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A new approach for solution of time dependent neutron transport equation based on nodal discretization using MCNPX code with feedback



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ABSTRACT

This paper proposes a new method for solving the time-dependent neutron transport equation based on nodal discretization using the MCNPX code. Most valid nodal codes are based on the diffusion theory with differences in approximating the leakage term until now. However, the Monte Carlo (MC) method is able to estimate transport parameters without approximations usual in diffusion method. Therefore, improving the nodal approach via the MC techniques can substantially reduce the errors caused by diffusion approximations. In the proposed method, the reactor core is divided into nodes of arbitrary dimensions, and all terms of the transport equation e.g. interaction rates and leakage ratio are estimated using MCNPX. They are then employed within the time-dependent neutron transport equation for each node independently to compute the neutron population. Based on this approach, a time-dependent code namely MCNP-NOD (MCNPX code based on a NODal discretization) was developed for solving time-dependent transport equation in an arbitrary geometry considering feed backs. The MCNP-NOD is able to simulate multi-group processes using appropriate libraries. Several test problems are examined to evaluate the method.

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1. Introduction

The kinetic behavior of neutrons can be simulated using the time-dependent Boltzman equation which is represented in a multi-group form as (Bell and Glasstone, 1970):

$$\frac{1}{\nu_{g}} \frac{\partial \int \Phi_{g}(r,\Omega,t) d\Omega}{\partial t}
+ \left(\int_{\Omega,n>0} \Omega.\nabla \Phi_{g}(r,\Omega,t) d\Omega - \int_{\Omega,n<0} \Omega.\nabla \Phi_{g}(r,\Omega,t) d\Omega \right)
+ \int \Sigma_{g,t}(r,t) \Phi_{g}(r,\Omega,t) d\Omega
= \chi_{g}^{p}(1-\beta) \sum_{g'} \int \bar{\nu} \Sigma_{g'f}(r,t) \Phi_{g'}(r,\Omega,t) d\Omega
+ \sum_{g'} \int \Sigma_{g'\rightarrow g,s}(r,t) \Phi_{g'}(r,\Omega,t) d\Omega + \sum_{j} \chi_{g}^{d_{j}} \lambda_{j} C_{j}(r,t)$$
(1)

The corresponding time-dependent precursor equation is:

$$\frac{\partial C_j(r,t)}{\partial t} = \beta_j \sum_{g'} \bar{\nu} \Sigma_{g'f}(r) \phi_{g'}(r,t) - \lambda_j C_j(r,t)$$
(2)

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https://doi.org/10.1016/j.anucene.2019.06.026 0306-4549/© 2019 Elsevier Ltd. All rights reserved. where $\sum_{g' \to g,s}(r,t)$ is the macroscopic scattering cross section that a neutron of energy group g' having a collision at time t results a neutron in energy group g, $\sum_{g,t}(r,t)$ and $\sum_{g,f}(r,t)$ are macroscopic total and fission cross section in energy group g and time t respectively, $\phi_g(r,t)$ is scalar flux and $\Phi_g(r,\Omega,t)$ is angular flux in energy group gand time t, C_j , λ_j and β_j are the population, decay constants and fraction of delayed neutron precursor of j^{th} group, β is the total fraction of delayed neutrons, ν_g is the neutron speed with energy group gand $\overline{\nu}$ is the average number of neutron released per fission.

Almost all valid existing codes use diffusion theory and approximate the streaming term $(\Omega.\nabla\Phi_g(r,\Omega,t))$ in form $D_g\nabla^2\phi_g(r,t)$ where D_g is the diffusion coefficient (Zarei, 2018; Zarei et al., 2017; Shaukat et al., 2017; Kotchoubey, 2015; Parhizkari et al., 2015; Yun et al., 2008; Aoki et al., 2007; Alcouffe and Baker, 2005; Abdou, 2005; Arzhanov, 2002; Goluoglu and Dodds, 2001; Bentley et al., 1997a,b; Gehin, 1992; Smith, 1979). These codes apply different approximations to evaluate the term $D_g \nabla^2 \phi_g(r,t)$ between different nodes. Based on these approximations, different nodal methods are obtained (Lawrence, 1986; Christensen, 1985). Of course, there are some ways to remove these restrictions recently e.g. method of the characteristics (Talamo, 2013) and Monte Carlo method (Sjenitzer and Hoogenboom, 2012).





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When the term $\Omega . \nabla \Phi_g(r, \Omega, t)$ in the transport equation (which represents the current on the node's boundaries in all directions) is approximated by $D\nabla^2 \phi_g(r, t)$ in the diffusion equation; it indicates that the current between the two nodes is always perpendicular to the surface (boundary) between two nodes and ignores the current in other directions on the surface. This assumption would cause

errors in the results for some problems. In order to solve this issue, lots of meshes is employed; as a result of that, the run time of the program and the requested memory of the computer increase. Triangular meshes are also used for better modeling of complex geometries whose formulation is more complicated than square mesh relationships (Lozano et al., 2010). Hopefully the Monte Carlo



Fig. 1. The flowchart of the MCNP-NOD.

(MC) method which directly simulates the particle transport phenomena as a stochastic process to estimates the result through the mean behavior of particles is a reliable alternative method to avoid the above restrictions might be.

In this paper, a time-dependent neutron transport method named MCNP-NOD (MCNPX code based on a NODal discretization) is developed for solving time-dependent transport equation in an arbitrary geometry using MCNPX code. MCNP-NOD extracts $\Omega.\nabla\Phi_g(r,\Omega,t)$ of transport equation from MCNPX code (Pelowitz, 2008) for transient analysis. In this method, we solve the transport equation without any approximation for the term $\Omega.\nabla\Phi_g(r,\Omega,t)$. Simulation results would therefore be more accurate. Several benchmark problems are examined to evaluate the performance of the developed method.

2. Methodology

The stochastic modifications of neutrons' population within a system (through absorption, scattering, leak out etc.) is normally too short compared to the system alterations. In other words, the neutron life time (tG) is generally far less than the system period and hence the system can be assumed as steady state during a t_{c} .

In MCNP-NOD, the total simulation time (T) is divided into time steps ΔT and the geometry is also divided into nodes of arbitrary dimensions. It should be noted that each node can consist of only one material but there is no restriction over the mesh size and shape. Therefore, arbitrary meshes can be defined in such a way that they cover all the problem geometry and its details. The conclusion was enriched to clarify this capability. The values of Ω . $\nabla \Phi_g(r, \Omega, t)$ (using F1 and FS tallies of MCNPX) and interaction rates (using F4 and FM tallies of MCNPX) in transport equation are calculated at the beginning of each time step by the MCNPX code. In the case of timevarying cross sections or changing of temperature or boundaries, variations are also assumed at the beginning of each time step. This method assumes that these values are constant during ΔT and the system will not change during this time step (ΔT). On the other hand, the neutron flux and precursors are interdependent and change after each mean generation time (t_G). Therefore, each time step (Δ T) divides into sub-steps each lasts t_G and the neutrons flux and the precursor population are calculated using time-dependent Eqs. (1) and (2) in each sub-steps. Then by integrating over the interval $t' - t_{\rm G}$ to t'(equal to a mean generation time (t_G)) The neutron flux and the power are express as follows:

$$\begin{split} \phi_{g}^{(t')} &= \phi_{g}^{(t'-t_{G})} + \sum_{g'=1}^{G} \chi_{g'}^{d_{g'}} \lambda_{g'} C_{g'}^{(t'-t_{G})} \times t_{G} \times \nu_{g} - \left(\int \Omega . \nabla \Phi_{g}^{(t)} d\Omega \right) \\ &\times M^{(t'-t_{G})} \times t_{G} \times \nu_{g} \\ &+ \left(\chi_{g}^{p} (1-\beta) \sum_{g'} \bar{\nu} \Sigma_{f,g'}^{(t)} \phi_{g'}^{(t'-t_{G})} - \Sigma_{t,g}^{(t)} \phi_{g}^{(t'-t_{G})} + \sum_{g'} \Sigma_{s,g' \to g}^{(t)} \phi_{g'}^{(t'-t_{G})} \right) \\ &\times t_{G} \times \nu_{g} P^{(t')} = \sum_{g=1}^{G} E_{f} \times \Sigma_{f,g}^{(t)} \times \phi_{g}^{(t')} \times V_{F} \end{split}$$
(3)

It is noteworthy that nodal codes also use implicit complex methods such as a predictor-corrector method to ensure the stability of their results; while, MCNP-NOD updates the flux of each node from Eq. (4) in order to keep the results stable, and it uses Eq. (3) only to extracts $P^{(t')}$.

$$M^{(t')} = \frac{p^{(t') \times \bar{\nu}}}{E_f \times K_{eff}^{(t)}}$$

$$\phi_{\sigma}^{(t')} = \phi_g^{(t)} \times M^{(t')}$$
(4)

If it is assumed that variation of ϕ_g is linear during t_G, then the precursors' concentration at each sub-step is expressed as follows through integrating over the interval $t' - t_G$ to t'(equal to a mean generation time (t_G)) on Eq. (2),:



Fig. 3. Schematic of problem ANL 16-A1 (Mazaher et al., 2019).



Fig. 2. Relative flux vs. time for benchmark problem 1.

$$C_{g'}^{(t')} = C_{g'}^{(t'-t_G)} \times e^{-\lambda_{g'}t_G} + \left(\frac{1 - e^{-\lambda_{g'}t_G}}{\lambda_{g'}t_G} - e^{-\lambda_{g'}t_G}\right) \frac{\beta_{g'}}{\lambda_{g'}} \\ \times \sum_{g=1} \nu \Sigma_f^g \phi_g^{(t'-t_G)} + \left(1 - \frac{1 - e^{-\lambda_{g'}t_G}}{\lambda_{g'}t_G}\right) \frac{\beta_{g'}}{\lambda_{g'}} \times \sum_{g=1} \nu \Sigma_f^g \phi_g^{(t')}$$
(5)

In the above equations $\Omega.\nabla\Phi_g^{(t)}$ is the normalized streaming term and $\varphi_g^{(t)}$ is the normalized scaler flux of g^{th} group extracted

Table 1Number of intervals in each zone for problem 16-A1.

Zone	Number of nodes	Number of nodes
1	20	1
2	25	1
3	6	1
4	17	1
5	6	1
6	25	1
7	20	1
Sum of nodes	119	7

by MCNPX code, $\phi_g^{(t')}$ is the scalar flux of g^{th} group, $C_{g'}^{(t')}$ is the number of the g'^{th} group the precursors, $\Sigma_{f,g}^{(t')}$ is the macroscopic fission cross section, v_g is the average speed of g^{th} group, E_f is the recoverable energy per fission, V_F is the volume of the fissile elements and $P^{(t')}$ is power generated from all energy groups after t' second. Besides, $M^{(t')}$ is flux multiplier to transform the MCNPX normalized flux into a real flux for the investigated problem (Hendricks et al., 2008).

It should be noted that t denotes the coarse time steps (the beginning time for each step) and t represent fine time sub-steps. Fig. 1 presents the flowchart of the MCNP-NOD for dynamic transient analysis and the way it is divided into time steps and sub-steps.

3. Numerical results

Each problem is simulated by the MCNPX using 300 cycles having omitted the first 100 as inactive. The number of source histories per cycle is set to 2×10^6 as well. The maximum relative



Fig. 4. Relative power vs. time for problem 16-A1.



Fig. 5. Normalized flux vs. radial position for problem 16-A1 (group 1).



Fig. 6. Normalized flux vs. radial position for problem 16-A1 (group 2).



Fig. 7. Schematic of the TWIGL (Mazaher et al., 2019).

standard deviation is given in the following test problems. To verify the proposed approach, we have opted a series of test cases from simple to hard to examine its all features.

3.1. Problem 1: A cube with time-varying cross sections

A bare cube of $10 \times 20 \times 24$ cm with cross sections varying with time is verified as the first example. The problem has been previously simulated with MC method (Sjenitzer and Hoogenboom, 2012). The absorption cross-section of the cube suddenly drops at t = 10 s and jumps to its initial value at t = 40 s.

MCNP-NOD estimated K_{eff} and t_G 0.99998(±0.00005) and 7.48E-6 (±3.5E-10) s, respectively. The time-dependent flux with time steps equal to $\Delta T = 0.1$ s is displayed in Fig. 2. A positive reactivity step followed by a negative one can be easily traced within the curve. As observed results are in excellent accord with what predicted by Dynamic Tripoli (Sjenitzer and Hoogenboom, 2012) which is also an MC code. In addition, the maximum relative standard deviation was estimated to be 6.89E-03 happening at t = 40 s when the flux experiences a sharp drop. In order to investigate the independency of this method with regards to the node size, the calculations are carried out with two different node sizes of 600 nodes with dimensions of 2 × 2 × 2 cm and 1 node with dimensions of 10 × 20 × 24 cm. The total calculation time was 11.5 CPU hours



Fig. 8. The relative power vs. time for the step transient in the TWIGL.

for 1 node and 14.8 CPU hours for 600 nodes (The processors used were 2.2 GHz AMD Opteron (tm)).

3.2. ANL 16-A1 benchmark problem

The ANL benchmark is a 1-D, 2-G, time-dependent fast reactor composed of seven homogeneous slabs ending to vacuum. Geometry of the problem is described in Fig. 3. Six delayed neutron precursor groups as defined in (Goluoglu and Dodds, 2001) are assumed for the problem. To perturb the system, the material density of Zone #2 is suddenly increased by 5% at t = 0 s while at the same time, a same reduction is imposed on Zone #6. The problem has been previously simulated with the TDTORT (Goluoglu and Dodds, 2001) which is a discrete ordinate transport code. The output of MCNP-NOD for Keff and tG are 0.99998 (±0.00005) and 3.75E-7 (±2.752E-10) s, respectively. In order to investigate stability of this method for any node size, the calculations are carried out with two different node sizes as listed in Table 1. The relative power versus time is shown in Fig. 4 (with time step $\Delta T = 0.000001$ s until t = 0.01 s and ΔT = 0.01 s until t = 0.1 s and ΔT = 0.1 s until t = 10 s) and the normalized flux for group 1 and 2 are shown in Figs. 5 and 6 respectively. MCNP-NOD shows excellent agreement with the TDTORT results. It can be clearly seen that the dimensions of the nodes will not affect the results, and the results of segmentation with 7 and 119 nodes are almost the same. This indicates that there is no dependency for this method with regards to the size and number of nodes. In addition, the maximum relative standard deviation was estimated to be 7.95E-03 happening at t = 10 s. The total calculation time for benchmark problem ANL 16-A1 was 17.2 CPU hours (The processors used were 2.2 GHz AMD Opteron (tm)).

3.3. TWIGL transient problems

The TWIGL is a 2D reactor with vacuum boundaries as displayed in Fig. 7. It is made of 2-G homogeneous materials with one group delayed neutron precursor (Goluoglu and Dodds, 2001). Two transient scenarios are modeled here: first, a ramp scale down in Σ_{a2} of region #1 during 0.2 s, and second, a step reduction equal to the total change in ramp transient ($\Delta \Sigma_{a2} = 0.0035$ cm-1). The problem has been previously simulated with the TDTORT (Goluoglu and Dodds, 2001) which is a discrete ordinate transport code.



Fig. 10. The schematic of the LRA (Mazaher et al., 2019).

The problem segmentation is shown in Fig. 7 with white lines. K_{eff} and t_{G} were evaluated as 1.00002 (±0.00004) and 4.14E-5 (±4.5E-08) s, respectively by MCNP-NOD. The relative power for step and ramp perturbation (with time step $\Delta T = 0.01$ s) calculated by MCNP-NOD agrees very well with the TDTORT and DeCART as shown in Figs. 8 and 9. Moreover, maximum relative standard deviations were obtained equal to 5.91E-03 for the step and 1.35E-03 for the ramp transients both at t = 0.5 s. The total calculation time was 11.4 CPU hours for the step transient and 115.6 CPU hours for the ramp transient (The processors used were 2.2 GHz AMD Opteron (tm)).

As shown in Fig. 8, following the early prompt jump in step transient, the power rises relatively slowly until the end of the period. In contrast, no such jump is forecasted for the ramp transient and the power rockets exponentially. Then, moderate increment is estimated for the rest of transient. As conceived from Fig. 8, this difference can be seen only for very early initial time (less than



Fig. 9. The relative power vs. time for the ramp transient in the TWIGL.



Fig. 11. The average core power for the LRA vs. time.

0.05 s), which is due to the difference in solution techniques, and the two methods forecast approximately same answers for long times after that.

3.4. LRA BWR benchmark problem

Here, the problem is a 2-D, 2-G BWR in transient condition and the Geometry of the benchmark is illustrated in Fig. 10. The transient starts with a linear approximation on Σ_{a2} of the region R and Doppler temperature feedback is modeled on Σ_{a1} of fuels regions (regions 1–4) (Mazaher et al., 2019). The problem has been previously simulated with the MOC (Shaner, 2014) which is based on MOC method and CONQUEST (Gehin, 1992) which is based on Diffusion method.

 K_{eff} and t_G were evaluated as 1.00000 (±0.00004) and 3.51E-5 (±2.03E-08) s, respectively by MCNP-NOD. The relative power versus time is calculated by the MCNP-NOD (with time step $\Delta T = 0.1$ s until t = 1.2 s and $\Delta T = 0.05$ s until t = 1.6 s and $\Delta T = 0.1$ s until t = 3 s and with node dimension of 15 × 15 cm) agrees very well with the MOC and CONQUEST results as shown in Fig. 11. The Maximum relative standard deviation for power was estimated to be 9.01E-03 at t = 1.41 s. The total calculation time was 323.9 CPU hours for the LRA transient problem (The processors used were 2.2 GHz AMD Opteron (tm)).

Fig. 11 indicates an exponential surge in power due to the positive reactivity of less absorption in reflector. The power is bound to rapid escalation if no Doppler feedback is taken into consideration. However, the Doppler feedback finally damps the surge, and following a few oscillations the power tends to a constant value at the end of the transient.

4. Conclusions

A new MC approach is proposed using MCNPX based on a nodal discretization for the multi-dimensional analysis of 3-D systems with explicit representation of delayed neutrons. This method, named MCNP-NOD is capable to simulate the systems with a time-varying arbitrary geometry and meshing style plus parallel processing with multi-groups cross section without the restrictions of previous methods (dependency on node size, approximate the leakage term, etc.). To evaluate the proposed idea a number of standard benchmarks such as TWIGL, LRA, and ANL were resorted to. The results prove satisfactory agreement with the reference values while being independent and stable for any size of nodes. To extend the work, a coupling is suggested between the MCNP-

NOD and some reliable thermal-hydraulics tool for the simulation of more realistic accident scenarios. This way MCNP-NOD would be capable of analyzing the dynamic behavior of complex reactors which form our next step forward.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.anucene.2019.06.026.

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