Numerical scheme to solve spatially-dependent kinetics equation*

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The first version of this text is based on a master thesis written by Y. Ban[1].

Spatially-dependent kinetics equation (SDKE) is written as follows:

$$\begin{aligned}
\frac{1}{v_g}\frac{\partial \phi_g(x,t)}{\partial t} &= \nabla D_g(x,t)\cdot\nabla\phi_g(x,t) - \Sigma_{r,g}(x,t)\phi_g(x,t) + \sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t)\phi_{g'}(x,t) \\
&\quad +(1-\beta)\chi_{p,g}\sum_{g'}\nu\Sigma_{f,g'}(x,t)\phi_{g'}(x,t) + \sum_m \chi_{d,m,g}\lambda_m C_m(x,t), \qquad (1)\\
\frac{\partial C_m(x,t)}{\partial t} &= \beta_m\sum_{g'}\nu\Sigma_{f,g'}(x,t)\phi_{g'}(x,t) - \lambda_m C_m(x,t), \qquad (2)
\end{aligned}$$

where m is an index for delayed neutron precursor family, C_m and λ_m denote the delayed neutron precursor density of the mth family and its decay constant, χ_p and χ_d are fission spectra for prompt and delayed neutrons, respectively. v_g is neutron speed of group g. β is the effective delayed neutron fraction and β_m is that of the delayed neutron precursor of family m.

SDKE can be simplified by using the following definition of fission neutron source:

$$P(x,t) = \sum_{g'}\nu\Sigma_{f,g'}(x,t)\phi_{g'}(x,t). \qquad (3)$$

With this equation, SDKE is rewritten as

$$\begin{aligned}
\frac{1}{v_g}\frac{\partial \phi_g(x,t)}{\partial t} &= R_g(x,t), \qquad (4)\\
\frac{\partial C_m(x,t)}{\partial t} &= \beta_m P(x,t) - \lambda_m C_m(x,t), \qquad (5)
\end{aligned}$$

where

$$\begin{aligned}
R_g(x,t) = \nabla D_g(x,t)\cdot\nabla\phi_g(x,t) - \Sigma_{r,g}\phi_g(x,t) + \sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t)\phi_{g'}(x,t) \\
+ (1-\beta)\chi_{p,g}P(x,t) + \sum_m \chi_{d,m,g}\lambda_m C_m(x,t). \qquad (6)
\end{aligned}$$

While there are various numerical methods to solve SDKE, those can be categorized into the direct method and the factorization method. Summary for these methods are shown in **Table 1**. In the

Table 1: Summary of numerical methods to solve SDKE

Factorization method	Direct method
Adiabatic method, quasi-static method	Implicit method, θ method,
Improved quasi-static method	Stiffness confinement method (SCM),
	frequency-transform method

factorization method, neutron flux is factorized to the amplitude function and spatial function, and these

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functions are independently solved. The amplitude function strongly depends on time while the spatial function does not. Therefore the amplitude function should be calculated with the fine time interval and the spatial function should not be. Recently, the improved quasi-static method is widely used.

In the direct method, neutron flux is NOT factorized and SDKE is directly solved. Thus the computational cost is heavier than that of the factorization method. Some schemes such as frequency-transform method and SCM employ some techniques and do not require fine time internal. Numerical procedure of the direct method is much simpler than the factorization method, so the direct method is more widely used than the factorization method.

Here the numerical procedure of the θ method is briefly described. Equation (4) is discretized on time as

$$\frac{1}{v_g}\frac{\phi_g(x,t+\Delta t)-\phi_g(x,t)}{\Delta t}\approx \theta R_g(x,t+\Delta t)+(1-\theta)R_g(x,t). \tag{7}$$

This equation can be transformed into

$$\frac{\phi_g(x,t+\Delta t)}{\theta v_g\Delta t}-R_g(x,t+\Delta t)=\left(\frac{1}{\theta}-1\right)R_g(x,t)+\frac{\phi_g(x,t)}{\theta v_g\Delta t}, \tag{8}$$

if $\theta\neq 0$. Equation (8) can be rewritten with explicit representation of $R_g(x,t+\Delta t)$ as

$$\begin{aligned}-\nabla D_g(x,t+\Delta t)\cdot\nabla\phi_g(x,t+\Delta t)+\left\{\Sigma_{r,g}(x,t+\Delta t)+\frac{1}{\theta v_g\Delta t}\right\}\phi_g(x,t+\Delta t)\\ -\sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t+\Delta t)\phi_{g'}(x,t+\Delta t)-(1-\beta)\chi_{p,g}P(x,t+\Delta t)\\ -\sum_m\chi_{d,m,g}\lambda_m C_m(x,t+\Delta t)=\left(\frac{1}{\theta}-1\right)R_g(x,t)+\frac{\phi_g(x,t)}{\theta v_g\Delta t}.\end{aligned} \tag{9}$$

As described later, delayed neutron precursor density is calculated as

$$C_m(x,t+\Delta t)=\mu_m C_m(x,t)+\eta_m P(x,t)+\xi_m P(x,t+\Delta t). \tag{10}$$

Using this equation, Eq. (9) can be written as

$$\begin{aligned}-\nabla D_g(x,t+\Delta t)\cdot\nabla\phi_g(x,t+\Delta t)+\Sigma'_{r,g}(x,t+\Delta t)\phi_g(x,t+\Delta t)\\ =\tilde{\chi}_g P(x,t+\Delta t)+\sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t+\Delta t)\phi_{g'}(x,t+\Delta t)+Q_{ex,g}(x,t),\end{aligned} \tag{11}$$

where

$$\Sigma'_{r,g} = \Sigma_{r,g}(x,t+\Delta t)+\frac{1}{\theta v_g\Delta t}, \tag{12}$$

$$\tilde{\chi}_g = \chi_{p,g}(1-\beta)+\sum_m\chi_{d,m,g}\lambda_m\xi_m, \tag{13}$$

$$Q_{ex,g}(x,t) = \sum_m\chi_{d,m,g}\lambda_m\left(\mu_m C_m(x,t)+\eta_m P(x,t)\right)+\left(\frac{1}{\theta}-1\right)R_g(x,t)+\frac{\phi_g(x,t)}{\theta v_g\Delta t}. \tag{14}$$

In actual coding, one should be careful about a fact that not $\tilde{\chi}$ but χ is used in Eq. (14). As shown in Eq. (11), SDKE discretized by the θ method has the same form with the fixed source diffusion equation. That is, to solve SDKE is to solve the fixed source problem.

Next, a calculation procedure for $R(x,t)$ is described. As shown in Eq. (6), the neutron current calculation is required to get $R(x,t)$, but neutron current calculation is sometimes cumbersome. The following numerical technique, which does not require neutron current calculation, is very convenient. SDKE discretized by the θ method at the preceding time step is written as follows:

$$\begin{aligned}-\nabla D_g(x,t)\cdot\nabla\phi_g(x,t)+\Sigma'_{r,g}(x,t)\phi_g(x,t)\\ =\tilde{\chi}_g P(x,t)+\sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t)\phi_{g'}(x,t)+Q_{ex,g}(x,t-\Delta t).\end{aligned} \tag{15}$$

Using this equation to Eq. (6), $R(x,t)$ can be calculated without neutron current as

$$R_g(x,t) = \frac{\phi_g(x,t)}{\theta v_g \Delta t} + \sum_m \chi_{d,m,g}\lambda_m \left(C_m(x,t) - \xi_m P(x,t)\right) - Q_{ex,g}(x,t-\Delta t). \tag{16}$$

Finally, a calculation procedure for delayed neutron precursor density is described. By multiplying $\exp(\lambda_m t)$ to the both sides of Eq. (5), the following equation is derived:

$$\exp(\lambda_m t)\frac{\partial C_m(x,t)}{\partial t} = \exp(\lambda_m t)\beta_m P(x,t) - \exp(\lambda_m t)\lambda_m C_m(x,t). \tag{17}$$

This equation can be rewritten as

$$\frac{\partial}{\partial t}\left(\exp(\lambda_m t) C_m(x,t)\right) = \exp(\lambda_m t)\beta_m P(x,t) \tag{18}$$

This equation is integrated on $[t, t+\Delta t]$:

$$\int_t^{t+\Delta t} dt' \frac{\partial}{\partial t'}\left(\exp(\lambda_m t') C_m(x,t')\right) = \beta_m \int_t^{t+\Delta t} dt' P(x,t') \exp(\lambda_m t'). \tag{19}$$

Then we can obtain

$$C_m(x,t+\Delta t) = C_m(x,t)\exp(-\lambda_m \Delta t) + \beta_m \int_t^{t+\Delta t} dt' P(x,t') \exp(-\lambda_m (t+\Delta t - t')). \tag{20}$$

To calculate the time integration in Eq. (20), fission source is approximated as follows:

$$P(x,t') = P(x,t) + \frac{1}{\Delta t}\left\{P(x,t+\Delta t) - P(x,t)\right\}(t'-t) \tag{21}$$

By using this equation to Eq.(20) we can obtain

$$\begin{aligned} C_m(x,t+\Delta t) = C_m(x,t)\exp(-\lambda_m \Delta t) &+ \frac{\beta_m}{\lambda_m}\left\{\frac{1-\exp(-\lambda_m\Delta t)}{\lambda_m \Delta t} - \exp(-\lambda_m \Delta t)\right\} P(x,t) \\ &+ \frac{\beta_m}{\lambda_m}\left\{1 - \frac{1-\exp(-\lambda_m\Delta t)}{\lambda_m \Delta t}\right\} P(x,t+\Delta t). \end{aligned} \tag{22}$$

From this equation, we can now define μ_m, η_m and ξ_m in Eq. (10) as

$$\mu_m = \exp(-\lambda_m \Delta t), \tag{23}$$

$$\eta_m = \frac{\beta_m}{\lambda_m}\left\{\frac{1-\exp(-\lambda_m\Delta t)}{\lambda_m \Delta t} - \exp(-\lambda_m \Delta t)\right\}, \tag{24}$$

$$\xi_m = \frac{\beta_m}{\lambda_m}\left\{1 - \frac{1-\exp(-\lambda_m\Delta t)}{\lambda_m \Delta t}\right\}. \tag{25}$$

Note that the following relation holds:

$$\eta_m + \xi_m = \frac{\beta_m}{\lambda_m}\left(1-\mu_m\right). \tag{26}$$

In a usual transient calculation, a critical and stationary state is assumed at an initial time step ($t=0$) and reactivity is inserted to the system in $t>0$. In this case, neutron flux distribution at $t=0$ may be calculated from the following equation:

$$\begin{aligned} \nabla D_g(x,t)\cdot\nabla\phi_g(x,t) - \Sigma_{r,g}(x,t)\phi_g(x,t) + \sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t)\phi_{g'}(x,t) \\ + \left\{(1-\beta)\chi_{p,g} + \sum_m \chi_{d,m,g}\beta_m\right\} P(x,t) = 0. \end{aligned} \tag{27}$$

This equation is obtained from Eqs. (1) and (2) with $\frac{\partial \phi_g(x,t)}{\partial t} = 0$ and $\frac{\partial C_m(x,t)}{\partial t} = 0$. Practically the following eigenvalue equation might be solved and then nuclear data such as ν is adjusted so as to make the eigenvalue k_{eff} unity:

$$\begin{aligned} \nabla D_g(x,t) \cdot \nabla \phi_g(x,t) - \Sigma_{r,g}(x,t)\phi_g(x,t) + \sum_{g' \neq g} \Sigma_{s,g' \to g}(x,t)\phi_{g'}(x,t) \\ + \frac{1}{k_{\text{eff}}} \left\{ (1-\beta)\chi_{p,g} + \sum_m \chi_{d,m,g}\beta_m \right\} P(x,t) = 0. \quad (28) \end{aligned}$$

After obtaining neutron flux, the delayed neutron precursor densities at $t = 0$ can be calculated by

$$C_m(x,0) = \frac{\beta_m P(x,0)}{\lambda_m}. \quad (29)$$

The following is an example of numerical procedure for kinetics calculations.

1. If a time step width is fixed, μ_m, η_m and ξ_m can be calculated in advance. Removal cross sections and fission spectra should be corrected according to Eqs. (12) and (13).
2. If the initial state is a stationary critical state, neutron flux at $t = 0$ can be obtained from an eigenvalue calculation, and then precursor densities at $t = 0$ can be determined from Eq. (29). Also R at $t = 0$ should be zero in such cases.
3. When neutron flux and precursor densities at t are known, $Q_{ex,g}(x.t)$ can be calculated by Eq. (14). If $t \neq 0$, $R_g(x,t)$ can be calculated from Eq. (16).
4. Neutron flux at $t + \Delta t$ can be calculated by solving a fixed-source equation (11).
5. Precursor densities at $t + \Delta t$ can be calculated from Eq. (10).
6. Go to the step 3.

When one develops their own kinetics program, he should apply it to the null-transient problem at first. In this case, if he uses neutron flux and precursor distributions in a critical and stationary state as a initial condition, numerical solution should be unchanged. Neutron diffusion equation at the next time step can be written as follows:

$$\begin{aligned} &- \nabla D_g(x,t+\Delta t) \cdot \nabla \phi_g(x,t+\Delta t) + \left\{ \Sigma_{r,g}(x,t+\Delta t) + \frac{1}{\theta v_g \Delta t} \right\} \phi_g(x,t+\Delta t) \\ &\quad = \chi_{p,g}(1-\beta)P(t+\Delta t) + \sum_m \chi_{d,m,g}\lambda_m\xi_m P(t+\Delta t) + \sum_{g' \neq g} \Sigma_{s,g' \to g}(x,t+\Delta t)\phi_{g'}(x,t+\Delta t) \\ &\quad\quad + \sum_m \chi_{d,m,g}\lambda_m \left(\mu_m C_m(x,t) + \eta_m P(x,t) \right) + \frac{1}{\theta v_g \Delta t}\phi_g(x,t) \quad (30) \end{aligned}$$

By using Eq. (26) and the following equation

$$C_m(x,t) = \frac{\beta_m}{\lambda_m} P(x,t), \quad (31)$$

which can be derived by the stationary condition, Eq. (30) is rewritten as

$$\begin{aligned} &- \nabla D_g(x,t+\Delta t) \cdot \nabla \phi_g(x,t+\Delta t) + \left\{ \Sigma_{r,g}(x,t+\Delta t) + \frac{1}{\theta v_g \Delta t} \right\} \phi_g(x,t+\Delta t) \\ &\quad = \chi_{p,g}(1-\beta)P(t+\Delta t) + \sum_m \chi_{d,m,g}\lambda_m\xi_m P(t+\Delta t) + \sum_{g' \neq g} \Sigma_{s,g' \to g}(x,t+\Delta t)\phi_{g'}(x,t+\Delta t) \\ &\quad\quad + \sum_m \chi_{d,m,g}\beta_m P(x,t) - \sum_m \chi_{d,m,g}\lambda_m\xi_m P(x,t) + \frac{1}{\theta v_g \Delta t}\phi_g(x,t). \quad (32) \end{aligned}$$

On the other hand, we know that the following equation should hold because we now consider the null-transient problem:

$$
\begin{aligned}
&-\nabla D_g(x,t+\Delta t)\cdot\nabla\phi_g(x,t+\Delta t)+\Sigma_{r,g}(x,t+\Delta t)\phi_g(x,t+\Delta t)\\
&\quad=\chi_{p,g}(1-\beta)P(t+\Delta t)+\sum_{g'\neq g}\Sigma_{s,g'\to g}(x,t+\Delta t)\phi_{g'}(x,t+\Delta t)+\sum_m\chi_{d,m,g}\beta_m P(x,t+\Delta t). \qquad (33)
\end{aligned}
$$

By comparing Eq. (32) and Eq. (33) with each other, we should know

$$
\begin{aligned}
\phi_g(x,t+\Delta t) &= \phi_g(x,t) \qquad (34)\\
P(x,t+\Delta t) &= P(x,t). \qquad (35)
\end{aligned}
$$

In other words, if he can properly solve Eq. (32) by his computer program, he should obtain the above results.

In null transient problems, stationary results should be obtained regardless with a time mesh width. If time mesh width Δt is large, a fixed-source in Eq. (11) becomes extremely small and correction to removal cross sections becomes also extremely small. In such cases, this problem is a sub-critical state, but quite near to critical, with a weak fixed source and it requires a large number of fission source iterations to attain convergence.

References

[1] Y.Ban, 'Development of unified numerical scheme for spatially dependent kinetics equation,' Master thesis of Nagoya university, (2011).[in Japanese]