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# KASKAD: Deterministic Two-Dimensional Neutral and Charged Particle Transport Code System

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## Abstract

The KASKAD code system simulates neutron- proton- pion- and photon transport in the Accelerator Driven Systems (ADS). The main code KASKAD-S solves the multigroup transport equation by the discrete ordinates method in two-dimensional geometries. The scattering anisotropy is treated in the $P_L$ approximation. Coupled multigroup cross sections for neutrons, protons, and pions are provided by CONSYST/ABBN for energies of up to 20 MeV, and SADCO-2 for energies from 20 MeV to 10 TeV. Coupled electron-photon multigroup cross-sections are generated by the adapted version of CEPXS (called by CEPXS-BFP).

Postprocessor KASF prints, verifies and processes the flux, source, and functional interface of KASKAD-S results. Several benchmark results are provided to illustrate the performance of the algorithm implemented in the KASKAD code system.

## 1. Introduction

Growing interest in the accelerator-driven system (ADS) is accompanied with development of a code system to simulate the elementary production of particles in spallation reactions and transport of these particles in the target. In the ADS, a high-power particle accelerator produces energetic protons that interact with a heavy metal target to produce neutrons. The source neutrons are generated by direct impingement of the accelerator proton beam onto a target material in a process called spallation. The spallations are subsequently multiplied in the surrounding subcritical blanket. Currently both Monte Carlo (such as MCNPX) and deterministic codes are taken into consideration for analyses of the static and dynamic behaviour of the system.

As a deterministic method, the discrete ordinate method gives an additional merit in comparison with Monte Carlo codes, to perform both neutronics and shielding calculations in spallation target design by decreasing computing times and memory requirements in calculation of energy, angular and spatial distributions of the spallation source and in deep penetration target shielding calculations.

We are installing a deterministic two-dimensional neutral and charged particle transport code system called KASKAD[1], which is suitable for high-energy coupled proton-pion-neutron-photon transport simulation in the ADS. It was originally developed in Keldysh Institute of Applied Mathematics, Moscow, and transferred to the Korea Atomic Energy Research Institute (KAERI), and is currently being improved and updated for the ADS-related applications.

Section 2 gives an outline of the code system; the cross section generation,

numerical algorithm and postprocessing. Section 3 describes numerical methods for coupled charged/neutral particle transport calculations adopted in the KASKAD system. In section 4, benchmark calculations are presented and their results are discussed.

## 2. Structure of the KASKAD code system.

The KASKAD code system consists of several codes. The CONSYST/ABBN[2] data code system is used to generate the low-energy neutron/photon multigroup cross sections. It is designed for supporting of various neutron and photon multigroup cross section applications with ABBN-93 coupled neutron/photon data. To operate with the cross section files in the FMAC-M[3] format which is used by KASKAD-S, a preprocessor for FMAC-M format, ARVES-2[3], is used. SADCO-2[4] which consists of FOROS and KOLYMA can be used to generate coupled multigroup cross sections for protons, pions and neutrons in a high-energy region (20 MeV < E < 10 TeV), coupled with standard coupled neutron/photon multigroup libraries. To prepare multigroup cross sections for solving electron-photon cascade problems, CEPXS-BFP[5] is used.

The proton/pion/neutron coupled cross section libraries for the current benchmark calculations are prepared in several stages. At the first stage, the low energy neutron/photon multigroup cross sections are generated from the ABBN-93 coupled neutron/photon data by the code CONSYST. The resulting cross section file in ANISN format is then prepared in FMAC-M format by the code ARVES. At the second stage, the multigroup high-energy cross sections are generated by the code FOROS. Finally, the multigroup high-energy cross sections are coupled with the low-energy ones by the code KOLYMA.

The prepared coupled libraries are fed into the code KASKAD-S. Postprocessor KASF can print, verify and process the flux/source/functional interface files of the code KASKAD-S. For graphical display of the computed results, KASF provides an option to create a data file for the contouring and surface plotting program Surfer.

## 3. Numerical algorithms implemented in KASKAD-S

Charged particles transport can be treated well by means of the Boltzmann-Fokker-Plank (BFP)[6] equation. The BFP equation uses the Boltzmann scattering integral to treat the large-angle (sufficiently smooth or regular) component of scattering and the differential Fokker-Plank operator to approximate the forward-peaked or "singular" component of scattering. For the case of r,z geometry, the BFP equation can be written as follows:

$$-r\frac{\partial}{\partial E}(\beta\psi)+\mu r\frac{\partial\psi}{\partial r}+\xi\frac{\partial}{\partial\psi}(\eta\psi)-\frac{\partial}{\partial\varphi}(\eta\psi)+\sigma r\psi(r,z,\mu,\varphi,E)=rS(r,z,\mu,\varphi,E) \qquad (1)$$

where $\beta=\beta(r,z,E)$ is the stopping power (for neutral particles $\beta=0$), $\xi=(1-\mu^2)^{1/2}\cos\varphi$ and $\eta=(1-\mu^2)^{1/2}\sin\varphi$, $\mu=\cos\theta$. The first four operators in this equation are Fokker-Plank operators. The energy operator is known as the continuous slowing-down (CSD) operator, and the angular operator is known as the continuous-scattering operator. The discrete direction $\overrightarrow{\Omega}\cdot\vec{\Omega}=(\xi,\eta,\mu)$ spans the hemisphere. As usual, for the purpose of angular quadrature, this hemisphere is divided into L bands in angular cosine $\mu$ of weight $w_l$ and each band $l, l=1,\ldots,L$, into $M_l$ sectors of weight $w_{l,m}$.

The balance equation is obtained by integration of Eq. (1) over a cell $(r_{i-1/2}, r_{i+1/2})\times(z_{k-1/2}, z_{k+1/2})\times(\psi_{l,m-1.2}, X_{l,m+1/2})\times(\mu_{l-1/2}, \mu_{l+1/2})\times(E_{q+1/2}, E_{q-1/2})$:

$$\frac{V}{\Delta E}(\beta^{+}\psi_E^{+}-\beta^{-}\psi_E^{-})+\mu v(\psi_z^{+}-\psi_z^{-})+\Delta z[X(A^{+}\psi_r^{+}-A^{-}\psi_r^{-})$$
$$+\ \frac{C}{w}(\alpha_{m+1/2}-\alpha_{m-1/2}\psi_{m-1/2}^{q})]+\sigma_t^{q}V\psi^{q} \qquad (2)$$
$$=\ V\sum_{p}\sum_{j=0}^{J}\frac{2j+1}{4\pi}\sigma_{s,j}^{p\to q}\sum_{n=0}^{j}Y_j^{n}(\mu,X)\Pi_j^{n,p}+VF^{q}$$

where

$$Y_j^{n}(\mu,X)=\left[(2-\delta_{0,n})\frac{(j-n)!}{(j+n)!}\right]^{1/2}P_j^{n}(\mu)\cos nX,\quad \Psi_{j,i,k}^{n,q}=2\sum_{l,m}w_{l,m}Y_j^{n}(\mu_l,X_{l,m})\psi_{i,k,l,m}^{q} \qquad (3)$$

Adding to balance equation (2) the WDD auxiliary equations for spatial and angular variables $r,z$ and $\xi$,

$$\psi_r^{+}=(1+P_r)\psi-P_r\psi_r^{-},\quad \psi_z^{+}=(1+P_z)\psi-P_z\psi_z^{-},\quad \psi_{m+1/2}=(1+P_\xi\psi_{m-1/2},\quad 0\le P_{r,z,X}\le 1, \qquad (4)$$

and the WDD or weighted 2Step (W2Step) auxiliary equation for energy variable E:

$$\psi_E^{+}=(1+P_E)\psi-P_E\psi_E^{-},\qquad 0\le P_E\le 1, \qquad (5)$$

$$\psi_{q+1/2}=(1+\frac{P_q}{2})\frac{\psi^{q}}{\Delta E_q}-\frac{P_q}{2}\frac{\psi^{q-1}}{\Delta E_{q-1}},\qquad 0\le P_q\le 2\Delta\frac{E_q}{\Delta E_q+\Delta E_{q-1}}=P_q^{opt}, \qquad (6)$$

where $q-1$ is the nearest upper group of particles of the same type, we obtain two variants of differencing schemes for Eq. (1). The weighting coefficients in Eqs. (4) and (5) can be calculated, for example, by the AWDD scheme[7] that ensures positivity and prevents large errors in some rough cells. The recommended value of the weighting coefficient $P_q$ in Eq. (6) is $P_q=P_q^{opt}$ for $q>1$, and $P_q=0$ for $q=1$.

To transform the WDD system (2)-(5) or the compound WDD/W2Step system, given by Eqs. (2), (4) and (6), to a form that is acceptable for an $S_n$ code for neutral particles, we must introduce an additional approximation of the type:

$$\sigma_\beta^{p\to q}\psi^{p}(r,z,\mu_l,\varphi_{l,m})\approx\sum_{j=0}^{J}\frac{2j+1}{4\pi}\sigma_\beta^{p\to q}\sum_{n=0}^{j}Y_j^{n}(\mu_l,\varphi_{l,m})\Phi_j^{n,p}. \qquad (7)$$

This approximation gives the possibility to prepare a modified cross-sections $\tilde{\sigma}^{p}{}_{t}$ $\tilde{\sigma}^{p\to q}{}_{s,j}$ that can be used by standard $S_n$ codes. For the case of the W2Step scheme they are:

$$\tilde{\sigma}_t^{\,q}=\sigma_t^{q}+\frac{1}{\Delta E_q}\beta_{q+1/2}(1+\frac{P_q}{2}),$$
$$\tilde{\sigma}_{s,j}^{\,q-1\to q}=\sigma_{s,j}^{q-1\to}+\frac{1}{\Delta E_{q-1}}(\beta_{q-1/2}(1+\frac{P_{q-1}}{2})+\beta_{q+1/2}\frac{P_q}{2}),$$
$$\tilde{\sigma}_{s,j}^{\,q-2\to q}=\sigma_{s,j}^{q-2\to q}-\frac{P_{q-1}}{2\Delta E_{q-2}}\beta_{q-1/2},\qquad j=0,\ldots,J. \qquad (8)$$

The similar formulas are also known for the case of using the WDD auxiliary equation (5) in energy variable E. But using these formulas together with a nonlinear fix-up algorithm in this variable, usually needed for acceptable choice of weighting coefficients in Eq. (5), is complicated.

The consistent $P_1SA$ acceleration scheme [8], earlier developed for 2D neutral particle transport equation, has been extended from scheme (2)-(5). But in the cascade part of problem the number of unaccelerated inner iterations is sufficiently small. So the use of the $P_1SA$ scheme in this range does not give an essential gain in

computing time.

For a narrow pencil beam sources approximation, Eq. (7) is poor and we must modify the $S_n$ code for direct treatment of the CSD term. For the case of the WDD scheme (2) - (5) such treatment requires additional memory to store in memory the group boundary angular fluxes $\psi_{i,k,l,m,q\pm1/2}$ for solved energy group $q$. To improve the accuracy of calculations we also need to perform calculation of the extended uncollided flux from pencil beam sources that are normally incident on the bottom of the 2D $r,z$ geometry region by analytical formulas[9].

## 4. Benchmark calculation and results.

Several benchmark results are provided to illustrate the performance of an algorithm which is implemented in the code KASKAD-S. The neutron yields for various materials bombarded by proton beams are presented in Tables 1 and 2. The neutron cross section libraries were obtained from ABBN-93, and then the proton-neutron coupled cross section libraries were prepared using the SADCO system. Figures 1 and 2 show distributions of neutron and proton fluxes created by Surfer which is a contouring and surface plotting program. The XYZ data file for Surfer was prepared by the postprocessing code KASF.

Figure 4 shows distribution of the neutron flux in the critical assembly[10] which is an unreflected cylinder of highly enriched uranium whose geometry is shown in Figure 3. The atom densities for the benchmark model is presented in Table 3. The neutron cross section libraries were prepared using the codes NJOY99 and TRANSX-1.5 with ENDF/B-VI libraries. The calculated $k_{eff}$ was $1.00299 \pm 0.0006$.

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## References

1. A. M. Voloschenko and A. V. Shwetsov, "KASKAD-S-2.0 - Two-Dimensional Discrete-ordinates Neutron, Photon and Charged Particles Transport Code," User's Guide, Report No. 7-2-2000, Keldysh Inst. of Appl. Math., Moscow, 2000 (in Russian).
2. G. N. Manturov, M. N. Nikolaev and A. M. Tsyboulia, "CONSYST/ABBN Data Code System," IPPE Report No. 9865, Obninsk, 1998.
3. A. M. Voloschenko, S. V. Gukov and A. V. Shwetsov, "ARVES-2 - a Package of Utilities for FMAC-M Format: a Multigroup Macroscopic Cross-section Format for Discrete-ordinates Transport Codes," User's Guide, Report No. 7-3-2000, Keldysh Inst. of Appl. Math., Moscow, 2000 (in Russian).
4. D. V. Gorbatkov and V. P. Kryuchkov, "SADCO-2: A Modular Code System for Generating Coupled Nuclear Data Libraries to Provide High-Energy Particle Transport Calculation by Multigroup Methods," *Nucl. Instr. & Meth. In Phys. Res.*, **A 372**, 297 (1966).
5. A. M. Voloschenko, O. V. Nikolaeva, S. V. Gukov, CEPXS-BFP/ROZ-6.5/ KASKAD-S-2.0 Package for Solving the Coupled Electron-Photon Transport Problems by the Discrete Ordinate Method in 1D and 2D Geometries," KIAM

Report No. 7-5-2000
6. K. Przybylski, J. Ligou, "Numerical Solution of the Boltzmann Equation Including Fokker-Plank Terms," *Nucl. Sci. Eng.*, **81**, 92 (1982).
7. A. M. Voloschenko, T. A. Germogenova, "Numerical Solution of the Time-Dependent Transport Equation with Pulsed Sources," *Transp. Theory and Stat. Phys.*, **23**, No. 6, 845 (1994)
8. A. M. Voloschenko, "Consistent P1 Synthetic Acceleration Scheme for Transport Equation in Two-Dimensional r,z Geometry," *Proc. Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, October 6-10, 1997, Saratoga Springs, NY USA, vol. 1, p.364.
9. A. M. Voloschenko, "An Sn Algorithm for Spallation Target Neutronics and Shielding Calculations," *Proc. of International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses in Nuclear Applications*, 27-30 September, 1999, Madrid, Spain, vol. 2, P.975.
10. "International Handbook of Evaluated Criticality Safety Benchmark Experiments," vol. 2, NEA Nuclear Science Committee (1999).

Table 1. Neutron yields for lead cylinder 20 cm in diameter 60 cm in length bombarded by proton beams of various energies. (Experimental data of R. Vassil'kov et al., MRTI).

| Proton energy, MeV | Experimental data | KASKAD-S/SADCO-2 |
|---|---|---|
| 1000 | 21.5 | 21.58 |
| 1500 | 32.5 | 33.21 |
| 2000 | 42.0 | 44.34 |
| 2650 | 53.5 | 56.41 |
| 3250 | 64.5 | 64.16 |
| 5000 | 89.8 | 88.66 |

Table 2. Neutron yields for tungsten cylinder 10.2 cm in diameter 40 cm in length bombarded by proton beams of various energies (Experimental data of M. Zucker et al., BNL).

| Proton energy, MeV | Experimental data | KASKAD-S/SADCO-2 |
|---|---|---|
| 800 | 15.11 | 11.52 |
| 1000 | 20.40 | 15.28 |
| 1200 | | 18.61 |
| 1400 | 28.46 | 21.60 |

Table 3. Atom densities for the critical assembly (atoms/barn-cm)

| Nuclide | Bottom | Top |
|---|---|---|
| $^{235}U$ | $4.5774 \times 10^{-2}$ | $4.5708 \times 10^{-2}$ |
| $^{238}U$ | $1.3381 \times 10^{-3}$ | $1.3404 \times 10^{-2}$ |
| $^{234}U$ | $5.6597 \times 10^{-4}$ | $5.6404 \times 10^{-2}$ |
| $^{12}C$ | $1.0270 \times 10^{-4}$ | $1.0256 \times 10^{-4}$ |
| Fe | $5.0251 \times 10^{-5}$ | $5.0131 \times 10^{-5}$ |
| W | $1.2199 \times 10^{-6}$ | $1.2183 \times 10^{-6}$ |

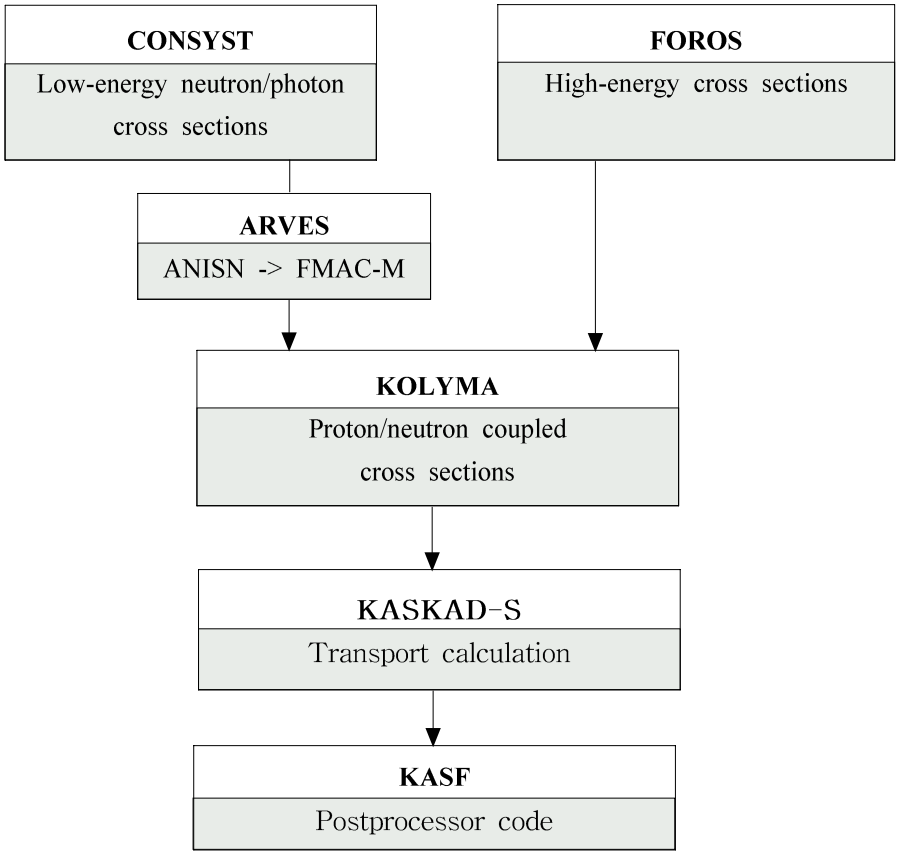
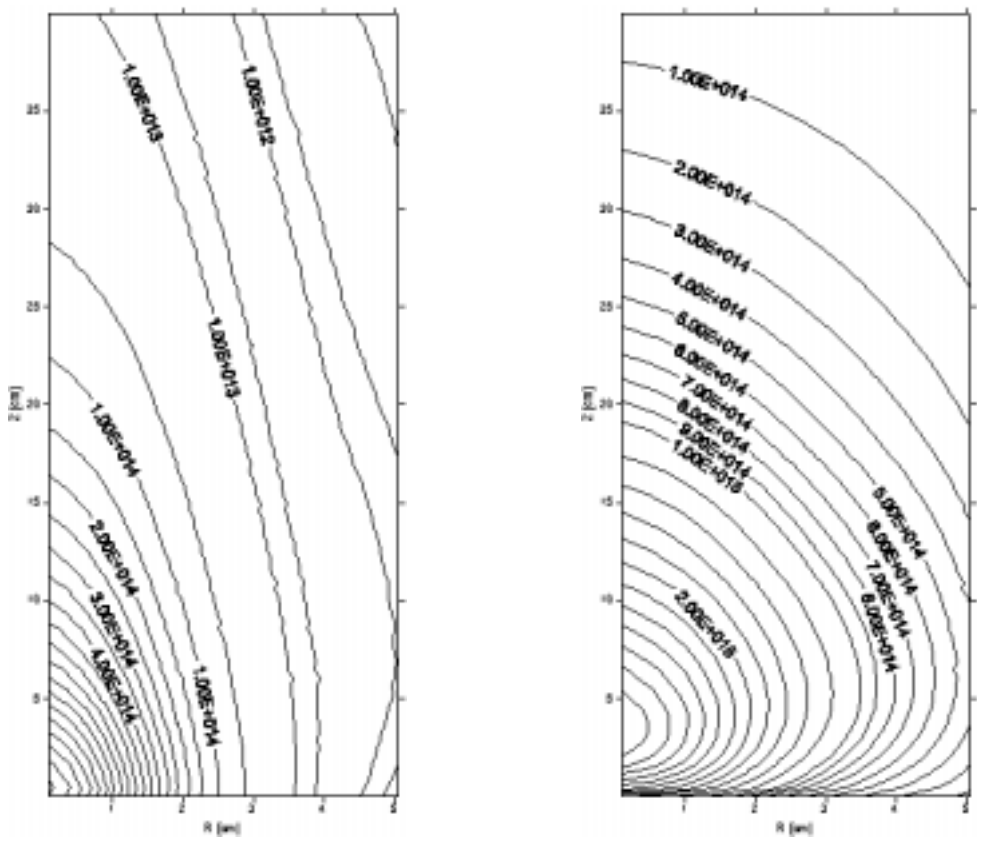



Fig 1. The procedure for proton/pion/neutron coupled benchmark calculations




(a) (b)

Fig. 2 Total proton (a) and neutron (b) flux in tungsten cylinder 10.2 cm in diameter 40 cm in length bombarded by 1400 MeV proton beam.

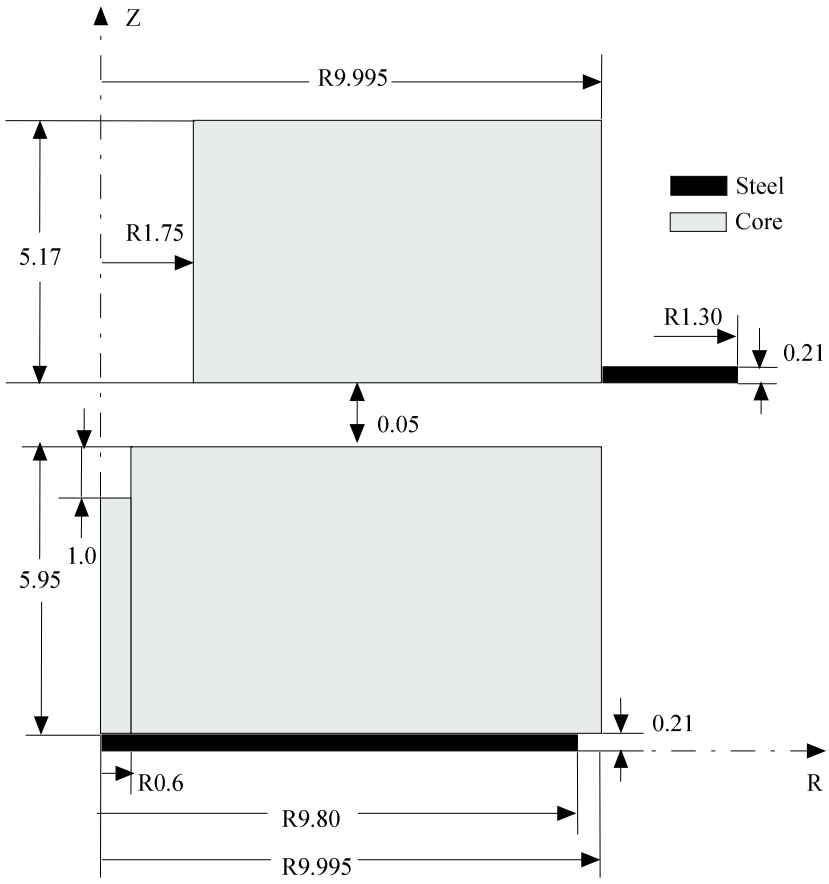



Fig 3. The critical assembly model geometry.

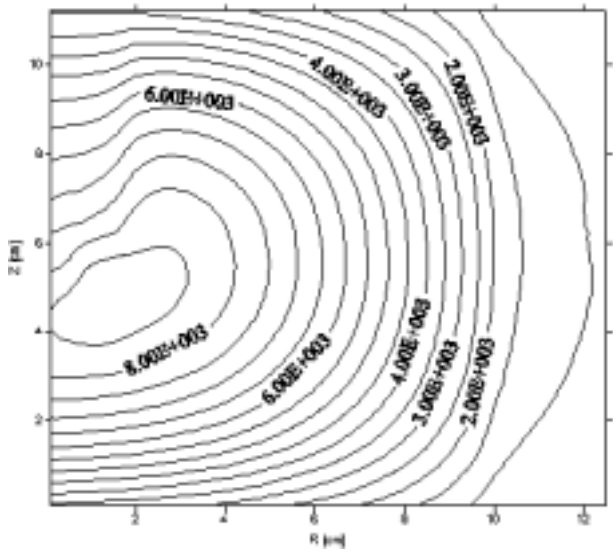


Fig 4. The total neutron flux in the critical assembly.