Polynomial Interpolation in the Predictor Corrector Quasi-Static Method for Transient Calculation

Tae-suk Oh ^a and Yonghee Kim ^{a*}

^aKorea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea ^{*}Corresponding author: yongheekim@kaist.ac.kr

1. Introduction

Being able to properly assess the dynamic behaviour of the reactor system is crucial for both design and safety analysis, which requires the solution of space- and timedependent neutron and precursor balance equations. Directly solving such equations, especially with the presence of thermohydraulic (TH) effects, often demands ample amount of computation resources. In order to render such calculation to be affordable, the quasi-static (QS) approach is widely employed, which factorizes the neutron flux into *amplitude* and *shape* functions [1,2].

The variation of the amplitude function is obtained from the point kinetic equation (PKE) with shorter time steps, i.e., *micro-step*, while the modified balance equation (in favor of the shape) is intermittently solved with bigger time steps, i.e., *macro-step*, to govern the time dependency of shape. The communication between two components is achieved by expressing PKE parameters in terms of the shape for intermediate time steps, i.e., *reactivity-step*, where variation in the crosssection information is taken into account. Three different time steps are illustrated in Fig. 1.

In the Improved Quasi-Static method (IQM), so-called *normalization iteration* must be made to incorporate interdependency between amplitude and shape [3]. On the other hand, Predictor Corrector Quasi-Static method (PCQM) deduces the shape and then determines the variation of the amplitude [4]. Both approaches postulate that shape does not vary within a certain *macro-step* while solving PKE, and thus retain the name Quasi-Static.

In this study, the prospect and implication of having relaxation in the QS approach through polynomial interpolation has been considered. Transient calculation for a two-group slab reactor with and without the presence of TH feedback was conducted to verify the applicability of such treatment.

2. Improved Quasi-Static Method (IQM)

Multi-group time dependent neutron balance equation and precursor concentration equation are written as

$$\begin{aligned} &\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} = \nabla \cdot D_g \nabla \phi_g - \Sigma_{r,g} \phi_g + \sum_{\substack{g'=1\\g'\neq g)}}^{G} \Sigma_{s,g' \to g} \phi_{g'} \\ &+ (1-\beta) \frac{\chi_g}{k_0} \sum_{g'=1}^{G} v \Sigma_{f,g'} \phi_{g'} + \sum_{k=1}^{6} \lambda_k \chi_{g,k} C_{k,} \end{aligned}$$
(1)



Fig. 1. Three different time steps for employing QS method, where Δt_s , Δt_ρ and Δt_K indicate *macro-*, *reactivity*, and *micro-steps* respectively.

$$\frac{\partial C_k}{\partial t} = -\lambda_k C_k + \frac{\beta_k}{k_0} \sum_{g=1}^G \nu \Sigma_{f,g} \phi_g , \qquad (2)$$

where ϕ_g and C_k denote neutron flux for group g and delayed neutron precursor concentrations, respectively.

The QS approach expresses the neutron flux $\phi(\mathbf{r}, E, t)$ to be the multiplication of amplitude function p(t) and shape function $\psi(\mathbf{r}, E, t)$

$$\phi(\mathbf{r}, E, t) = p(t)\psi(\mathbf{r}, E, t), \qquad (3)$$

which requires the following quantity to be constant in time

$$K = < \frac{\phi_0^{\dagger}(\mathbf{r}, E)}{v(E)}, \psi(\mathbf{r}, E, t) >$$

$$:= \iint dEdV \frac{\phi_0^{\dagger}(\mathbf{r}, E)}{v(E)} \psi(\mathbf{r}, E, t) = K_0, \qquad (4)$$

where $\phi_0^{\dagger}(\mathbf{r}, E)$ indicates initial adjoint flux of the system.

The point kinetic equation (PKE) can be obtained by integrating Eqs. (1) and (2) over the space and energy [5],

$$\frac{dp}{dt} = \left[\frac{\rho(t) - \beta(t)}{\Lambda(t)}\right] p(t) + \frac{1}{\Lambda_0} \sum_k \lambda_k \xi_k(t), \quad (5)$$
$$\frac{d\xi_k}{\Lambda(t)} = \frac{F(t)}{\Lambda(t)} - \frac{F(t)}{\Lambda(t)} -$$

$$\frac{d\xi_k}{dt} = -\lambda_k \xi_k(t) + \frac{F(t)}{F_0} \beta_k(t) p(t).$$
(6)

Each parameters of PKE is expressed in terms of the shape as

$$F(t) = \langle \phi_0^{\dagger}, F\psi \rangle,$$

$$\Lambda(t) = \frac{K_0}{F(t)},$$

$$\beta_k(t) = \frac{1}{F(t)} \langle \phi_0^{\dagger}, \beta_k v \Sigma_f \psi \rangle,$$

$$\xi_k(t) = \frac{1}{F_0} \langle \phi_0^{\dagger}, \chi_{dk}(E) C_k(\mathbf{r}, t) \rangle,$$

$$\rho(t) = \frac{1}{F(t)} \langle \phi_0^{\dagger}, [\Delta \mathbf{F} - \Delta \mathbf{M}] \psi \rangle,$$

(7)

where matrices M and F are expressed as

$$\boldsymbol{M}_{\boldsymbol{g}}\boldsymbol{\psi}_{\boldsymbol{g}} := \left(-\nabla \cdot D_{\boldsymbol{g}}\nabla + \boldsymbol{\Sigma}_{r,\boldsymbol{g}}\right)\boldsymbol{\psi}_{\boldsymbol{g}},\tag{8}$$

$$\boldsymbol{F}_{\boldsymbol{g}}\boldsymbol{\psi}_{\boldsymbol{g}} := \boldsymbol{\nu}\boldsymbol{\Sigma}_{f,\boldsymbol{g}}\boldsymbol{\psi}_{\boldsymbol{g}}.$$
(9)

The IQM hinges on the modified balance equation for the shape, which is obtained from Eq. (1) while taking factorization into account.

$$\frac{1}{v_g} \frac{\partial \psi_g}{\partial t} + \frac{1}{v_g} \frac{\dot{p}}{p} \psi_g = \nabla \cdot D_g \nabla \psi_g - \Sigma_{r,g} \psi_g + \sum_{\substack{g'=1\\(g'\neq g)}}^{G} \Sigma_{s,g' \to g} \psi_{g'} + (1-\beta) \frac{\chi_g}{k_0} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \psi_{g'} + \frac{1}{p} \sum_{k=1}^{6} \lambda_k \chi_{g,k} C_k, \quad (10)$$

Since Eqs (5), (6), and (10) are interconnected, nonlinear iteration is required to properly determine the variation in the shape. The overall procedure for IQM is depicted in Fig. 2.

3. Predictor Corrector Quasi-Static Method (PCQM)

In contrast to IQM, PCQM directly solves Eqs. (1) and (2) from the current macro-step t_{s-1} to evaluate the (temporary) neutron flux at the next macro-step t_s , which is denoted as $\phi^*(t_s)$. By assuming the shape function at t_s is proportional to $\phi^*(t_s)$, one can express $\psi(t_s)$ as

$$\psi(t_s) = \phi^*(t_s) \cdot \frac{K_0}{<\phi_0^{\dagger}, \frac{1}{\nu}\phi^*(t_s) >},$$
(11)

which mathematically satisfies Eq. (4).

PKE parameters are then obtained from the updated information through Eq. (7). Note that original QS method assumes a time independent shape function within a certain macro-step Δt_s ; however, it does not imply that PKE parameters are also stagnant. Such variables must be re-evaluated for each reactivity step to encompass variation in the cross-section.

After the acquisition of the amplitude at t_s through Eq. (5) and (6), the flux is corrected as $\phi(t_s) = p(t_s)\psi(t_s)$. The overall procedure for PCQM is illustrated in Fig. 3.

4. Relaxation of Quasi-Static Approach

The conventional QS method assumes negligible variation in the shape for a certain macro-time interval of



Fig. 2. Overall procedure for IQM.



Fig. 3. Overall procedure for PCQM.

interest. However, such premises can be un-realistic if the size of the macro-step Δt_s becomes considerably large [6].

To stifle such disparity, the authors propose a new method that allows the variation of shape through polynomial interpolation. Specifically, both linearinterpolation and quadratic interpolation cases were scrutinized in this study. It is noteworthy to mention that interpolated shape must be re-normalized to suffice the factorization criterion

5. Consideration of Feedback Effect

In order to acquire a realistic dynamic behaviour of the reactor system, a proper thermohydraulic equation must be solved coupled with the neutronic consideration. In the proposed study, both mass and energy balance equations were solved for fluids interacting with the fuel rods to determine the adjustment in the cross-section.

For both IQM and PCQM, the TH module was solved for each reactivity step from the power density calculated based on the estimated flux as $\phi(t_m^{\rho}) = p(t_m^{\rho})\psi(t_m^{\rho})$. Since TH module can be readily solved, re-evaluation of PKE parameters were sufficiently performed.

6. Numerical Results

One-dimensional two-group slab reactor coupled with a simple TH module was subjected to a localized perturbation to assess the applicability of relaxation of Quasi-Static treatment of the shape.

Ramp-up perturbation in the thermal group absorption cross-section has been introduced in the bottom region of the fuel by 60 [cm]. The configuration and the imposed perturbation are illustrated in Fig. 4.



Fig. 4. Configuration and introduced perturbation.

6.1 Without the Presence of Feedback Effect

Three different treatments, namely static, linear, and quadratic interpolation for the shape, had been made for both IQM and PCQM. The computational burden and relative power error (P_{err}) are depicted in Fig. 5. and Table. 1. Every calculation was done for having macrostep of 0.2 [s], reactivity step of 0.01 [s], and micro-step of 0.5 [ms] on a single 3.1 GHz Intel Core i5 processor.



Fig. 5. Estimated power from IQM and PCQM

TABLE. 1. TH feedback non-considered calculation

reference = 524.56 [s]				
Method	Time	$P_{err}(t=4)$	$P_{err}(t=6)$	
w/o QS	30.34 [s]	16.93 [%]	21.45 [%]	
IQM (ψ static)	54.37 [s]	25.15 [%]	24.16 [%]	
PCQM (ψ static)	29.16 [s]	24.57 [%]	24.24 [%]	
IQM (ψ linear)	54.59 [s]	2.477 [%]	0.484 [%]	
PCQM (ψ linear)	28.81 [s]	4.340 [%]	0.795 [%]	
IQM (ψ quad)	55.90 [s]	1.333 [%]	0.361 [%]	
PCQM (ψ quad)	29.65 [s]	3.346 [%]	0.829 [%]	

With a static treatment of the shape, the estimated power variation became worse compared to that of the brute force calculation (denoted as w/o QS) for both IQM and PCQM. On the other hand, with a linear and quadratic interpolation of the shape, a salient increase in the accuracy was obtained.

In terms of the computation, due to the presence of a normalization loop for IQM, such method required about twice as much computing time to that of PCQM.

6.2 With the Presence of Feedback Effect

In order to mimic the accident during the start-up, the same perturbation was introduced for HZP condition (0.01% of HFP). Conspicuous difference originating from the feedback effect is depicted in Fig. 6.



Calculated result for having linear and quadratic interpolation of shape for both IQM and PCQM for such case is illustrated in Fig 7. and Table. 2. To assess the performance of each approach, the following quantity, which is named as integrated error (ε_{OS}), was evaluated.

$$\varepsilon_{\rm QS} := \int_{t_{start}}^{t_{end}} dt \left| P_{ref}(t) - P_{QS}(t) \right|. \tag{12}$$

It can be observed that having a quadratic treatment of the shape results in better estimation of power for both IQM and PCQM. Furthermore, the relative additional computational burden for IQM to that of PCQM had dwindled compared to the case of not having TH feedback effect.



Fig. 7. Estimated power from IQM and PCQM

TABLE. 2. TH	feedback considered calculation

reference = 534.74 [s]			
Method	Time	Integrated Error	
w/o QS	58.47 [s]	3.19291E+02	
IQM (ψ linear)	59.04 [s]	8.41267E+01	
PCQM (ψ linear)	48.51 [s]	4.67825E+01	
IQM (ψ quad)	58.94 [s]	7.81011E+01	
PCQM (ψ quad)	48.49 [s]	4.54856E+01	

7. Conclusions

In this paper, relaxation of Quasi-Static approach has been achieved through either linear or quadratic interpolations in the framework of IQM and PCQM, and its applicability was investigated by solving transient problems for slab reactor.

It has been shown that for neutronics calculation only, although a marginal enhancement in the accuracy was obtained by employing IQM based approaches, the presence of normalization loop renders computational burden of it to be substantial compared to that of PCQM based approaches.

For the case of having a finite TH feedback effect, transient at HZP was simulated to resemble an accident

during a start-up of the power plant. For such scenario, quadratic interpolation of shape in the framework of PCQM resulted in the most accurate estimation of power at an affordable cost.

Validation of appropriateness of relaxation of Quasi-Static approaches will be expanded to more realistic problems and a sensitivity analysis regarding the time step(s) will be investigated in the near future.

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