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CAD-based interface programs for fusion neutron transport simulation

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ABSTRACT

Describing and verifying of the models for three-dimensional (3D) neutron transport simulation based on Monte Carlo (MC), discrete ordinates (S_N) and MC–S_N coupled methods are time-consuming and error-prone. The conversion algorithm and corresponding CAD-based interface programs have been developed to achieve the bi-directional conversion between commercial CAD systems and the neutron transport simulation codes including MCAM program for MC simulation, SNAM program for S_N simulation and RCAM program for MC–S_N coupled simulation. This paper introduces the main functions of the three interface programs and a benchmark test based on the ITER model.

1. Introduction

Neutronics analysis is the foundation of reactor physics design, shielding analysis, fuel management optimization and nuclear safety analysis. The neutronics simulation methods can be classified into two categories: Monte Carlo (MC) method and deterministic method. The MC method is increasingly preferred for transport calculations due to its powerful capability to accurately model the physics of particle in complicated three-dimensional (3D) problem. A number of MC codes (e.g. MCNP/MCNPX [1,2], TRIPOLI [3]) have been developed by different scientific and industrial institutions over the last decades. In spite of the dramatic improvements of computer speed, the application of the MC method to generate the detailed profile or map with plenty of parameter values is still constrained because of its inherent limitations.

The deterministic method, especially the discrete ordinates (S_N) method, is most widely used for the solution of the neutron transport equation. Various 1D/2D/3D S_N codes (e.g. DOORS/TORT [4–6], VisualBUS [7]) have been developed and used to treat the deep penetration problems to get the parameters distribution map. However, the S_N method still suffers from the limitation of the geometry representation when dealing with complex 3D problems.

Therefore, in order to meet the requirements to calculate and analyze the advanced nuclear facilities such as fusion devices and accelerator systems which complex geometry and large scale as well, the coupled MC–S_N particle transport computational scheme has been developed to realize the combination of the strength and the complement of the weakness of the different MC and S_N methods.

Three integrated CAD-based interface programs between CAD systems and transport simulation codes have been developed for MC simulation (named MCAM—Monte Carlo Automatic Modeling system [8–17]), for S_N simulation (named SNAM–S_N Automatic Modeling system [18,19]) and for MC–S_N coupled simulation (named RCAM—Radiation Coupled Automatic Modeling System) to address the predicaments of transport simulation modeling. MCAM, SNAM and RCAM have been tested with the complex 3D geometry of the International Thermonuclear Experimental Reactor (ITER) benchmark model. The results and analyses have demonstrated the feasibility, effectiveness and maturity of the three programs for the complex fusion applications.

2. CAD-based interface programs

2.1. MCAM

MCAM is an interface program and an integrated modeling system implementing the bi-directional conversion between CAD model and MC simulation model and supports a series of supplementary functions such as creation and repair of CAD model and analysis of physics properties. MCAM employed a mature CAD kernel as the geometry engine and adopted component-based architecture shown in Fig. 1. With MCAM, analyzers can conveniently and rapidly create the MC models of a complex and large-scale nuclear device.

"Fixer" is to check and fix geometry errors existing in CAD model, such as small collisions and gaps between adjacent solids, which

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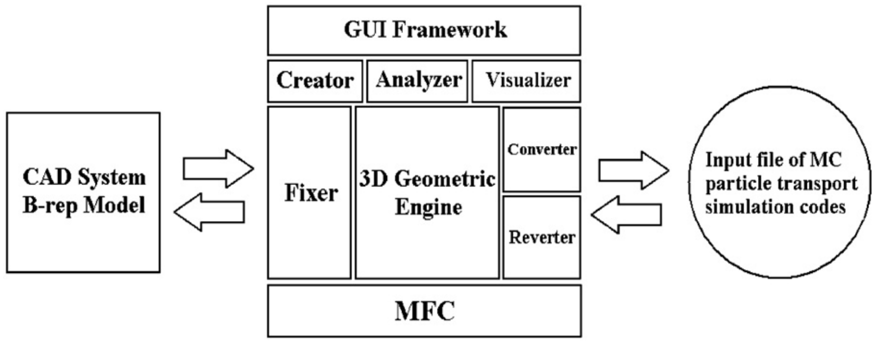

Fig. 1. MCAM architecture.

are not allowed by any particle transport simulation. "Converter" is to convert CAD model into MC simulation model. The geometry and topology information of CAD model is converted into geometry description cards such as cell card and surface card, and physics properties assigned on model are also translated into physics properties description cards, such as the cards of material, source and tally, to constitute a complete input data for MC calculation. Furthermore, void space filling function was developed to generate the void description which was not implemented in a normal CAD model created by commercial CAD software. "Reverter" is a reverse processor to produce a CAD model, which can be exported in various CAD file formats such as STEP and IGES-formats widely supported by the state-of-the art commercial CAD systems, deriving from an existing MC input file to be visualized to display not only geometry but also the physic properties. "Analyzer" enables users to add, modify, delete and edit the geometry and physics properties of a model. "Creator" supplies a variety of modeling functions of basic primitives such as box, sphere, cylinder and torus and Boolean operations (union, intersection and subtraction) so as to enable the users to create 3D geometry models directly with MCAM.

The current version of MCAM supports the MC codes MCNP and TRIPOLI. The advanced function of human body modeling in the Advance/Accurate Radiation Therapy System (ARTS) for cancer treatment [20] has been developed as well.

2.2. SNAM

Similar to MCAM, SNAM has been developed to implement the automatic conversion between CAD model and S_N model. By means of specified computer graphic algorithms, irregular geometry of CAD model can be discretized and normalized to generate regular geometries suitable for S_N simulation codes.

SNAM has four basic function modules as follows. The module "Preprocessor" checks and fixes interferences and unnecessary gaps in CAD model that are not allowed for S_N particle simulation, and generate the void description which is necessary for S_N particle simulation, but not existing in a normal CAD model. The module "Convertor" is capable of translating a normal CAD geometry into the S_N transport calculation model through discretization and normalization of model, assignment and parsing of physics properties, etc. The module "Reverter" can read a S_N input file and revert it into a CAD model with assignment of corresponding physics properties on it. The module "Creator" is used to construct a CAD solid model directly with SNAM like a normal commercial CAD system.

2.3. RCAM

The coupled MC–S_N calculation is to combine the advantages of the MC method and the S_N method to treat deep penetration problems. To perform a coupled calculation, the whole model should be split up into two parts: the source region and the bulk shield region. The MC method is used to calculate the source region with complex geometry; the S_N method is used to simulate the bulk shield region.

To achieve the coupled calculation, a transitional zone needs to be specified as a link between the MC geometric model and the S_N meshing model. In general, a common surface or a common volume should be selected as a geometric link. Since an anisotropic volume source option is currently not available for some S_N codes, a common surface is more usually used as geometric link between the models of the two methods. The MC simulation is performed to obtain the information of particle tracks (e.g. particle type, weight, flight direction, spatial position, energy) which cross the common surface. The S_N angular flux source for S_N code can be generated by using a mapping approach based on the recorded Monte Carlo particle tracks.

RCAM has been developed by combining the conversion functions of MCAM and SNAM. RCAM is used to divide a CAD model into two parts with an overlapped zone: one is the MC model and the other is the S_N model. Moreover, RCAM can be used to achieve the multi-directional conversion among a normal CAD model, a S_N model and a MC model for the solution of a specific problem. The flow chart of the RCAM is displayed in Fig. 2.

3. Testing and analysis

In order to test the capability of the above three programs for complex fusion application, the benchmarks have been performed based on the complex ITER geometric model. Neutron fluxes in various areas in the model are calculated by using the MC, S_N and MC–S_N coupled codes.

3.1. ITER benchmark model

ITER benchmark model, a toroidal 40 degree sector of the ITER device created with CATIA V5, was issued by the ITER International Organization (IO) to benchmark all the CAD-based interface programs being developed by the ITER Participant Teams (PTs).

3.1.1. Geometry

All significant components of ITER are included in the model, as shown in Fig. 3. Details have been suppressed properly and geometric simplifications were performed mainly to discard free form surfaces and reduce complexity in order to suit for all the interface programs developed by the ITER PTs. It contains 15 components composed of approximately 1000 solids with 9000 surfaces. Reflecting boundary conditions is implemented on poloidal planes that are located at $\pm 20^{\circ}$ from the center of the mid-plane port in order to create a 40 degree model. Although this model does not capture the full details of the engineering design (e.g. PF coil casings, PFC layer on dummy plugs), it is sufficient for the purpose of

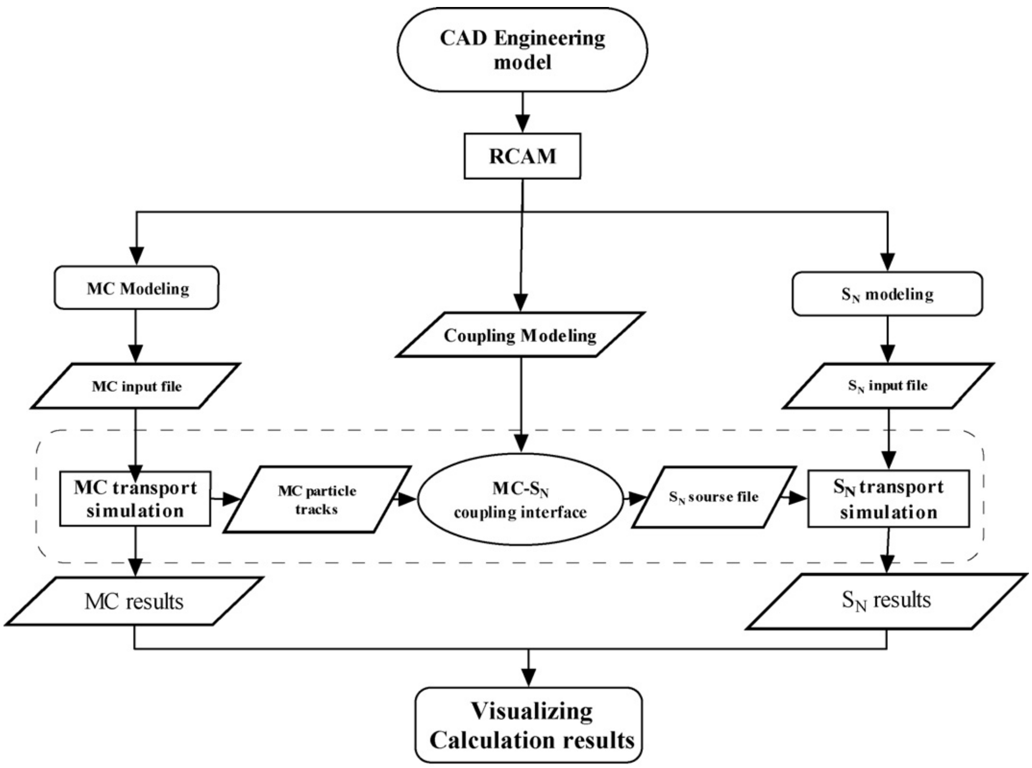

Fig. 2. Flow chart of the MC–S_N coupling modeling and calculation.

this benchmark and even may be used in some nuclear analyses although some simplifications are involved.

3.1.2. Materials and neutron cross-sections

In the model there are distributed 17 different materials shown in Table 1. The neutron cross-sections are based on FENDL 2.1 [21], with FENDL 2.0 [22] and ENDF/B-VI [23] used as alternatives for missing isotopes, in that order of preference.

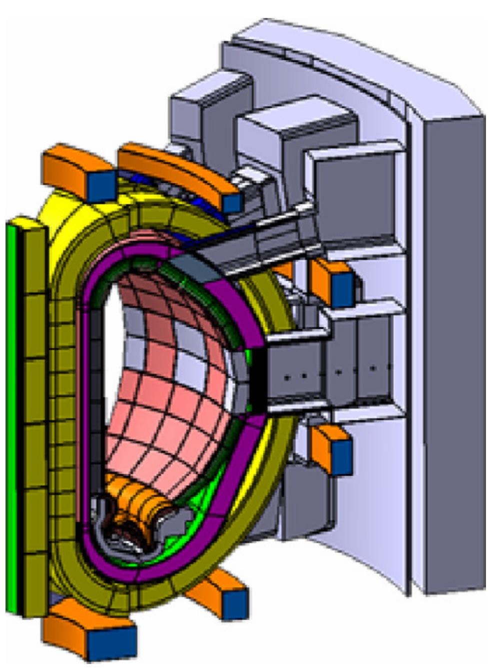

Fig. 3. ITER benchmark model in CATIA.

3.1.3. Source

The official ITER source description of 500 MW fusion power was provided as a set of FORTRAN subroutines for use with MCNP. These subroutines randomly sample the starting location from a probability table in an *r*–*z* mesh and uniformly within the 40° of the problem bounds, from −20 to 20°, with the *x*-axis defined as 0°.

3.2. Testing of MCAM and SNAM

The CAD model was converted into the input files of simulation codes automatically with MCAM and SNAM, and neutron fluxes in the inboard blanket modules of ITER benchmark model were calculated using MC and S_N codes. The conversion processing is shown in Fig. 4, including the following steps:

(1) The CAD model in STEP format is imported into the three modeling programs. Geometry errors generated in CAD file formats transformation were fixed, and unnecessary gaps and overlaps in the model were checked and removed automatically.
(2) All the solids in the model were grouped according to the material definition given in Table 1, and relevant physics properties are assigned on them. The prepared model is converted into different neutronics models, respectively for MC, S_N and MC–S_N calculations.
(3) In order to check and verify the converted neutronics model, the input files were reverted into the CAD model. The geometry, material and physics information were examined according to the original CAD model.

The MC transport calculation was performed by using MCNP/4C with the data library FENDL-2.1 and TRIPOLI with the data library ENDF/B-VI, with the statistical errors of the results of less than 3%. The S_N transport calculation was carried out by TORT with the data library MATXS10 (30 neutron groups, 12 gamma groups) [24]. The

Table 1
Main components and material composition.

Main components	Material composition (homogenized with vol.%)
PF coil stainless steel case, cryostat wall	SS304L, 100%
Bioshield	Boron concrete, 100%
PF3&PF4 support structure, TF coil stainless steel case, CS outer/inner tie plates	SS316LN, 100%
Thermal shield	SS304L, 100%
Vacuum vessel outer/inner shell, equatorial port and upper port	SS316L(N)-IG, 100%
Vacuum vessel in wall shield	SS304B7, 55%; water, 45%
Blanket module first wall	SS316L(N)-IG, 44%; water, 16.3%; Be, 14.3%; CuCrZr-IG, 25.4%
Blanket module shield block, Equatorial port and Upper port dummy plugs	SS316L(N)-IG, 70%; water, 30%
Blanket module rear layer	SS316L(N)-IG, 52.5%; water, 22.5%
TF coil winding pack	SS316LN, 47.6%; SS316L, 1.5%; He, liq., 12.9%; Nb3Sn, 6.3%; r-epoxy, 18%; Cu, 13.7%
PF coil winding pack	r-epoxy, 39%; SS316L, 41%; He, liq., 9.1%; NbTi, 1%; Cu, 9.8%; Inconel, 0.1%
Divertor body	SS316L(N)-IG, 65%; water, 35%
SS part of PFC (plasma facing component) on divertor	SS316L(N)-IG, 55%; water, 45%
PFC cooling structure on divertor	SS316L(N)-IG, 33%; water, 7.1%; CuCrZr-IG, 59.9%
PFC units on divertor	Cu, 20%; W, 80%
PFC units on divertor	CFC
CS winding pack	JK2 stainless steel, 54.7%; SS316L, 1.2% Inconel, 0.6%; He, liq., 11.2%; Cu, 11% Nb3Sn, 5.5%; r-epoxy, 15.8%

Legendre expansion of the scattering kernel is P_1 and the angular quadrature set used by TORT was S_4. The neutron fluxes in the inboard blanket (Module 4) were compared. As shown in Table 2, the calculation results by different codes agreed well and the peak difference was 12%. These differences may lie on the different data libraries used, as well as the different simulation methods, which need to be investigated further.

3.3. Testing of RCAM

The shielding calculation of ITER based on conversional methods, e.g. only MC simulation or S_N simulation is difficult due to the complex geometry and the large dimension, especially including bio-shield of meters thickness. In this benchmark, RCAM is used to generate the input files of MC and S_N codes, respectively as

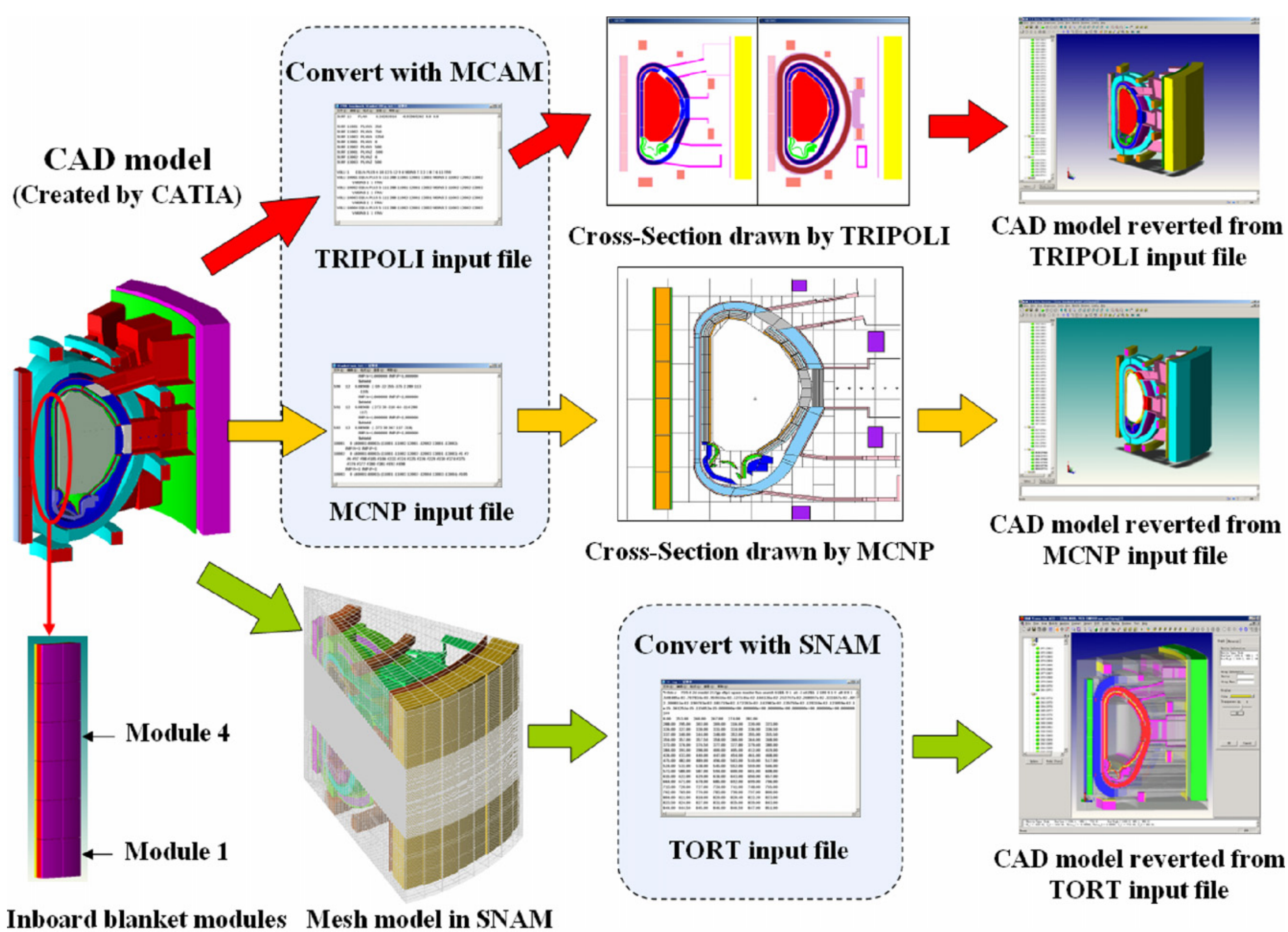

Fig. 4. Processing of ITER benchmark model by MCAM and SNAM.

Table 2
Neutron flux in module 4.

Radial range	Neutron flux (l/cm^2 s)				
	TORT	MCNP		TRIPOLI	
		Result	Error	Result	Error
359.35–370	1.359E+12	1.550E+12	2.16%	1.493E+12	2.73%
370.35–381.5	4.841E+12	4.967E+12	1.12%	4.723E+12	1.45%
381.5–393	1.940E+13	1.828E+13	0.61%	1.785E+13	0.74%
393–397.35	4.486E+13	4.153E+13	0.50%	4.092E+13	0.63%
397.35–404.5	7.465E+13	6.999E+13	0.35%	6.959E+13	0.40%

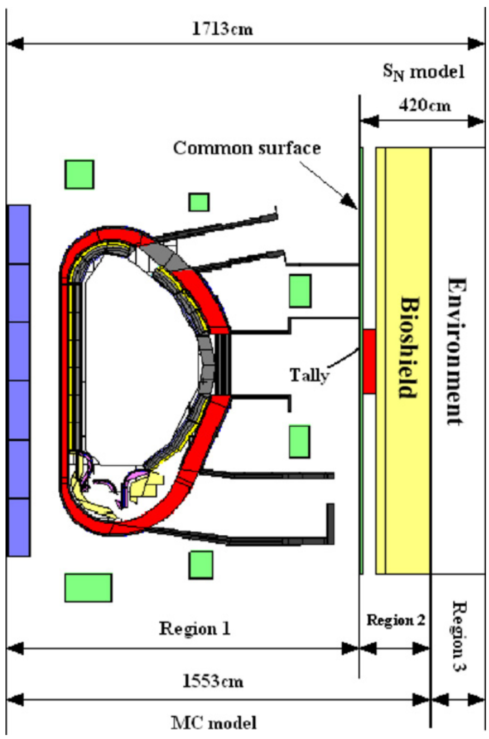

Fig. 5. Processing of ITER benchmark model by RCAM.

schematically shown in Fig. 5. The whole model was divided by the common surface (the inner surface of the cryostat) and the outer surface of bioshield into three parts: the source modeling region (Region 1) inside the common surface, transitional region (Region 2) between the common surface and the outer surface of bioshield and the environment region (Region 3). For the purpose of testing RCAM, the neutron flux in the tally area was calculated, respectively, by MCNP with the data library FENDL-2.1 based on the MC model (Region 1 + Region 2) and by the S_N code TORT the data library MATXS10 based on the S_N model (Region 2 + Region 3) with the surface source obtained from the MCNP calculation. The calculated results given in Table 3 have shown an acceptable difference (∼13%) between the two approaches, which may be caused by different transport methods (MC and S_N methods) and different nuclear data libraries (point-wise and multi-group libraries), etc.

Table 3
Neutron flux in tally area.

MCNP	
Result	1.609E+08
Stat. error	6.14%
MC–S_N coupled	1.817E+08
Error	12.95%

4. Summary

Three CAD-based modeling programs named MCAM, SNAM and RCAM have been developed as bridges between the engineering CAD models and particle transport simulations. The main functions of them have been tested by using the complex geometry of the 3D ITER benchmark model. The benchmarking processing and results have demonstrated the feasibility, effectiveness and maturity of the three modeling programs for fusion applications with complex geometry. It can be expected that the interface program system can significantly reduce the manpower needed for modeling complex geometry for particle transport calculation and play even more important roles in the quality assurance of nuclear analysis for complex systems in the future.

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References

[1] J.F. Briesmeister (Ed.), MCNP—A General Monte Carlo N-Particle Transport Code, Version 4C, Los Alamos National Laboratory, Report LA-13709-M, April 2000.
[2] J.S. Hendricks, G.W. McKinney, L.S. Waters, T.L. Roberts, H.W. Egdorf, J.P. Finch, et al., “MCNPX, Version 2.5.E” Los Alamos National Laboratory, Report LAUR-04-0569, February 2004.
[3] J.P. Both, H. Derriennic, B. Morillon, J.C. Nimal, A survey of TRIPOLI-4, in: Proceedings of the 8th International Conference on Radiation Shielding, Arlington, TX, USA, April 24–28, 1994, pp. 373–380.
[4] W.W. Engle, Jr., ANISN, A One-dimensional Discrete Ordinates Transport Code with Anisotropic Scattering, ORNL Report, K-1693, March 1967.
[5] W.A. Rhoades, R.L. Childs, The DORT two-dimensional discrete ordinates transport code, Nucl. Sci. Eng. 99 (May 1) (1988) 88–89.
[6] Y.Y. Azmy, F.X. Gallmeier, D.A. Lillie, TORT solution for the 3D radiation transport benchmarks for simplegeometries with void region, Prog. Nucl. Energy 39 (2) (2001) 155–166.
[7] Y. Wu, J. Li, Y. Li, Q. Zeng, M. Chen, S. Zheng, et al., An integrated multifunctional neutronics calculation and analysis code system: VisualBUS, Chin. J. Nucl. Sci. Eng. 27 (4) (2007) 365–373.
[8] Y. Wu, Y. Li, L. Lu, A. Ding, H. Hu, Q. Zeng, et al., Research and development of the automatic modeling system for Monte Carlo particle transport simulation, Chin. J. Nucl. Sci. Eng. 26 (1) (2006) 20–27.
[9] Y. Li, L. Lu, A. Ding, H. Hu, Q. Zeng, S. Zheng, et al., Benchmarking of MCAM 4.0 with the ITER 3D model, Fusion Eng. Des. 82 (2007) 2861–2866.
[10] Y. Wu, FDS team, conceptual design activities of FDS series fusion power plants in China, Fusion Eng. Des. 81 (2006) 2713–2718.
[11] Y. Wu, X.G. Xu, The need for further development of CAD/MCNP interface codes, Invited Presentation at the American Nuclear Society Annual Meeting, Boston, USA, June 24–28, 2007.
[12] Q. Zeng, L. Lu, A. Ding, Y. Li, H. Hu, S. Zheng, et al., Update of ITER 3D basic neutronics model with MCAM, Fusion Eng. Des. 81 (2006) 2773–2778.
[13] H. Iida, L. Lu, Y. Wu, Nuclear Analysis of the Port Limiter and Neutron Flux Monitor in the Equatorial Port, ITER International Analysis Report, ID: NAG-264, 2007.
[14] S. Zheng, Y. Wu, Nuclear Analysis of the Upper Port-dose Rate Analysis of the Upper Port to Confirm Sufficiency of Shielding Capacity of Final Port Geometry, ITER International Analysis Report, ID: ITA 73-01, 2005.
[15] Q. Zeng, Y. Meng, S. Zheng, Y. Wu, Update of the ITER 3-D Model for MCNP and the Nuclear Data Library for Dose Calculation, ITER International Analysis Report, ID: ITA 73-03, 2008.
[16] L. Lu, Q. Zeng, Y. Li, S. Zheng, Y. Wu, Testing and Application of MCAM for ITER Benchmark Model, ITER International Analysis Report, ID: ITA 73-08, 2008.
[17] Q. Huang, S. Zheng, L. Lu, R. Hiwatari c, Y. Asaoka, K. Okano, et al., Neutronics analysis for a compact reversed shear Tokamak CREST, Fusion Eng. Des. 81 (2006) 1239–1244.
[18] H. Hu, J. Li, Y. Li, S. Zheng, Y. Wu, Study on key issues of automatic modeling for the S_N-method based particle transport simulation codes program, Chin. J. Nucl. Phys. Rev. 23 (2) (2006) 134–137.
[19] H. Hu, Y. Wu, M. Chen, Q. Zeng, A. Ding, S. Zheng, et al., Benchmarking of SNAM with the ITER 3D model, Fusion Eng. Des. 82 (2007) 2867–2871.
[20] Y. Wu, G. Song, R. Cao, A. Wu, M. Cheng, Z. Tang, et al., Development of accurate/advanced radiotherapy treatment planning and quality assurance system (ARTS), Chin. Phys. C (HEP & NP) 32 (Suppl. II) (2008) 177–182.

[21] The IAEA Nuclear Data Section, FENDL-2.1 Fusion Evaluated Nuclear Data Library, Vienna, Austria, INDC (NDS)-467, Version December 2004.
[22] H. Wienke, M. Herman, FENDL/E2.0, The Processed Cross-section Libraries for Neutron-photon Transport Calculations, IAEA-NDS-176 Rev 0, February 1998.
[23] J.S. Hendricks, S.C. Frankle, J.D. Court, ENDF/B-VI Data for MCNP, and Errata [R], Los Alamos National Laboratory Report LA-12891, 1994.
[24] R.E. Macfarlane, MATXS10, 30-Neutron, 12-Group Photon Cross Sections from ENDF/B-IV with TRANSX-2, Los Alamos National Laboratory, 1994.