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α-Adjoint Weighted Kinetics Parameter Estimation in the Monte Carlo α-Iteration Calculations

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1. Introduction

Nowadays the accelerator-driven subcritical system (ADS) has been widely studied as a candidate of transmutation reactor.[1] Applications of the conventional point kinetics equation (PKE) [2] using the *k*-adjoint weighted kinetics parameters may be invalid for the time-dependent ADS analysis because it assumes [3] that its nominal state is critical. In order to enhance the accuracy of the point kinetics analysis for an ADS, Nishihara et al. [3] proposed a PKE using kinetics parameters weighted by Green's function [4]. In our previous research [5], we proposed a PKE formulation with kinetics parameters weighted by the *α*-adjoint flux, the fundamental mode solution to the adjoint *α*-mode eigenvalue equation, because the *α*-mode eigenvalue equation can accurately represent an off-critical system.

In this paper, the physical meaning of the α-adjoint flux is derived by applying the power iteration method for the *α*-mode eigenvalue equation. Using this physical meaning, algorithms to calculate the *α*-adjoint weighted kinetics parameters in the Monte Carlo (MC) *α* iteration method [6] are developed and tested in an infinite homogeneous 2-group problem and the KUCA Th-ADS experimental benchmark.[7]

2. Methods

2.1 New point kinetic equation

The PKE based on the adjoint *α*-mode eigenvalue equation has been derived as [5]

$$\frac{dP(t)}{dt}=\left[\Delta\alpha(t)-\frac{\beta_{eff,\alpha}(t)}{\Lambda_{eff}(t)}\right]P(t)+\alpha_0 P(t)+\sum_i \lambda_i C_i(t)+Q(t); \quad (1)$$

$$\Delta\alpha(t)\equiv\frac{1}{\left\langle \phi_0^\dagger,\frac{\phi}{v}\right\rangle}\left[-\left\langle \phi_\alpha^\dagger,(\mathbf{L}-\mathbf{L}_0)\phi\right\rangle+\left\langle \phi_\alpha^\dagger,(\mathbf{F}-\mathbf{F}_0)\phi\right\rangle\right], \quad (2)$$

$$\beta_{eff}(t)\equiv\sum_i \beta_{eff,i}(t), \quad (3)$$

$$\beta_{eff,i}(t)\equiv\left\langle \phi_\alpha^\dagger,\beta_i\mathbf{F}_i\phi\right\rangle\Big/\left\langle \phi_\alpha^\dagger,\mathbf{F}\phi\right\rangle, \quad (4)$$

$$\Lambda_{eff}\equiv\left\langle \phi_\alpha^\dagger,\phi/v\right\rangle\Big/\left\langle \phi_\alpha^\dagger,\mathbf{F}\phi\right\rangle, \quad (5)$$

$$C_i(t)\equiv\left\langle \phi_\alpha^\dagger,c_i\right\rangle\Big/\left\langle \phi_\alpha^\dagger,\phi/v\right\rangle, \quad (6)$$

$$Q(t)\equiv\left\langle \phi_\alpha^\dagger,Q\right\rangle\Big/\left\langle \phi_\alpha^\dagger,\phi/v\right\rangle. \quad (7)$$

$\phi_\alpha^\dagger$ denotes the *α*-adjoint flux. $c_i(\mathbf{r},E,\mathbf{\Omega},t)$ is defined by $\left(\chi_i(E)/4\pi\right)C_i(\mathbf{r},t)$ where $\chi_i(E)$ and $C_i(\mathbf{r},t)$ are the fission spectrum and the delayed neutron precursor density, respectively, for the *i*-th precursor group. Other notations follow standards.

The time-dependent loss and fission production operators, denoted by **L** and **F**, respectively, are defined as

$$\mathbf{L}\phi=\left[\mathbf{\Omega}\cdot\nabla+\Sigma_t(\mathbf{r},E,t)\right]\phi(\mathbf{r},E,\mathbf{\Omega},t)-\int dE'\int d\mathbf{\Omega}'\Sigma_s(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\,|\,\mathbf{r},t)\phi(\mathbf{r},E',\mathbf{\Omega}',t), \quad (8)$$

$$\mathbf{F}\phi=\frac{\chi(E)}{4\pi}\int dE'\int d\mathbf{\Omega}'\nu(E')\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},E',\mathbf{\Omega}',t), \quad (9)$$

while their counter operators for the nominal state are defined by

$$\mathbf{L}_0\phi=\left[\mathbf{\Omega}\cdot\nabla+\Sigma_{t0}(\mathbf{r},E)\right]\phi(\mathbf{r},E,\mathbf{\Omega})-\int dE'\int d\mathbf{\Omega}'\Sigma_{s0}(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\,|\,\mathbf{r})\phi(\mathbf{r},E',\mathbf{\Omega}'), \quad (10)$$

$$\mathbf{F}_0\phi=\frac{\chi(E)}{4\pi}\int dE'\int d\mathbf{\Omega}'\nu(E')\Sigma_{f0}(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}'). \quad (11)$$

The subscript "0" indicates the nominal state of the subcritical system.

The *i*-th delayed neutron production operator, $\mathbf{F}_i$ is defined by

$$\mathbf{F}_i\phi=\int dE'\int d\mathbf{\Omega}'\frac{\chi_i(E)}{4\pi}\nu(E')\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},E',\mathbf{\Omega}',t). \quad (12)$$

2.2 Physical meaning of the α-adjoint

The adjoint form of *α*–mode eigenvalue equation can be expressed as [6]

$$\phi_\alpha^\dagger=\alpha\mathbf{R}^\dagger\phi_\alpha^\dagger; \quad (13)$$

$$\mathbf{R}=\frac{1}{v\Sigma_t}\sum_{j=0}^{\infty}\int d\mathbf{r}'\int dE_0\int d\mathbf{\Omega}_0 K_j(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r},E,\mathbf{\Omega})\times\int d\mathbf{r}_0 T(E_0,\mathbf{\Omega}_0;\mathbf{r}_0\to\mathbf{r}'), \quad (14)$$

where the *j*-th transport kernel K_j is defined with transport kernel *K*, free flight kernel *T* and collision kernel *C* as

$$\begin{aligned}&K_j(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r},E,\mathbf{\Omega})\\&=\int d\mathbf{r}_1\int dE_1\int d\mathbf{\Omega}_1\cdots\int d\mathbf{r}_{j-1}\int dE_{j-1}\int d\mathbf{\Omega}_{j-1}\\&\times K(\mathbf{r}_{j-1},E_{j-1},\mathbf{\Omega}_{j-1}\to\mathbf{r},E,\mathbf{\Omega})\cdots K(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r}_1,E_1,\mathbf{\Omega}_1),\end{aligned} \tag{15}$$

$$\begin{aligned}&K(\mathbf{r}',E',\mathbf{\Omega}'\to\mathbf{r},E,\mathbf{\Omega})\\&=T(\mathbf{r}'\to\mathbf{r}\,|\,E,\mathbf{\Omega})\cdot C(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\,|\,\mathbf{r}'),\end{aligned} \tag{16}$$

$$C(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\,|\,\mathbf{r}')=\sum_r\frac{\nu_r\Sigma_r(\mathbf{r}',E')}{\Sigma_t(\mathbf{r}',E')}f_r(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}), \tag{17}$$

$$\begin{aligned}&T(\mathbf{r}'\to\mathbf{r}\,|\,E,\mathbf{\Omega})=\frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2}\times\\&\exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|}\Sigma_t(\mathbf{r}-s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|},E)ds\right]\delta\left(\mathbf{\Omega}\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}-1\right).\end{aligned} \tag{18}$$

An application of the power iteration method for Eq. (13) gives

$$\phi^\dagger_{\alpha,i+1}=\alpha\mathbf{R}^\dagger\phi^\dagger_{\alpha,i}\,, \tag{19}$$

$$\phi^\dagger_{\alpha,n}=\left(\alpha\mathbf{R}^\dagger\right)^n\phi^\dagger_{\alpha,init}=\alpha^n\left(\mathbf{R}^\dagger\right)^n\phi^\dagger_{\alpha,init}\,. \tag{20}$$

Equation (20) can be expressed in an integral form as

$$\phi^\dagger_{\alpha,n}=\alpha^n\int dr'\int dE'\int d\mathbf{\Omega}'\mathbf{R}^n\left(r,E,\mathbf{\Omega}\to r',E',\mathbf{\Omega}'\right)\phi^\dagger_{\alpha,init}. \tag{21}$$

$\mathbf{R}^n\left(\mathbf{r},E,\mathbf{\Omega}\to\mathbf{r}',E',\mathbf{\Omega}'\right)$ is number of time source at $\mathbf{r}',E',\mathbf{\Omega}'$ produced in the n-th iteration due to a unit time source located at $\mathbf{r},E,\mathbf{\Omega}$. When $\phi^\dagger_{\alpha,init}\left(\mathbf{r},E,\mathbf{\Omega}\right)=1$, $\phi^\dagger_{\alpha,n}\left(\mathbf{r},E,\mathbf{\Omega}\right)$ can be interpreted as the number of time source produced in the n-th iteration due to a unit time source located at $\mathbf{r},E,\mathbf{\Omega}$. If n is large enough to converge, $\phi^\dagger_\alpha$ can be approximated by $\phi^\dagger_{\alpha,n}$.

$$\phi^\dagger_\alpha=\lim_{n\to\infty}\phi^\dagger_{\alpha,n} \tag{22}$$

2.3 Calculation of the α-adjoint weighted kinetics parameters in α-iteration

The definition of the α-adjoint weighted kinetics parameters are Eq. (3), (4), (5). The shape function ψ is approximated as ϕ, eigenfunction of α-mode eigenvalue equation.

$$\bar{\Lambda}^i_\alpha=\frac{\left\langle\phi^\dagger_\alpha,\phi/v\left(E\right)\right\rangle}{\left\langle\phi^\dagger_\alpha,\mathbf{F}\phi\right\rangle} \tag{23}$$

$$\left\langle\phi^\dagger_\alpha,\frac{1}{v\left(E\right)}\phi\right\rangle=\frac{1}{M^i}\sum_{j=1}^{M^i}\left(\sum_{k=1}^{K^{ij}}\frac{w^{ijk}\alpha^i}{\Sigma_t^{ijk}v^{ijk}}\right)\left(\frac{1}{\alpha^{i-n}}\right) \tag{24}$$

$$\left\langle\phi^\dagger_\alpha,\mathbf{F}\phi\right\rangle=\frac{1}{M^i}\sum_{j=1}^{M^i}\left(\sum_{k=1}^{K^{ij}}\frac{w^{ijk}\alpha^i}{\Sigma_t^{ijk}v^{ijk}}\right)\left(\sum_{k''\in Fission}^{k'}\frac{w^{(i-n+1)j'k''}}{w^{(i-n+1)j'k''}}\right) \tag{25}$$

Superscripts i, j and k are iteration, history and collision indices. Superscripts j' and k' are the history and collision indices of the (i-n+1)-th iteration from which the j-th time source of iteration i is generated. k'' is collision index of (i-n+1)-th iteration and j'-th history neutron.

In the denominator term, $\mathbf{F}\phi$ is weight of neutron generated from fission. In $\left\langle\phi^\dagger_\alpha,\mathbf{F}\phi\right\rangle$, adjoint of $\mathbf{F}\phi$ is number of time source which one neutron generated from fission. Then, $\mathbf{F}\phi$ is divided by weight. In the numerator, when i-n+1 iteration, j'-th history neutron induce a time source at k'-th collision, this one time source represents 1/α time source.

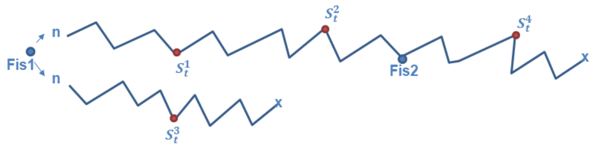

Figure 1. Fission neutrons and induced time sources

Like figure 1, we can suppose that one neutron produces two neutron by fission and induces 4 time source and fissions again during this flight. The adjoint of upper neutron between two fission neutrons produced by first fission expressed as Fis1 is number of time source after n iteration induced by time sources S_t^1, S_t^2, S_t^4. The adjoint of lower neutron between two fission neutrons produced by Fis1 is number of time source after n iteration induced by time source S_t^3. The adjoint of neutron produced by second fission expressed as Fis2 is number of time source after n iteration induced by time source S_t^4. Fis1 and Fis2 share time source S_t^4. Therefore, when j'-th history of time source induce fission, we sum 1 for each fission neutron before k'-th collision inducing time source as form of $\sum_{k''\in Fission}^{k'}$ to calculate $\mathbf{F}\phi$.

The weight function for the denominator and numerator, α adjoint is $\sum_{k=1}^{K^{ij}}w^{ijk}\alpha^i\Big/\Sigma_t^{ijk}v^{ijk}$ which is number of time source induced in i-th iteration. The term $\frac{w^{ijk}\alpha^i}{\Sigma_t^{ijk}v^{ijk}}$ is number of time source induced at k-th collision of j-th history neutron in i-th iteration.

$$\bar{\beta}^i_{eff,\alpha}=\frac{\left\langle\phi^\dagger_\alpha,\beta\,\mathbf{F}\,\phi\right\rangle}{\left\langle\phi^\dagger_\alpha,\mathbf{F}\phi\right\rangle} \tag{26}$$

$$\left\langle \phi_{\alpha}^{\dagger}, \beta\, \mathbf{F}\, \phi \right\rangle = \frac{1}{M^{i}} \sum_{j=1}^{M^{i}} \left(\sum_{k=1}^{K^{ij}} \frac{w^{ijk} \alpha^{i}}{\Sigma_{t}^{ijk} v^{ijk}} \right) \left(\sum_{k'' \in \substack{Delayed \\ Fission}}^{k'} \frac{w^{(i-n+1)j'k''}}{w^{(i-n+1)j'k''}} \right) \quad (27)$$

Indices and denominator term is same with prompt neutron generation time. In the numerator $\left\langle \phi_{\alpha}^{\dagger}, \beta \mathbf{F} \phi \right\rangle$, $\beta \mathbf{F} \phi$ is weight of neutron generated from delayed fission.

3. Numerical Results

3.1 The adjoint weighted kinetics parameters in the infinite homogeneous problem

The proposed method to calculate the α-adjoint weighted kinetics parameters is verified for an infinite homogeneous problem characterized by two-group cross sections given in Table 1. The precursor decay constant is 0.2. By multiplying constants to fission cross section, multiplication factors are modified to 0.65, 0.7, 0.8, 0.9, 0.95, 0.98, 0.99.

The MC α iteration and *k*-eigenvalue calculations were conducted with 200 active iterations on 1,000,000 sources per iteration except k_{inf} 0.98, 0.99 cases for MC α iteration calculations, which were conducted with 200 active iterations on 500,000 sources per iteration. Table 2 shows the comparison of MC estimates of α and *k*-eigenvalue and their analytic solutions. Table 3, 4 show the comparison of MC estimates of the adjoint weighted kinetic parameters and their analytic solutions. From table 2, 3, 4, one can see that the MC estimates agree well with the references within their 95% confidence intervals.

Table 1. 2-group cross-section for the infinite homogeneous problem

Cross section	g=1	g=2
Σ_{tg}	0.507132083	1.247472
Σ_{fg}	0.00268023	0.0522913
ν_{pg}	2.400	2.400
Σ_{sgg}	0.4798	1.085
$\Sigma_{sg'g}$(g≠g')	0.01453	0.001889
β_0	0.006	0.006
$1/v_g$[sec/cm]	2.286261×10^{-10}	1.293291×10^{-6}

Table 2. Estimated value of α and k_{inf} for the infinite homogeneous problem

k_{inf}	α (Rel. SD)	Analytic Value (Rel. error)	k_{inf} (Rel. SD)	Analytic Value (Rel. error)
0.65	57104.49 (0.002%)	57104.10 (0.001%)	0.65502 (0.003%)	0.65000 (0.003%)
0.7	50129.70 (0.007%)	50128.48 (0.002%)	0.70000 (0.003%)	0.70000 (0%)
0.8	35111.44 (0.009%)	35114.70 (-0.009%)	0.79999 (0.003%)	0.80000 (-0.001%)
0.9	18498.65 (0.014%)	18495.48 (0.017%)	0.90003 (0.003%)	0.90000 (0.003%)
0.95	9498.36 (0.020%)	9501.50 (-0.033%)	0.95002 (0.003%)	0.95000 (0.002%)
0.98	3864.74 (0.055%)	3864.21 (0.014%)	0.97998 (0.003%)	0.98000 (-0.002%)
0.99	1943.62 (0.070%)	1942.94 (0.035%)	0.98997 (0.003%)	0.99000 (-0.003%)

Table 3. Effective delayed neutron fraction in the infinite homogeneous problem

k_{inf}	$\beta_{eff,\alpha}$ (Rel. SD)	Analytic Value (Rel. error)	β_{eff} (Rel. SD)	Analytic Value (Rel. error)
0.65	6.00701×10^{-3} (0.326%)	0.006 (0.117%)	6.00436×10^{-3} (0.314%)	0.006 (0.073%)
0.7	5.97281×10^{-3} (0.303%)	0.006 (-0.453%)	5.98630×10^{-3} (0.297%)	0.006 (-0.228%)
0.8	6.00965×10^{-3} (0.270%)	0.006 (0.161%)	5.99542×10^{-3} (0.281%)	0.006 (-0.076%)
0.9	5.99175×10^{-3} (0.217%)	0.006 (-0.138%)	6.00175×10^{-3} (0.286%)	0.006 (0.029%)
0.95	5.99864×10^{-3} (0.228%)	0.006 (-0.023%)	5.98765×10^{-3} (0.306%)	0.006 (-0.206)
0.98	6.01570×10^{-3} (0.293%)	0.006 (0.262%)	6.00477×10^{-3} (0.287%)	0.006 (0.080%)
0.99	5.97947×10^{-3} (0.260%)	0.006 (-0.342%)	6.01814×10^{-3} (0.312%)	0.006 (0.302%)

Table 4. Effective prompt neutron generation time in the infinite homogeneous problem

k_{inf}	$\Lambda_{eff,\alpha}$ (Rel. SD)	Analytic Value (Rel. error)	Λ_{eff} (Rel. SD)	Analytic Value (Rel. error)
0.65	1.12961×10^{-5} (0.014%)	1.12939×10^{-5} (0.019%)	7.87479×10^{-6} (0.038%)	7.87379×10^{-6} (0.013%)
0.7	1.00011×10^{-6} (0.043%)	9.99816×10^{-6} (0.029%)	7.31210×10^{-6} (0.040%)	7.31137×10^{-6} (0.010%)
0.8	7.92799×10^{-6} (0.052%)	7.92347×10^{-6} (0.057%)	6.39569×10^{-6} (0.033%)	6.39745×10^{-6} (-0.028%)
0.9	6.34388×10^{-6} (0.068%)	6.34651×10^{-6} (-0.041%)	5.68743×10^{-6} (0.036%)	5.68662×10^{-6} (0.014%)
0.95	5.69330×10^{-6} (0.082%)	5.69556×10^{-6} (-0.040%)	5.39100×10^{-6} (0.036%)	5.38732×10^{-6} (0.068%)
0.98	5.32463×10^{-6} (0.193%)	5.34092×10^{-6} (-0.305%)	5.22147×10^{-6} (0.035%)	5.22241×10^{-6} (-0.018%)
0.99	5.23616×10^{-6} (0.251%)	5.22814×10^{-6} (0.153%)	5.17151×10^{-6} (0.035%)	5.16965×10^{-6} (-0.036%)

3.2 Application results of the α–PKE in the KUCA A Core Th-ADS Experiment

The α–PKE was be tested by thorium-loaded accelerator-driven system (Th-ADS) at Kyoto University Critical Assembly (KUCA) [7] by comparing MC PNS results. Th-HEU-5PE fuel case was tested. The $\boldsymbol{\alpha}$-PKE and *k*-PKE were applied and compared with MC PNS results. MC PNS experiment result with

14 MeV neutrons source was detected at ^{3}He #1, 2 detector.[6]

The prompt neutron decay constant is compared at table 5. We can see that the α iteration results are quite comparable with the experimental results because two estimates from different detectors show good agreements.

The kinetics parameters are compared at table 6. Effective delayed neutron fractions agree well with the references within their 95% confidence intervals. Relative difference of prompt neutron generation times is 27.33% because of different spectrum.

Table 5. Prompt neutron decay constants

	Measurements		MC PNS simulation[6]	MC α iteration
	^{3}He #1[6]	^{3}He #2[6]		
α_p (SD)	-3110 (11)	-3104 (10)	-2977.1 (1.4)	-2948.6 (1.8)

Table 6. Effective delayed neutron fraction and prompt neutron generation time

	Effective delayed neutron fraction		Prompt neutron generation time	
	$\bar{\beta}_{eff,\alpha}$	$\bar{\beta}_{eff}$	$\bar{\Lambda}_{eff,\alpha}$	$\bar{\Lambda}_{eff}$
Estimated Value (Rel. sd)	8.06946×10^{-3} (0.789%)	8.06183×10^{-3} (0.131%)	6.92151×10^{-5} (0.202%)	5.43591×10^{-5} (0.016%)
Rel. Difference	0.10%		27.33%	

Fitting was conducted to the amplitude functions $P_\alpha(t)$ and $P_k(t)$, solutions of PKEs, with MC PNS data from t=0.001 to t=0.003 using least square method with mathematica.

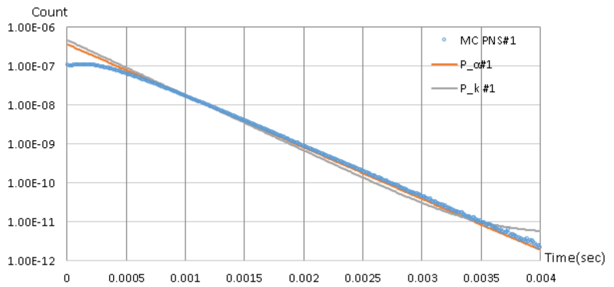

Figure 2. Comparison of amplitude function fitted to count rate at detector #1

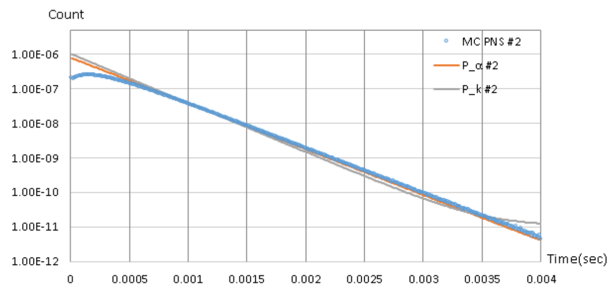

Figure 3. Comparison of amplitude function fitted to count rate at detector #2

In two graph, $P_\alpha(t)$ is closer to MC PNS results. From t=0.001 to t=0.003, average relative errors are compared at table 7. The average relative error of $P_k(t)$ is bigger than $P_\alpha(t)$ about 143% at detector 1 and 182% at detector 2.

Table 7. Average relative error of fitting function

	^{3}He #1		^{3}He #2	
	$P_\alpha(t)$	$P_k(t)$	$P_\alpha(t)$	$P_k(t)$
Rel. error[%]	-8.694%	-21.123%	-7.065%	-19.934%

4. Conclusions

The physical meaning of the α-adjoint is explained. The algorithms to calculate the required kinetics parameters is suggested for the MC α iteration calculations. In the two group infinite homogeneous problem, the MC estimated the adjoint weighted kinetics parameters agree well with the references within their 95% confidence intervals. In the KUCA A Core Th-ADS Experiment, α–PKE and k-PKE were applied and compared. When shape of fitting graphs and average relative errors are considered, estimation of α–PKE is more accurate at the KUCA A Core Th-ADS PNS Experiment.

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