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Extension of KIN3D, a Kinetics Capability of VARIANT, for Modeling Fast Transients in Accelerator Driven Systems

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The time-dependent second-order PN equation is discretized by a fully implicit finite-difference scheme; the obtained pseudo-steady-state PN equations are then used in the framework of the Variational Nodal Method (VNM). This scheme is implemented in the VARIANT/KIN3D code. A new code option is presented that takes in account neutron wave phenomena. The code has been validated for a very simple case against an analytic solution; other simple tests are performed in order to investigate differences compared to the original version of KIN3D/VARIANT.

KEYWORDS: Neutron kinetics, variational nodal method, even-parity neutron transport equation, neutron waves.

1. Introduction

Innovative nuclear waste burning concepts, such as Accelerator Driven Systems (ADSs), are under investigation and development worldwide and also at Forschungszentrum Karlsruhe. To prove safety of an ADS and to simulate experiments related to ADS studies, transient analyses are carried out [1, 2]. These analyses require use of modern codes based on advanced neutron transport models. In particular, the Variational Nodal Method (VNM) implemented in the VARIANT code [3-6] shows a great potential for 3-D transport calculations. Initially, VARIANT was developed for solving the steady-state neutron transport equation based on the nodal method applied to the second-order (even-parity) transport equation. Later a neutron kinetics model, KIN3D [7], was coupled with VARIANT for dealing with time-dependent problems. KIN3D was originally developed for critical reactor analyses, though an option for taking into account an external neutron source was implemented for generality. Recently transient simulations for an external neutron source driven system were performed with VARIANT/KIN3D [2]. The fast transients (in the following we consider that a transient is fast if the corresponding time scale is comparable to the neutron lifetime) were caused by rapid source variations. For this new VARIANT/KIN3D application capability related to ADS transient analyses, we have recently extended the KIN3D model aiming at improving the accuracy and reliability of the code. In the paper we present these extensions and numerical results for simplified cases that show and compare the performance of initially available and newly introduced computation options.

2. Mathematical Formulation

The variational nodal method is based on the search of the minimum of a functional. The Euler-Lagrange equation of this functional is the second-order (in space) neutron transport equation: this methodology was developed by E. E. Lewis et al. [3-6]. For the readers convenience we show briefly the path leading to the mathematical formulation of this method.

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2.1 Second Order Transport Equation: Time Independent

To explain the VNM, let us consider the within-group neutron transport equation:

$$\vec{\Omega}\cdot\vec{\nabla}\varphi\left(\vec{r},\vec{\Omega}\right)+L[\varphi]\left(\vec{r},\vec{\Omega}\right)=S\left(\vec{r},\vec{\Omega}\right), \qquad (1)$$

$\varphi\left(\vec{r},\vec{\Omega}\right)$ is neutron flux,

$S\left(\vec{r},\vec{\Omega}\right)$ is sum of fission, up- and down-scattering, and external sources,

$L[\ ]\left(\vec{r},\vec{\Omega}\right)$ is self scattering and absorption operator,

group index is omitted, other notations are standard.

By introducing even- and odd- parity (with respect to angle) flux components

$$\begin{cases}\psi\left(\vec{r},\vec{\Omega}\right)=\dfrac{1}{2}\left(\varphi\left(\vec{r},\vec{\Omega}\right)+\varphi\left(\vec{r},-\vec{\Omega}\right)\right) & \text{even flux}\\ \chi\left(\vec{r},\vec{\Omega}\right)=\dfrac{1}{2}\left(\varphi\left(\vec{r},\vec{\Omega}\right)-\varphi\left(\vec{r},-\vec{\Omega}\right)\right) & \text{odd flux}\end{cases} \qquad (2)$$

one can get a system of coupled equations:

$$\begin{cases}\vec{\Omega}\cdot\vec{\nabla}\chi\left(\vec{r},\vec{\Omega}\right)+L^{+}[\psi]\left(\vec{r},\vec{\Omega}\right)=S^{+}\left(\vec{r},\vec{\Omega}\right),\\ \vec{\Omega}\cdot\vec{\nabla}\psi\left(\vec{r},\vec{\Omega}\right)+L^{-}[\chi]\left(\vec{r},\vec{\Omega}\right)=S^{-}\left(\vec{r},\vec{\Omega}\right).\end{cases} \qquad (3)$$

Here L^+, L^-, and S^+, S^-, are the even (+) and odd (-) parity components of L and S, which are defined following the approach of Eq. (2). For the P1 approximation, L^+ corresponds to the removal cross section and L^- corresponds to the transport one. By eliminating χ from Eq. (3), one can get an equation for the even flux (angular and spatial variables are omitted):

$$\vec{\Omega}\cdot\vec{\nabla}\left(-\left(L^{-}\right)^{-1}[\vec{\Omega}\cdot\vec{\nabla}\psi]\right)+L^{+}[\psi]=S^{+}-\vec{\Omega}\cdot\vec{\nabla}\left(\left(L^{-}\right)^{-1}[S^{-}]\right). \qquad (4)$$

The main advantages of solving Eq. (4) instead of Eq. (1) by the PN (spherical harmonics) method are the following ones: (a) the number or unknowns is reduced (as the even-parity flux is expanded within spatial meshes with the even harmonics only) and (b) Eq. (4) is self-adjoint. Due to the latter feature, one can construct a positively defined functional, the minimum of which corresponds to the solution of Eq. (4). The corresponding "Variational" problem can be solved numerically by the Ritz method.

2.2 KIN3D Model: Original Approach

In the following only the direct option (a fully implicit scheme with respect to time) of KIN3D is considered. The delayed neutrons are ignored (as their treatment was not changed) for brevity. The time-dependent within-group transport equation in the even-parity form can be written as (the fluxes/operators are time-dependent):

$$\begin{cases}\dfrac{1}{v}\dfrac{\partial\psi}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}\chi+L^{+}[\psi]=S^{+},\\ \dfrac{1}{v}\dfrac{\partial\chi}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}\psi+L^{-}[\chi]=S^{-}.\end{cases} \qquad (5)$$

For a time interval *i*, $\Delta t_i=\left(t_i-t_{i-1}\right)$, the implicit scheme gives:

$$\begin{cases}\left(v\Delta t_i\right)^{-1}\left(\psi_i-\psi_{i-1}\right)+\vec{\Omega}\cdot\vec{\nabla}\chi_i+L^{+}[\psi_i]=S_i^{+},\\ \left(v\Delta t_i\right)^{-1}\left(\chi_i-\chi_{i-1}\right)+\vec{\Omega}\cdot\vec{\nabla}\psi_i+L^{-}[\chi_i]=S_i^{-}.\end{cases} \qquad (6)$$

This finite-difference representation transforms the original Eq. (5) into a set of steady-state-like problems of the Eq. (3) type. According to the original KIN3D approach, the term $\left(v\Delta t_i\right)^{-1}\left(\chi_i-\chi_{i-1}\right)$ in the last equation is neglected giving rise to an approximate treatment of the time dependence. This approximation is usually quite accurate for reactor perturbations caused by relatively slow variations (in time) of cross-sections (e.g. due to material density or temperature variations) and of the external source. For the lowest angular order (the even- and odd-parity flux components are the scalar flux and current), this treatment corresponds to the time-dependent diffusion equation (i.e. Fick's law is assumed being valid under transient conditions and, in particular, the time derivative of the current is neglected).

2.3 KIN3D Model: New Option

In case of fast source variations, the approximate treatment discussed above may no longer be sufficiently accurate. A new KIN3D option does take into account the term related to the time derivative of the odd-parity flux as described in the following. One may note that the factor $(v\Delta t_i)^{-1}$ can be seen as an additional absorption cross-section (time absorption), while $(v\Delta t_i)^{-1}\psi_{i-1}$ and $(v\Delta t_i)^{-1}\chi_{i-1}$ are known and can be added (as a "time source") to the source terms. By assigning

$$\begin{cases} \tilde{L}_i[\ ] = L_i[\ ] + (v\Delta t_i)^{-1}, \\ S_{T,i} = (v\Delta t_i)^{-1}\varphi_i; \end{cases} \tag{7}$$

one can transform Eq. (6) into (index *i* is omitted hereafter):

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}\chi + \tilde{L}^+[\psi] = S_T^+ + S^+, \\ \vec{\Omega}\cdot\vec{\nabla}\psi + \tilde{L}^-[\chi] = S_T^- + S^-; \end{cases} \tag{8}$$

then the even-parity equation can be derived:

$$\vec{\Omega}\cdot\vec{\nabla}\left(-\left(\tilde{L}^-\right)^{-1}[\vec{\Omega}\cdot\vec{\nabla}\psi]\right) + \tilde{L}^+[\psi] = S^+ + S_T^+ - \vec{\Omega}\cdot\vec{\nabla}\left(\left(\tilde{L}^-\right)^{-1}[S_T^- + S^-]\right). \tag{9}$$

By introducing a group index g (and rearranging) one gets:

$$\vec{\Omega}\cdot\vec{\nabla}\left(-\left({}_g\tilde{L}^-\right)^{-1}[\vec{\Omega}\cdot\vec{\nabla}{}_g\psi]\right) + {}_g\tilde{L}^+\left[{}_g\psi\right] = {}_gS^+ - \vec{\Omega}\cdot\vec{\nabla}\left(\left({}_g\tilde{L}^-\right)^{-1}{}_g\breve{S}^-]\right) + {}_gS_T^+ \underbrace{-\vec{\Omega}\cdot\vec{\nabla}\left(\left({}_g\tilde{L}^-\right)^{-1}{}_g\hat{S}_T^-]\right)}_{(a)}, \tag{10}$$

where:

$${}_g\hat{S}_T^- = {}_gS_T^- + \sum_{g'\neq g}\Sigma_{g'\to g}^-\left({}_{g'}\tilde{L}^-\right)^{-1}\left[{}_{g'}\hat{S}_T^-\right] \tag{11}$$

$${}_g\breve{S}^- = \sum_{g'\neq g}\Sigma_{g'\to g}^-\left({}_{g'}\tilde{L}^-\right)^{-1}\left[-\vec{\Omega}\cdot\vec{\nabla}{}_{g'}\psi + {}_{g'}\breve{S}^-\right], \tag{12}$$

and $\Sigma_{g'\to g}^-$ is the odd part of the group-to-group transfer operator. The complexity of the procedure is related to a specific feature of the VARIANT solution scheme: only even-parity external source moments are allowed, therefore the contribution related to the term (a) in Eq. (10), has to be computed outside of VARIANT and added to the even-parity source.

We have shown that the time-dependent equation can be transformed into a set of steady-state like problems (Eq. (10)), which are similar to the original problem (Eq. (4)). The corresponding cross-section and external source files are generated by KIN3D at each time step and supplied to VARIANT. The cross-sections include the "time absorption". The external source (even-parity moments only) includes "additional" components: the two last right-hand part terms of Eq. (10).

Compared to the original approach (S_T^- was set to zero and L^- was used instead of $\tilde{L}^-$ in Eq.(9)), the new KIN3D option computes **in addition** the following (at each time step):

- it reconstructs the odd-parity flux from the even-parity flux computed by VARIANT (by solving the second equation of the system (8), iteration are needed in case of up-scattering);
- it solves Eq. (11)) (iterations are needed in case of up-scattering) and adds the corresponding term to the external source file;
- it modifies the odd part of the scattering/absorption operator (to obtain $\tilde{L}^-$ instead of L^-).

For the lowest angular order (P1), one may transform Eq. (5): $\psi\to\phi$ (scalar flux), $\chi\to\vec{J}$ (current), $S^+\to Q$ (isotropic source), $L^+\to\Sigma_r$ (removal cross section), $L^-\to\Sigma_{tr}$ (transport cross section, i. e. the total cross-section minus the anisotropic self-scattering one). If the source is isotropic, (we consider the 1-group equation here):

$$\begin{cases} \left(\frac{1}{v}\frac{\partial}{\partial t}+\Sigma_r\right)\phi+\vec{\nabla}\vec{J}=Q, \\ \left(\frac{1}{v}\frac{\partial}{\partial t}+\Sigma_{tr}\right)\vec{J}+\frac{1}{3}\vec{\nabla}\phi=0. \end{cases} \tag{13}$$

Eliminating the current yields the telegraph equation:

$$\left(\frac{\Sigma_r}{v\Sigma_{tr}}\frac{\partial\phi}{\partial t}+\frac{1}{v^2\Sigma_{tr}}\frac{\partial^2\phi}{\partial t^2}-\frac{1}{v\Sigma_{tr}}\frac{\partial Q}{\partial t}\right)+\frac{1}{v}\frac{\partial\phi}{\partial t}+\Sigma_r\phi-\vec{\nabla}\frac{1}{3\Sigma_{tr}}\vec{\nabla}\phi=Q \tag{14}$$

For the lowest angular order, Eq. (10) corresponds to the discretized (in time) Eq. (14). Compared to the conventional time-dependent diffusion equation,

$$\frac{1}{v}\frac{\partial\phi}{\partial t}+\Sigma_r\phi-\vec{\nabla}\frac{1}{3\Sigma_{tr}}\vec{\nabla}\phi=Q\,, \tag{15}$$

the P1/telegraph equation includes additional terms (in brackets in Eq. (14)). These terms give rise to neutron transport wave phenomena.

2.4 Angular and Space Discretization

According to the angular and space discretization used in VARIANT, we introduce a complete set of ortho-normal functions in space $f_l(\vec{r})$ and in angle $g^{\pm}_{m^{\pm}}(\vec{\Omega})$ that yields the following expansion:

$$\begin{aligned} {}_g\psi(\vec{\Omega},\vec{r}) &= \sum_l f_l(\vec{r})\sum_{m^+} {}_g\xi_{l,m^+}\, g^+_{m^+}(\vec{\Omega}), \\ {}_g\chi(\vec{\Omega},\vec{r}) &= \sum_l f_l(\vec{r})\sum_{m^-} {}_g\xi_{l,m^-}\, g^-_{m^-}(\vec{\Omega}), \end{aligned} \tag{16}$$

where $\xi_{l,m^{\pm}}$ are the of even- and odd-parity flux moments.

By expanding (employing the same set of basis functions) the source and scattering kernel (see the second equation of Eq. (8)) it is possible to get the following explicit expression for the odd-parity flux moments (odd flux moments at previous time step being assumed known):

$$\begin{aligned} {}_g\xi^{(i)}_{l,m^-} = &-\left[{}_g\tilde{\Sigma}^{(i)}_{tot}-{}_g\Sigma^{-(i)}_{s,m^-}\right]^{-1}\sum_{l'}\sum_{m^+}{}_g\xi^{(i)}_{l',m^+}\times\int dV\int_{4\pi} d\vec{\Omega}g^-_{m^-}(\vec{\Omega})\,g^+_{m^+}(\vec{\Omega})\vec{\Omega}f_l\vec{\nabla}(f_{l'})+\left[{}_g\tilde{\Sigma}^{(i)}_{tot}-{}_g\Sigma^{-(i)}_{s,m^-}\right]^{-1}\times \\ &\times\left[\sum_{g'\neq g}\Sigma^{-(i)}_{s,m^-}(g'\to g)\,{}_{g'}\xi^{(i)}_{l,m^-}+\left({}_g v\Delta t_i\right)^{-1}\,{}_g\xi^{(i-1)}_{l,m^-}\right] \end{aligned} \tag{17}$$

where:

${}_g\Sigma^{(i)}_{tot}$ is total cross section for group g,

${}_g\Sigma^{\pm(i)}_{s,m^-}$ is even (+) and odd (-) moments of the scattering kernel in group g,

$\Sigma^{\pm(i)}_{s,m^{\pm}}(g'\to g)$ is even (+) and odd (-) moments of the scattering cross section from group g to g'.

In order to take into account the additional time absorption, we have introduced:

$${}_g\tilde{\Sigma}^{(i)}_{tot}={}_g\Sigma^{(i)}_{tot}+\left({}_g v\Delta t_i\right)^{-1}. \tag{18}$$

Eq. (11) then could be transformed:

$${}_g\hat{S}^-_T\Big|_{l,m^-}=\frac{1}{v_g\Delta t}\,{}_g\xi^{(i)}_{l,m^-}+\sum_{g'\neq g}\frac{\Sigma^{-(i)}_{s,m^-}(g'\to g)}{{}_{g'}\tilde{\Sigma}^{(i)}_{tot}-{}_{g'}\Sigma^{-(i)}_{s,m^-}}\left[{}_{g'}\hat{S}^-_T\Big|_{l,m^-}\right]. \tag{19}$$

At this point it is possible to take in account the contributions to the source even-parity moments arising from terms (a) in Eq. (10) by adding to the external source terms: ${}_g\mathbb{S}_{l,m^+}$

$$ {}_g\mathbb{S}_{l,m^+} = \sum_{l'} \sum_{m^-} \frac{ {}_g\widehat{S}_T^- \Big|_{l',m^-} }{ {}_g\tilde{\Sigma}_{tot}^{(i)} - {}_g\Sigma_{s,m^-}^{-(i)} } \times \left\{ \int dV \int d\vec{\Omega} f_{l'} \vec{\Omega} \vec{\nabla} \left(f_l \right) g_{m^-}^- \left(\vec{\Omega} \right) g_{m^+}^+ \left(\vec{\Omega} \right) \right\}. \tag{20} $$

3. Results

This chapter consists of two parts. In the first one we consider a benchmark case, for which an analytic solution can be obtained [8, 9], in order to test the new KIN3D option. In the second part, a comparison between the new and old KIN3D options is performed for a simplified reactor model related to an experiment [2] in order to get an impression: how the options affect a practical case.

3.1 Analytical Benchmark

We consider a thick non-fissile 1-D slab. All neutrons have the same velocity: $v = 10^8\, cm/s$. The total and scattering cross-sections are: $\Sigma_{tot} = 0.8 cm^{-1}$, $\Sigma_s = 0.4 cm^{-1}$; the neutron scattering is isotropic. The source variation is triangular in time: the source is zero t=0, reaches the maximum of $1000\, cm^{-1} s^{-1}$ at t=$0.5 \cdot 10^{-9} s$ and goes down to zero at $10^{-9} s$. The source is isotropic, flat (in space) within a "source region", being zero outside this region. Two options are considered in the following: a "narrow" source region (the boundaries are at $\pm$ 0.001 cm) and a "broad" source region (the boundaries are at $\pm$ 0.1 cm). The geometry model, physical properties (i. e. cross sections, neutron velocity, etc.), and source variation for this test case were chosen in order to have a strong difference between the diffusion and P1 options (we use "P1" instead of "P1/telegraph" hereafter). For this model we obtained a reference (assuming the P1 equation being valid) solution (time-dependent neutron flux) as described in the following. One may get the time-dependent flux for a source pulse that is proportional to the Dirac delta function in space (x) and time (t), $Q(x,t) = Q\delta(t)\delta(x)$ by the Laplace transformation in time and the Fourier transformation in space [8,9]:

$$ \phi(x,t) = \frac{e^{-at}}{2} Q \left\{ \delta\left(ct - |x|\right) + \beta h\left(ct - |x|\right) \left[\frac{ct}{\sqrt{(ct)^2 - x^2}} I_1(\theta) + I_0(\theta) \right] \right\}; \tag{21} $$

where:

$a = v\left(\Sigma_{tot} - \frac{1}{2}\Sigma_s \right)$, $b = \frac{v}{2}\Sigma_s$, $c = \frac{v}{\sqrt{3}}$, $\beta = \frac{b}{c}$, $\theta = \beta\sqrt{(ct)^2 - x^2}$, $\delta(z)$ is Dirac's function, $h(z)$ is Heaviside's step-function, $I_0(\theta)$ is the 1st kind modified Bessel function of order 0; $I_1(\theta) = \frac{dI_0(\theta)}{d\theta}$ is the modified Bessel function of the 1st order. This solution is valid for a thick slab until the wave reaches the boundary. By employing this result as Green's function, we got (employing some analytics and numerical integration) the reference solution. The reference solution shows a wave front that travels at the velocity of $v/\sqrt{3}$ away from the source. Wave phenomena are neglected in the diffusion approximation because the current varies promptly when the scalar flux changes (a time-space localized perturbation in the source term is seen in the whole domain instantaneously [10]). For the same model we computed the time-dependent flux by employing the original diffusion and new P1 options of KIN3D (the spatial mesh Δx of 0.001 cm, 4th order spatial expansion within nodes, surface 2nd order spatial expansion for the node interfaces being used). The corresponding results for the narrow and broad source regions are shown in Figures 1 and 2, two different time step being employed in KIN3D: fine (0.001 ns) and coarse (0.1 ns). In the wave front area, the numerical solution converges to the reference one with time step decreasing. The flux amplitude in the region between the source position and the wave front is not appreciable in Figure 1 since it is about 100 times smaller than the maximum flux value. However, the convergence (with time step decreasing) of P1 results to the analytic ones is faster in this region than near the wave front. If the source region is larger (0.1 cm instead of 0.001 cm), the numeric solution is more accurate for same time step due to a lower mutual influence of approximation errors at the front and back sides of the wave.

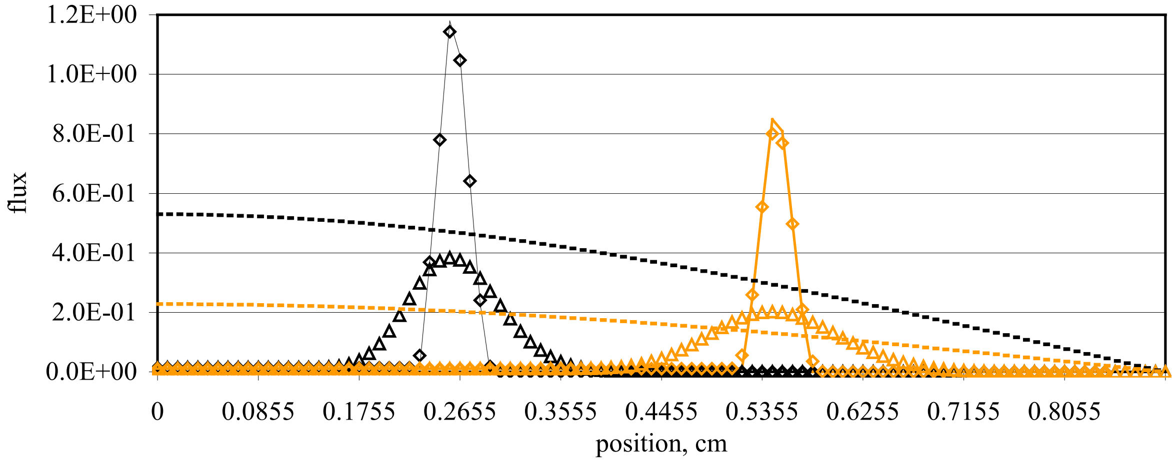

Fig. 1 Flux: numerical and analytic solution, source boundary at 0.001 cm, the following notations being used:

reference, t=5 ns — P1, fine, t=5 ns — P1, coarse, t=5 ns — reference, t=10 ns

P1, fine, t=10 ns — P1, coarse, t=10 ns — Diffusion*10, t=5 ns — Diffusion*10, t=10 ns

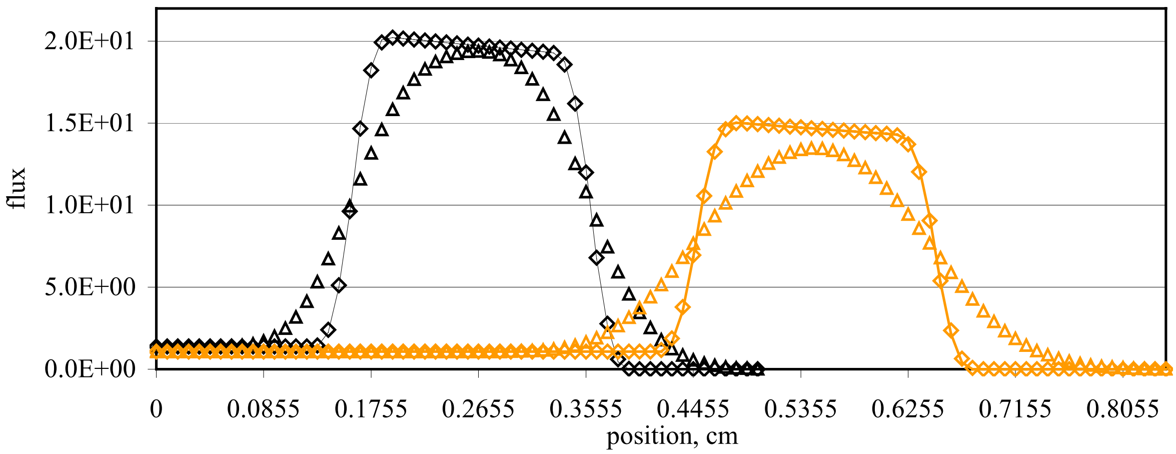

Fig. 2 Flux: numerical and analytic solution, source boundary at 0.1 cm

3.2 Simplified case related to the MUSE experiment

We consider a 1-D model that is related to the MUSE experiment [2]. Though the geometry model is simplified significantly, we suppose that it is representative for estimating possible deviations between the original and new KIN3D options for this case. The 1-D model is shown in Figure 3, positions of 2 detectors (in the core and in the reflector, the detector cross-section is the U-235 fission cross-section) being indicated. The k_{eff} value for this configuration is about 0.975. The number of energy groups is 33. We consider relative detector rate variations to an almost square (in time) source pulse of 1 μs. The corresponding results - relative detector rate variations - are given in Figures 4 and 5. These variations are proportional to the pulse amplitude. Therefore the curves are similar for any source amplitude (as relative units are employed). As expected, the results don't show substantial changes in the detector response to an external source pulse. On the other hand, the effect of employing the P1 option is not negligible: it may shift the results by several percents. The option implies higher neutron flux inertia as one may observe in the Figures 4, 5. It should be noted that both options correspond to the lowest angular approximation. Therefore the both options can not be considered as a reference for the moment. More refined modeling by employing higher order PN and SPN options is planned.

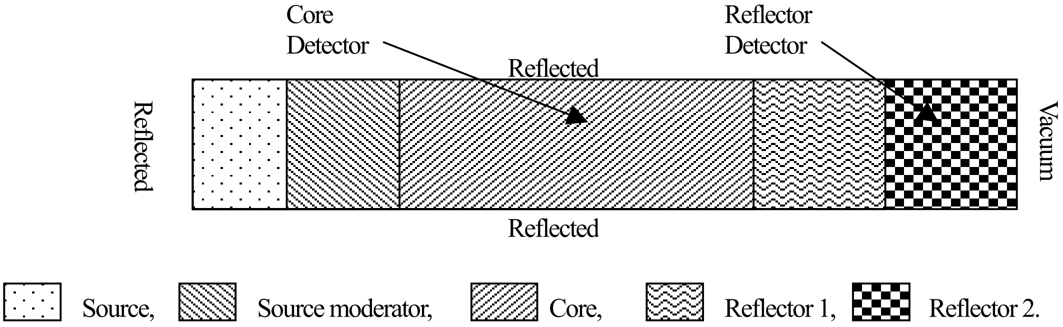

Fig. 3 Geometry (not at scale)

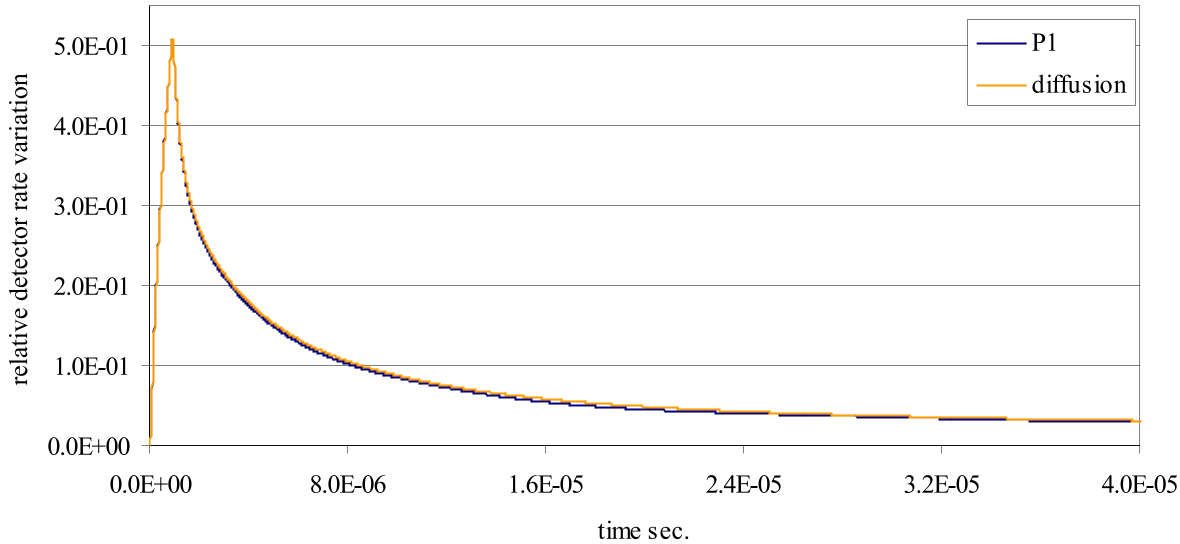

Fig. 4 Core detector rate for the P1 and diffusion option

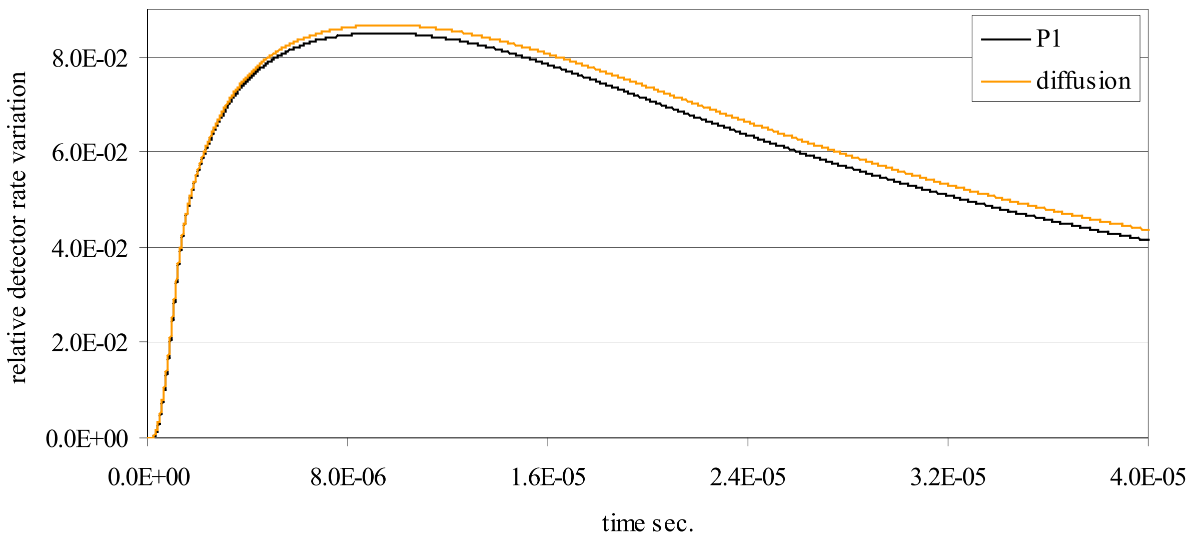

Fig. 5 Reflector detector rate for the P1 and diffusion option

4. Conclusion

The time-dependent second-order PN equation (even-parity transport equation) can be discretized in time by a fully implicit finite-difference scheme that results in a set of pseudo steady-state PN equations solved at each time step by the Variational Nodal Method. For this procedure we consider employment of two techniques corresponding - for the lowest angular approximation - to (1) the transient diffusion and (2) to the P1/telegraph equation.

The first scheme was implemented originally in the VARIANT/KIN3D code; the second one was implemented there recently. In the paper, the second scheme is presented and validated in P1 for a benchmark case by comparing with a result based on the analytical technique. In addition, a simplified experimental model is analyzed in order to get an impression: how the results (detector response to an external source pulse) obtained by following the new technique may differ from those obtained by the original KIN3D version earlier. As expected, the results don't show substantial changes. On the other hand, the effect of employing the new option is not negligible: it may shift the detector rate traces by several percents.

Further investigations are planned in order to study the stability of the method and performance of the new option for higher angular approximations (P3, P5, etc.), 2-D and 3-D geometry models.

The presented technique seems to be promising due to its stability proved in the simple test case. The correctness was proved with analytical solutions. Compared to the original approach, the increase of the computer time is not too high. An additional effort for implementing the SPN (simplified PN) approximation is foreseen. That would hopefully results in a fast multi-dimensional transport code applicable for a large variety of time-dependent problems.

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