibrium process exists between the two stages. This process allows the highly excited residual nucleus to transition to an equilibrium compound nucleus by emitting a neutron or a light charged particle with slightly higher energy than those evaporated during the de-excitation process. In many Monte Carlo programs, the pre-equilibrium process is often not explicitly considered, mainly because many INC models have already implemented it.

The reliability of using the INCL model to simulate particle-nucleus interactions within the GMT framework has been meticulously substantiated [36], along with the ABLA [43] model for heavy residual nucleus de-excitation and the Fermi Break-up model for light nuclei. MATS has integrated these three models, making them more modular and easily disabled or replaced with minor modifications, thus facilitating subsequent program updates. For elastic interactions, MATS employs the well-established Glauber model, effectively simulating the elastic nuclear scattering process. It is noteworthy that the electron knock-out process mentioned in the electromagnetic module is also classified as one type of elastic interaction in the program.

## III. Benchmark Calculations

### A. The Benchmark Model

The OECD-ADS model, a 377 MWth small-size ADS sub-critical blanket, is chosen for numerical validation of MATS. Proposed by the Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) in collaboration with seven institutions (ANL, CIEMAT, KAERI, JAERI, PSI/CEA, RIT, and SCK • CEN), this benchmark model is designed to compare

ADS neutronics parameters utilizing various programs and evaluated nuclear data libraries [45]. In the benchmark calculations, a predefined spallation neutron source produced with HETC was provided to participants for reactor calculations, assuming a proton energy of 1 GeV and a beam radius of 10 cm.

[Figure 3: see original paper] shows the OECD-ADS benchmark model. The concept includes four fuel regions. The central region represents the target area, with a void region above it housing the beam pipe space. Encircling the target area is the fuel region, and the outermost layer is the reflector region. Details of the materials in the target, fuel, and reflector regions can be found in the reference for the OECD/NEA benchmark work [45].

A cylindrical target made of lead-bismuth eutectic (LBE) material was modeled, with a height of 150 cm and a radius of 20 cm. The Cartesian coordinate system was adopted, with the origin set at the center of the target's bottom surface, and the cylinder axis defined as the Z-axis. Surrounding the target, a fuel region was modeled with a height of 100 cm, an inner radius of 20 cm, and an outer radius of 92 cm. A cylindrical reflector region with a thickness of 50 cm was constructed to encompass the fuel region. An ideal beam of uniformly distributed protons with a radius of 10 cm was directed towards the target at coordinates (0, 0, 150) with a direction vector of (0, 0, -1). In the simulation, the ENDF/B-VII.0 database was used for neutron calculations, while photon data was obtained from the ENDF/B-VII.1 database.

### B. Benchmark Calculations of Spallation Target

**1. Neutron Fluence and Neutron Yield** The physical processes within the target, including electromagnetic and hadronic interactions, directly determine the yield and energy spectrum of leakage neutrons, both of which are crucial for computation of the sub-critical reactor system. The simulation was carried out with 1 million proton particles, each with an energy of 1 GeV, directed towards the target as described in the previous subsection. The resulting neutron fluence distribution, heat deposition distribution within the target, and leakage neutron energy spectrum were obtained.

The results from MATS were compared with those from other Monte Carlo programs, including MCNPX 2.5.0, Geant4, and PHITS. For both MATS and Geant4 simulations, the INC model used was INCL++ [46], with MATS employing version 5.1 and Geant4 employing version 6.28. To minimize discrepancies caused by different physical models, the INCL model was also selected for PHITS and MCNPX simulations. PHITS used INCL4.6 [47], while MCNPX used INCL4.2. Both programs are written in Fortran. It is worth noting that INCL4.6 is the last Fortran version of the INCL model; after that, it was only distributed in C++.

[Figure 4: see original paper] illustrates the axial (H) and radial (R) distributions of neutron fluence within the target calculated by different programs. Meanwhile, [Figure 5: see original paper] displays the two-dimensional spatial distributions in H and R directions. The axial and radial distributions of neutron fluence exhibit discernible differences among different programs. As demonstrated in the figures, MATS agrees more closely with Geant4 and PHITS, yet gives a lower estimation than MCNPX. This may be attributed to the fact that MATS has adopted the newer version of the INCL model, similar to Geant4 and PHITS. INCL++ is based on INCL4.6 and has evolved significantly since it was completely redesigned and rewritten in C++ in 2012. The difference between MATS and MCNPX is about 10%. As depicted in [FIGURE:5(a-d)], the spatial distribution of neutron fluence within the target computed by MATS is roughly the same as those obtained by other programs. [FIGURE:5(e-g)] illustrate the differences in spatial distributions of neutron fluence between MATS and other programs (MCNPX, PHITS, and Geant4). It is evident that MATS has the smallest discrepancy with Geant4.

Disparities in neutron fluence within the target can lead to variations in the yield and distribution of leaked neutrons, resulting in different beam requirements for the ADS subcritical system. In addition to flux, the energy spectrum of leaked neutrons from the target also has a significant impact on the neutronics performance of the ADS sub-critical blanket. The normalized spectra of leaked neutrons calculated with MATS, MCNPX, Geant4, and PHITS are presented in [Figure 6: see original paper]. For neutrons with energies greater than 0.1 MeV—fast neutrons and high-energy neutrons that are absolutely dominant—the differences among the four programs are relatively indistinguishable. As detailed in , MATS agrees very well with Geant4 in the range of 1 MeV to 20 MeV, while generally providing a lower prediction than MCNPX. Compared with PHITS, MATS tends to underestimate the yield of high-energy neutrons by less than 5% and overestimate the number of neutrons below 20 MeV by a similar margin. Regarding the total neutron yield, the difference between MATS and Geant4 is less than 1%, while the difference between MATS and MCNPX is about 10%.

**2. Energy Deposition in Spallation Target** The calculation of energy deposition in the target is crucial for spallation target design. [Figure 7: see original paper] shows the R-Z distributions of energy deposition simulated with MATS (a), MCNPX (b), PHITS (c), and Geant4 (d), and the absolute deviations of other programs (MCNPX (e), PHITS (f), Geant4 (g)) compared to MATS, in units of $MeV/cm^3/proton$. It is evident that the heat distributions within the target calculated by different programs are generally similar, except that MCNPX gives an overall underestimation, while MATS provides a slightly lower profile at the end of the range. The total energy deposition and its relative deviation are detailed in , in units of MeV/proton. MATS's result is about 3% higher than PHITS's result and is nearly equivalent to Geant4's result. Interestingly, MCNPX underestimates the energy deposition while overestimating the neutron yield, with the magnitude of underestimation in energy deposition being nearly equivalent to the overestimation in neutron yield. This can be easily understood through energy conservation, since the overestimated neutrons take away more energy.

### C. Benchmark Calculations of Target-Reactor System

**1. External Source Efficiency** In ADS R&D, the external source efficiency $\phi^*$ serves as a crucial parameter for assessing system performance [48]. It plays a pivotal role in determining beam requirements, and its value can be evaluated by Monte Carlo simulation [10]. The $\phi^*$ is calculated with the following formula:

$$\phi^* = \frac{1 - 1/k_{\text{eff}}}{1 - 1/k_s} = \frac{\bar{\nu}R}{(\bar{\nu} + S_0)}$$

where $k_s$ is the external source multiplication factor, $R$ denotes the fission rate in the sub-critical blanket, $\bar{\nu}$ is the average number of neutrons released per fission, and $S_0$ is the intensity of the external neutron source. Normalizing each value to one external source neutron, the following equation is obtained:

$$k_{\text{eff}} = \frac{\bar{\nu}R}{\bar{\nu}R + S_0}$$

showing $\phi^*$ as equivalent neutrons induced by an external source. A larger $\phi^*$ means a smaller ratio of absorption loss to fission yield. The external source efficiencies obtained with MCNPX and MATS are compared in [Figure 8: see original paper]. One sees that the higher the energy, the larger the external neutron efficiency. Furthermore, the efficiency tends to increase exponentially with log(E) above 10 MeV. Within the energy range of 0.01 MeV to 1000 MeV, MCNPX and MATS basically agree with each other. MATS exhibits a deviation of around 4% relative to MCNPX in the energy range of 100 MeV to 1000 MeV.

**2. Notable Contributions from High-Energy Neutrons** Conventional two-step simulations using reactor-oriented programs like OpenMC often neglect high-energy neutrons in sub-critical blanket calculations due to database limitations. To mitigate this error, one approach is to reset the energy of high-energy neutrons to a value within the database energy range. However, the external source efficiency of high-energy neutrons is significantly higher than that of low-energy neutrons. To discuss the impact of neglecting high-energy neutrons in the sub-critical blanket, we consider the scenario where high-energy neutrons entering the fuel region from the target surface are reset to 20 MeV.

[FIGURE:9(a)] and [FIGURE:9(b)] show the distributions of neutron fluence in the x-y plane at z=100 cm, with and without high-energy neutrons in the fuel region, respectively. The differences are evident. The energy cutoff of neutrons results in an overall underestimation of neutron fluence. [FIGURE:10(a)] presents the neutron fluence along the x-axis at z = 100 cm and y = 0 cm, showing a relative deviation of approximately 10%. As previously mentioned, the larger the energy of a neutron, the higher its external source efficiency.

Since the neutron fluence in the target region is partly contributed by neutrons from the fuel, the energy cutoff not only leads to an underestimation of neutron fluence in the fuel region but also results in reduced fluence within the target.

As shown in [FIGURE:9(c)], [FIGURE:9(d)], and [FIGURE:10(b)], the heat density is nearly identical within the target region where the proton beam plays the dominant role in energy deposition. The deviation in the fuel region is similar to that observed for neutron fluence. An underestimation of neutron fluence will lead to an overestimation of the beam requirement [49]. The beam requirement represents the proton beam current needed to drive the reactor to operate at a fixed total power, which is expressed as:

$$I_{\text{beam}} = \frac{W_R}{Q}$$

where $W_R$ is the thermal power of the sub-critical blanket, and $Q$ denotes the average heat released in the sub-critical blanket per proton.

With a total thermal power of 377 MW, the heat released in the sub-critical blanket is 55.9 GeV/proton for complete transport simulation and 49.8 GeV/proton for energy-cut transport simulation, respectively, as detailed in . Consequently, the energy-cut transport simulation overestimates the beam requirement by more than 12%. In conclusion, the energy-cut transport method leads to significant deviations in design parameters. The capability to perform complete transport simulation of wide-energy-range particles in the sub-critical system is important not only for ADS design but also for in-core measurements and operational controls.

**3. Cross Validations** So far, only MCNPX and MCNP6 can be used for direct validation of MATS. To perform comprehensive verification and validation (V&V), two-step methods have been employed in addition to MCNPX. These methods involve using the neutrons leaking from the outer surface of a naked target, obtained from the first-step simulation, as an external source for the target-reactor in the second step. In all two-step simulations, neutrons across the full energy range are transported.

[Figure 11: see original paper] and [Figure 12: see original paper] present comparisons of neutron fluence and energy deposition distribution between direct simulation and two-step simulation. In the two-step simulation denoted as MATS-MATS, full-energy-range external neutrons are transported in the sub-critical blanket, while other external particles are neglected. [FIGURE:11(a)] shows the radial neutron distribution at z = 100 cm, while [FIGURE:11(b-d)] display the axial neutron distributions at R = 0 cm, R = 22 cm, and R = 56 cm, respectively. As shown in [Figure 11: see original paper] and [Figure 12: see original paper], the deviation in neutron fluence is at the level of 1%, while that in heat density is about 2%. These deviations can be eliminated when other external particles, including protons, pions, gammas, and light-nucleus particles, are considered in the second-step simulation. Since these deviations are smaller than those caused by differences in external neutrons from different programs, as previously described, the external particles other than neutrons are neglected in the two-step simulations to simplify the validation process, which will be detailed in the following section.

In [Figure 13: see original paper] and [Figure 14: see original paper], the direct MATS simulation is compared with the direct MCNPX simulation, and the two-step simulations that employ MCNPX, PHITS, and Geant4 for the first-step simulation of the neutron source. Since the second-step program is MATS, the conducted two-step simulations are denoted as MCNPX-MATS, PHITS-MATS, and Geant4-MATS, respectively. For the radial distributions in [FIGURE:13(a)] and [FIGURE:14(a)], the target region ranges from -20 cm to 20 cm along the X-axis, while the fuel region ranges from -92 cm to 92 cm. The axial distributions in [FIGURE:13(b-d)] and [FIGURE:14(b-d)] display the results at three typical radial distances from the central axis. [FIGURE:13(b)] and [FIGURE:14(b)] show distributions in the beam-target region, while [FIGURE:13(c-d)] and [FIGURE:14(c-d)] show distributions in the fuel region.

Clearly, one sees that the neutron fluences in both the target and fuel regions, as well as the heat density in the fuel region, are significantly higher from MCNPX and MCNPX-MATS simulations than those from MATS, PHITS-MATS, and Geant4-MATS simulations. This finding is consistent with the results of neutron fluence and yield in the naked target simulation, as previously detailed. The difference between the results of MCNPX and MCNPX-MATS is much smaller than that between MCNPX and MATS. When considering the heat power in the sub-critical blanket and the beam requirement, as listed in , the difference between MCNPX and MATS is about 10%, while the difference between MCNPX and MCNPX-MATS is about 1%. These results demonstrate that the target simulation dominantly influences the observed differences. It is noteworthy that the neutron fluence and heat density in the sub-critical blanket depend not only on the number of external neutrons but also on their energy. Although the external neutron yield from Geant4 is smaller than that from MATS, Geant4-MATS results in higher heat density in the sub-critical blanket, leading to a reduced beam requirement.

## IV. Conclusions and Outlook

Based on the Monte Carlo simulation programs OpenMC and GMT, a program named MATS has been developed, dedicated to simulation studies of the ADS target-reactor system. The physical calculation functions of MATS rely on an electromagnetic interaction module, a hadronic interaction module, a high-energy cross-section module, traditional reactor-oriented calculation functions, and the nuclear data library. This equips MATS with the capability to simulate the transport processes of particles across a wide energy range, which is essential for ADS R&D. This is because the external source efficiency is also sensitive to neutron energy. It is revealed that there is an underestimation of neutron fluence and heat density, resulting in an overestimation of beam requirement at the level of 10% or more, when neutrons with energies above 20 MeV are treated as 20 MeV neutrons. Additionally, the deviations of heat in the sub-critical blanket and beam requirement are at the level of 2% when protons, gammas, pions, and light-nucleus particles from the target are not transported in the sub-critical blanket.

The V&V of ADS spallation target simulations indicate that MATS provides a medium estimation of neutronics characteristics and heat compared to MCNPX, PHITS, and Geant4. The comparisons reveal that the differences in neutron yield and total heat between MATS and MCNPX are about 8% and 10%, respectively. MATS tends to predict higher heat and lower neutron yield than MCNPX. However, the differences between MATS simulation and those of PHITS and Geant4 are less than 5% for both neutron yield and total heat.

Regarding the target-reactor system, the difference between MCNPX and MATS is similar to that observed in target simulation. We find that the difference is primarily due to different predictions in target simulation. Additionally, there are differences in the simulations of high-energy neutrons in the sub-critical system. In terms of external source efficiency, the deviation is approximately 4% within the energy range from 100 MeV to 1000 MeV.

To perform extensive V&V, we employed the two-step method in addition to direct MCNPX simulation. In these two-step methods, the first-step simulation was performed with different programs, while the second-step simulation was done using MATS. We find that the differences in neutron fluence and heat among Geant4-MATS, PHITS-MATS, and MATS-MATS are all smaller than 5%. Our study also demonstrates that the neutron fluence and heat density in the sub-critical blanket depend not only on the number of external neutrons but also on neutron energy. Compared to the benchmark exercise [45] organized by OECD/NEA in 1999, which emphasized code and data validation in the energy region below 20 MeV, the benchmark presented in this paper represents a significant step forward. In the future, more benchmark exercises based on experimental results may be conducted to clarify discrepancies.

In summary, the development of the MATS program with fundamental calculation functions for ADS R&D has been demonstrated to be successful. Further efforts should focus on upgrading reaction models [50–52] based on an overall evaluation of calculations of high-energy neutron-induced reactions on actinide nuclides, and on developing more neutronics calculation functions [53–56] dedicated to the study of sub-critical reactors and ADS facility R&D. A user-friendly interface and more widely demanded functions including variance reduction calculations [57], radioactivity and shielding simulation [58,59], and irradiation dose assessment [60,61] are also on the to-do list to make MATS a state-of-the-art radiation simulation program for multidisciplinary applications of accelerator beams [62–64].

## V. Acknowledgments

All authors would like to extend special thanks to the OpenMC development team, and also to Davide Mancusi for providing the source code of the INCL++ model.

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