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An Algorithm to Obtain the Dynamics From Step Responses Measured at Two Detected Points - Step Testing Method -

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Abstract

A step testing method that can obtain the dynamics of a desired test section from the step responses measured at the points before and behind the test section is proposed. Discussion was made on the processing accuracy of this testing method by numerical experiments. As a practical application of this method, the dynamics of a desired part in a packed bed along the flow direction were computed from the experimental step responses.

The results are as follows; the step testing method has been found to be a useful tool for the observation of the dynamics in chemical equipments. The procedure developed here for the dynamic analysis of a desired test section has been proved to be useful when the section has non-linearity.

Introduction

In the study of chemical processes, it is often necessary to determine the dynamics of a desired part or section, but the position of tracer input is restricted in some degree. In such cases, a conventional method to determine the dynamics is a frequency response method. In its implementation, a sinusoidal input, when imposed upon a real process, requires such a complicated input facility that its setting-up and operation are more time consuming than step or impulse input, since several frequencies must be tested and transients eliminated before measurement. A second method, a statistical approach using auto- and cross-correction functions⁷, needs a very long measurement time. In addition, if the process contains some non-linearity, an error is unavoidable in the dynamics and the error can not be estimated. As the other more convenient method to determine the dynamic analysis across-the-board from the components to the complete plant. This method has been playing a very important role in process analysis to obtain the dynamics of the desired part of the plant, in a short observation time.

In the present study, as another process dynamics testing algorithm using a short observation period, the step testing method is proposed. This method utilizes step responses in a manner analogous to the way the pulse testing method employes impulse responses. A step response can sometimes simplify the experimental facility compared with a statistical signal or a frequency response. For instance, step changes in the inlet concentration and flow rate of the process are often imposed instantaneously, so the dynamics of the desired part can be easily obtained

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without any special facility. Furthermore, in the step testing method proposed, a step input does not always necessitate an exact step function.

The scope of our investigation is as follows.

(1) For dynamic analysis of the two points detection type, the computational error caused by the data processing is investigated. (1-1) For both methods, the usual pulse testing method and the newly proposed step testing method, formulae of the first and the second order approximation have been derived. (1-2) Utilizing the Nth delay system, $G(S)=1/(S+1)^N$ as a model, the processing errors with these formulae are examined by numerical experiments. Also, the processing error is discussed with the data including a round off error.

(2) For an example of application, the effectiveness of the step testing method is demonstrated in the measurement of the mixing dynamics of a shallow packed bed.

Derivation of Formulae

For the first order approximate formula (derived as the sum of all the small triangle pulses) of the pulse testing method, Hougen and Walshs' formula is well known. But, when $(Y(t))_{t=0}$ is not equal to zero, their formula needs to make a correction of a right triangle pulse as shown in Fig. 1-(a).

For the formula of the step testing method, the first order formula (as the sum of all the narrow step wise stripes) is derived easily as shown in Fig. 1-(b) (see Appendix).

With formulae for the second order approximation, pulses (Figs. 1-(c), (e)) or steps (Figs. 1-(d), (f)) are approximated by applying the parabola that passes through three points: Y_{k-1} , Y_k , Y_{k+1} . Further, the formulae are derived as the sum of all stripes after Laplace transformation of each stripe⁶. When summing up the stripes, two kinds of formulae are conceivable both for the single stripe (Figs. 1-(e), (f)) and double stripes (Fig. 1-(c), (d)). All the formulae obtained are listed in Table 1.



Fig. 1 Pulse and step testing methods (a) Correction for Hougen eqn.; eqn. (P1) (b) Step testing method; eqn. (S1)

(c), (e) Pulse testing method (2nd order); eqns. (P2), (P3)

(d), (f) Step testing method (2nd order); eqns. (S2), (S3)

METHODS ORDER	PULSE TESTING METHOD (Y (S)) $s=j\omega$	STEP TESTING METHOD (Y (S)) $s=j\omega$
1ST ORDER BROKEN LINE)	$\left\{\frac{\sin(\Delta t \omega/2)}{\Delta t \omega/2}\right\}^{2} \sum_{k=1}^{n-1} Y_{k} \Delta t e^{-jk\Delta t \omega} + Y_{0}(0) \left[(1-e^{-\Delta t \omega})/\omega^{2} \Delta t + 1/j\omega\right]$	$\frac{1-e^{j\Delta t\omega}}{\Delta t\omega^2}\sum_{k=1}^n (Y_k-Y_{k-1})e^{-jk\Delta t\omega}$
	eqn. (P1)	eqn. (S1)
2 ND ORDER (PARABOLA) DOUBLE STRIPS	$\sum_{k=1}^{n-1} \left[\frac{4 \sin \Delta t \omega}{\omega} \left(-\frac{a_k}{\omega} j + \frac{a_k}{2} - a_k \Delta t \right) + Y_{k-1} e^{j \Delta t \omega} \right]$	$\frac{-4}{\omega^2} \sum_{k=1}^{n-1} \left[\left\{ \left(\frac{1}{\omega} - j \Delta t \right) a_k + \frac{d \kappa}{2} j \right\} (\sin \Delta t \omega) \right.$
	$-\left(Y_{k+1}+\frac{4a_{k}}{j\omega}\Delta t\right)e^{-j\Delta t\omega}\left]\frac{e^{-jk\Delta t\omega}}{j\omega}\right]$	$-a_{k}\Delta t e^{-j\Delta t\omega} \bigg] e^{-jk\Delta t\omega}$
	$k = 1, 3, 5, \cdots$ eqn. (P2)	$k = 1, 3, 5, \cdots$ eqn. (S2)
2ND ORDER (PARABOLA)	$\sum_{k=1}^{n-1} \left[\left\{ -\frac{2a_k}{\omega^2} + \frac{1}{j\omega} (d_k - 2a_k \Delta t) \right\} (e^{j\Delta t \omega} - 1) \right]$	$-\frac{1}{\omega^2}\sum_{k=1}^{n-1}\left[\left(d_k-2a_k\Delta t-\frac{2a_k}{\omega}j\right)\left(e^{j\Delta t\omega}-1\right)\right]$
SINGLE STRIPS	$+\frac{2a_{k}\Delta t}{\omega}j+Y_{i-1}e^{j\Delta t\omega}-Y_{i}\left]\frac{e^{-jk\Delta t\omega}}{j\omega}\right]$	$-2a_{k}\Delta t \left] e^{-jk\Delta t\omega} \right]$
	$k = 1, 2, 3, \cdots$ eqn. (P3)	$k = 1, 2, 3, \cdots$ eqn. (S3)
	$a_{k} = \frac{1}{2(\Delta t)^{2}} (Y_{k+1} + Y_{k-1} - 2Y_{k}), d_{k} = \frac{1}{2\Delta t} (Y_{k+1} - Y_{k-1})$,

Numerical Experiments

The procedure for the numerical experiment is as follows:

First, the dynamics of the test section in frequency domain are obtained as the ratio of eqn. (S1), (S2) or (S3), at the outlet of the section to that at the inlet. That is, frequency response, gain $|G(j\omega)|$ and phase angle, $\angle G(j\omega)$ of the test section can be computed for the given frequency, ω .

Second, we can obtain the residence time curve (RTC) about the test part or section from these gain and phase angle, by Johnson's method⁴ of harmonic analysis given in eqn. (4).

$$\psi(\tau) = \frac{1}{2} + \frac{2}{\pi} \sum_{m=1,3,5,\cdots} \frac{|G(jm\omega)|}{m} \sin[m\omega\tau + \angle G(jm\omega)]$$
(4)

The RTC of the test section is of importance for the mixing model identification.

Third, the error which is calculated as the difference between the analytical solution for the RTC of the test section and the above-mentioned numerical solution for the RTC through harmonic analysis of the test section, is evaluated on the basis of the root mean square criterion.

Numerical experiments for all the formulae in Table 1 are carried out with a model system as shown in Fig. 2. The test section of the system is first order delay. The delay order, N between tracer input and the first detection point is set equal to 1, 2, 3, 4, 5 and 10, and notch times (sampling time intervals), Δt are set to 0.1, 0.2 and 0.3. Frequency responses of the test section are calculated for two hundred frequencies, ω , in the interval (0.2–79.8) with an interval size $\Delta \omega \doteq 0.4$. The final tailing value of the response curves, Y_1 , Y_2 (generated in the computer by analytical impulse and step functions of Nth order) at two detected points utilized for the numerical experiments are terminated when the residuals (impulse: Y_1 , Y_2 , step: $1-Y_1$, $1-Y_2$) are less than 0.0001.

Figure 3 shows the test results obtained with the calculation of RTC, $|G(j\omega)|$ and $\angle G(j\omega)$ for the N=1, $\Delta t=0.1$ case by the pulse and step testing methods. At high frequency, the difference from the analytical G(S)=1/(S+1) becomes large. In general, difference in the errors for both testing methods is not significant.

In Figure 4, the processing errors on the RTC, gain and phase angle are plotted against N (the delay order between tracer input and the first detected point) for $\Delta t = 0.1$. Computation was carried out to seven significant figures (exponential part; 8 Bits, mantissa part; 24 Bits). There is no significant difference between the step testing method and the pulse testing method processing errors. As the value of N becomes larger, the difference between the first and second detection signals becomes less, and the processing error increases considerably in both methods. In this model system, N, i.e., the delay order between the tracer input and the first detected signals, must be less than four to keep the R.M.S. error on the RTC within 0.1 or 10%. When



Fig. 2 Model system for numerical experiments

the two detected signals become very similar and close owing to the big order of delay between the tracer input point and the first detected point, exact estimation with the dynamics of the test section is difficult in both methods.



Fig. 3 R.M.S. error vs. delay order between tracer input and 1st detected point



Fig. 4 Processing errors on RTC, gain and phase angle vs. delay order between tracer input and 1st detected point

In practice, experimental response curves usually involve some noise. Owing to the noise, experimental data, which may also depend upon the precision of experiments, may not be accurate to the 7 significant figures discussed above. To evaluate this consideration, the processing error with delay order was recalculated with Y_1 and Y_2 preset to 1, 2, 3 and 7 significant digits. Generation of the test data, Y_1 , Y_2 having the desired significant figures was accomplished by rounding off the seven significant digits data to the nearest requested whole number. Fig. 5-(a), (b) and (c) present the R.M.S. error for RTC, gain and phase angle, respectively, against the significant figures of test data. Figure 5 shows that the processing errors are almost the same for the first and second order approximate formulae (single stripe and double stripes), when the significant figures of the data are less than three digits. Therefore, when the experimental data have not enough significant figures, the formula of the first order approximation, which surpasses the second order approximation in computation speed, should be used for the step testing method and the pulse testing method.



Fig. 5 R.M.S. error on RTC, gain and phase angle vs. significant figures of test data

Computation Error of Model Parameter Estimation through the Integral Method

As a method to estimate model parameters from experimental response curves, a moment method in which integration of the response curves by adding various weights is made, is often employed. By equating the moments of models and experiments, the model parameter, such as number of tanks, is estimated. By utilizing the integral method, the error is examined for the kinds of response from which the moments are calculated. The computation error through impulse and step responses was discussed for numerical experiments, N-series tanks model was used as a model system. The transfer function of N-series tanks model can be described as eqn. (5).

$$G(S) = \frac{\psi^{\text{out}}(S)}{\psi^{\text{in}}(S)} = \frac{1}{(S/N+1)^{N}}$$
(5)

Its impulse response is developed analytically by eqn. (6) and its step response is eqn. (7).

$$\psi_{I}(\tau) = \frac{N(N\tau)^{N-1}}{(N-1)!} e^{-N\tau}$$
(6)

$$\psi_{s}(\tau) = 1 - \left[1 + (N\tau) + \frac{(N\tau)^{2}}{2!} + \dots + \frac{(N\tau)^{N-1}}{(N-1)!} \right] e^{-N\tau}$$
(7)

For the N-series tanks model, the mean and the variance of its residence time distribution can be derived analytically as $\overline{\tau}=1.0$ and $\overline{\tau}^2=1/N$. On the other hand, by applying the numerical moment integration in impulse response, $\psi_1(\tau)$ or step response, $\psi_{\underline{S}}(\tau)$, the variance of $\overline{\tau}^2$ is calculated from eqn. (9) or (12). For the impulse response, $\psi_1(\tau)$, $\overline{\tau}$ and $\overline{\tau}^2$ can be expressed by eqn. (8) and (9) from their definition.

$$\overline{\tau} = \int_0^\infty \psi_I(\tau) \ \tau \ d \ \tau \ / \int_0^\infty \psi_I(\tau) \ d \ \tau \tag{8}$$

$$\overline{\tau^2} = \left[\int_0^\infty \psi_i(\tau) \tau^2 d\tau \right] / \left[\int_0^\infty \psi_i(\tau) d\tau \right] - \left[\int_0^\infty \psi_i(\tau) \tau d\tau / \int_0^\infty \psi_i(\tau) d\tau \right]^2$$
(9)

For the step response, $\psi_S(\tau)$, $\overline{\tau}$ and $\overline{\tau^2}$ are defined as eqns. (11) and (12) by paying attention to the difference, $\psi_S(\tau)$ from steady state value¹.

$$\overline{\psi}_s \equiv G(0) - \psi_s(\tau) \tag{10}$$

$$\bar{\tau} = \int_0^\infty \bar{\psi}_s(\tau) \, d\tau \tag{11}$$

$$\overline{\tau^2} = 2 \times \int_0^\infty \overline{\psi}_s(\tau) \tau \, d\tau - [\int_0^\infty \overline{\psi}_s(\tau) \, d\tau]^2$$
(12)

Consequently, the variance for the step response is computed by the τ -weighted numerical integration with $\psi_{\rm S}(\tau)$. But, the variance for the impulse response is computed by the τ^2 -weighted numerical integration with $\psi_{\rm I}(\tau)$. τ^2 -weighted integration gathers much noise at large τ values. So, it is forecasted that the step response has less error in its processing than that the impulse response. To prove the above-mentioned forecast, the test data were generated from impulse or step response according to eqn. (6) (impulse) or (7) (step), and from these data respective variances are computed by eqn. (9) or (12). These computed variances, $\overline{\tau^2}$ were set equal to the analytical variance of the N-series tanks model, $\overline{\tau^2}=1/N$. Thus, the model parameter N (number of tanks) could be estimated as N_{computed}= $1/\overline{\tau^2}$.

As the criterion to evaluate numerical integration error with the number of tanks, relative error, Er_N defined by eqn. (13) was employed.

$$Er_N = |N_{analytical} - N_{computed}| / N_{analytical} \times 100$$
 (13)

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Fig. 6 Relative error vs. number of tanks

In Figure 6, the relative error, Er_N is plotted against the number of tanks, N for a notch time, i.e., sampling time interval of the test data sets equal to 0.3. The computation was operated at significant bits of 32 and 64, but there was not so great difference in their results. Figure 6 shows that integration through the step response is more accurate than that through the impulse response, as was forecasted. The same tendency was confirmed when a notch time of test data was varied at several values; 0.1, 0.2, 0.4 and 0.5.

Application of the Step Testing Method for the Measurement of Residence Time Curve at a Test Section in a Shallow Packed Bed

The procedure which is thought to be a convenient way for the measurement of RTC via frequency domain and its mean and variance at a desired part of a shallow packed bed (see Fig. 7) is outlined as follows.

(1) Measurement of experimental response curves

The procedure involves the step change in the inlet concentration into the packed bed and the measurement of its concentration at the points before and behind a desired part downstream from the inlet point. This gives a pair of experimental step response curves.

(2) Computation of frequency responses by the step testing method

By utilizing the formula of the step testing method (eqn. S1, S2 or S3), the frequency responses of the desired part of the packed bed can be computed from the experimental step response curves observed at the first and the second detected points in a packed bed along the flow direction.



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shallow packed beds

Fig. 7



(3) Computation of RTC by Johnson's method

The RTC of the test part or section is computed from the frequency responses by Johnson's method of harmonic analysis (eqn. (4)).

(4) Computation of the mean and the variance

The mean and the variance of experimental step responses are computed by moment integration. The moment will be used for the model parameter estimation.

Figure 7 shows the tube bundle bed which was constructed as a model bed to obtain the mixing dynamics in a shallow beads-packed-bed. Step-wise concentration changes, Y_1 , Y_2 both at the first void inlet and the fourth void outlet were detected by electric conductivity measurement, when a step change in concentration was imposed on the fluid at the up-stream flow distributor. The concentration change was given by a switch cock. The fluids, distilled water at 25±0.2°C, containing, respectively, 0.02N (d=0.9974g/cm³) and 0.04N (d=0.9978g/cm³) hydrochloric acid were switched by the cock to select either, and to give a step change in concentration into the bed. When the fluid was changed from the solution of low concentration (0.02N-HCl) to that of high concentration (0.04N-HCl) the obtained response was defined as the positive response, and inversely, when the fluid was changed from the high concentration to the low concentration the obtained response was the negative response.

The experimental residence time curves, Y_1 , Y_2 at the two detection points in a shallow packed bed were shown in Fig. 8-(a). The residence time curves in the desired test section which were computed by the step testing method and Johnson's method from the curves, Y_1 , Y_2 were shown in Fig. 8-(b). By use of the step testing method, we could measure the residence time curves in the shallow bed which was only four folds of packing diameter in height.

In Figure 8, the full line shows a positive response and the broken line shows a negative one. The difference in density between the two fluids was about $4 \times 10^{-4} \text{ g/cm}^3$. These curves are response curves at the laminar flow region. Figure 8-(b) shows that the response for the inputs between positive and negative are clearly distinguished. This difference in the response may be due to difference in density. For the experiments in which direction of the fluid flow to the

bed was changed from up-flow to down-flow with respect to the gravity force, the responses were the inverse of the shapes shown in Fig. 8-(b). Positive and negative change can be easily imposed on the input by the step testing method, and the non-linearity of the system can be discussed. Since all the derivations of the formulae have been based on linear algebra, strict evaluation of the non-linearity with the tested section in the process is not possible, but a qualitative feature of the non-linearity is sure to be grasped by our procedure developed for the measurement of the fluid mixing dynamics in a shallow packed bed.

Conclusion

The foregoing results lead to the following conclusions.

(1) The step testing method has been a useful technique for the measurement of dynamics of a desired part in chemical equipments. As positive and negative change on the signal can be easily applied by this testing method, non-linearity of the system, though qualitatively, can be examined by the procedure developed here.

(2) For the estimation of parameters in a chemical process model, the procedure through the step response is more accurate than the impulse response.

Nomenclature

- Er_N relative error with N-series tanks model
- G(S) transfer function
- N number of tanks or delay order
- S Laplace operation
- t real time, sec
- Y(t) response (experimental)

Greek symbol

- Δt notch time, sampling time interval
- $\psi(\tau)$ response (theoretical or computational)
- $\overline{\psi}(\tau)$ the difference from steady state value in response
- au dimensionless time
- $\overline{\tau}$ mean of residence time distribution, in term of τ
- $\overline{\tau}^2$ variance of residence time distribution from $\overline{\tau}$, in terms of τ

Subscript

- 1 1st detection
- 2 2nd detection
- cal numerical calculation
- exact theoretical analysis
- I impulse response
- S step response

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Appendix

This appendix shows how the results eqns. (S1) and (S2) can be obtained. The response curves at the detected points, $Y_1(t)$ and $Y_2(t)$ are approximated as the sum of all the step wise stripes, as shown in Fig. 1-(b) and (d).

Linear approximation Note the step-wise stripe passing through the two points, (t_{k-1}, Y_{k-1}) and (t_k, Y_k) , and apply unit step function $U(t-t_{k-1})$ to let $Y_{k-1}=0$. (See Fig. A) A simple step wise stripe is expressed by eqn. (A1).

$$D_{L}(t) = \frac{Z_{k} - Z_{k-1}}{\Delta t} (t - t_{k-1}) \times U(t - t_{k-1}) - \frac{Z_{k} - Z_{k-1}}{\Delta t} (t - t_{k}) \times U(t - t_{k})$$
(A1)

where $Z=Y-Y_{k-1}$ and $\Delta t=t_k-t_{k-1}$.

Laplace transformation of eqn. (A1) results in eqn. (A2).

$$D_{L}(S) = \frac{Z_{k} - Z_{k-1}}{\Delta t S^{2}} \left(e^{-t_{k-1}S} - e^{-t_{k}S} \right)$$
(A2)

Equation (A2) is expressed as eqn. (A3) by setting $S=j\omega$.

$$D_{s}(j\omega) = \frac{Z_{k} - Z_{k-1}}{\Delta t \,\omega^{2}} (1 - e^{j\Delta t \,\omega}) \, e^{-jt_{k}\,\omega} \tag{A3}$$

Since $Y_k - Y_{k-1} = Z_k - Z_{k-1}$, the first order approximate formula, which is expressed as the sum of eqn. (A3), becomes eqn. (S1).

Parabola approximation Note the step-wise stripes using the three points, $(t_{k-1}, Y_{k-1}), (t_k, Y_k)$ and (t_{k+1}, Y_{k+1}) . (See Fig. B) When $Z = Y - Y_{k-1}$, a parabola approximated function throughout the three points, $(t_{k-1}, Z_{k-1}), (t_k, Z_k)$ and (t_{k+1}, Z_{k+1}) is rewritten by eqn. (B1).

$$D = A (t - t_{k-1})^2 + B (t - t_{k-1})$$
(B1)

where
$$A = \frac{Z_{k+1} - 2Z_k + Z_{k-1}}{2(\Delta t)^2}$$
, $B = \frac{1}{2\Delta t} (Z_{k+1} - Z_{k-1}) - A + 2At_{k-1}$ and

 $\Delta t = t_{k+1} - t_k = t_k - t_{k-1}$.

The parabola equation which is symmetrical to eqn. (B1) with respect to the axis of $Z = (Z_{k+1}-Z_{k-1})/2$, passes through the three points, (t_{k-1}, Z_{k+1}) , $(t_k, Z_{k+1}-Z_k)$ and $(t_{k+1}, 0)$. The eqn. (B1) is rewritten as eqn. (B2).

$$D = \overline{A}(t - t_{k+1})^2 + \overline{B}(t - t_{k+1})$$
(B2)
where $\overline{A} = -\frac{Z_{k+1} - 2Z_k + Z_{k-1}}{2(At)^2}, \ \overline{B} = -\frac{Z_{k+1} - Z_{k-1}}{2At} - \overline{A} - 2\overline{A}t_{k+1}.$

A parabola approximated step wise stripe is expressed by eqn. (B3).

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$$D_{P}(t) = [A(t - t_{k-1})^{2} + B(t - t_{k-1})] \times U(t - t_{k-1}) + [A(t - t_{k+1})^{2} + B(t - t_{k+1})] \times U(t - t_{k+1})$$
(B3)

Laplace transformation of eqn. (B3) gives rise to eqn. (B4).

$$D_{P}(S) = \left(\frac{2A}{S^{3}} + \frac{B}{S^{2}}\right)e^{-t_{k-1}s} + \left(\frac{2\overline{A}}{S^{3}} + \frac{\overline{B}}{S^{2}}\right)e^{-t_{k+1}s}$$
(B4)

Equation (B4) is written as eqn. (B5) by setting $S=j\omega$.

$$D_{P}(j\omega) = \frac{e^{-jA_{E}}\omega}{j\omega} \left[\left(-\frac{2A}{\omega^{2}} + \frac{B}{j\omega} \right) e^{j\Delta t\omega} + \left(-\frac{2A}{\omega^{2}} + \frac{B}{j\omega} \right) e^{-j\Delta t\omega} \right]$$
(B5)

since, $Y_{k-1} - 2Y_k + Y_{k+1} = Z_{k-1} - 2Z_k + Z_{k+1}$ and $Y_{k+1} - Y_{k-1} = Z_{k+1} - Z_{k-1}$, $Y_p(j\omega)$ is expressed by eqn. (B6) as the sum of eqn. (B5).

$$Y_{P}(j\omega) = \frac{1}{j\omega} \sum_{k=1,3,5,\cdots}^{n-1} \left[\left(e^{j\Delta t\omega} - e^{-j\Delta t\omega} \right) \left(-\frac{2A}{\omega^{2}} \right) + \frac{B}{j\omega} e^{j\Delta t\omega} + \frac{\overline{B}}{j\omega} e^{-j\Delta t\omega} \right] e^{-jt_{k}\omega}$$
(B6)

Thus, the second order (parabola) approximate formula becomes eqn. (S2).

Equation (S3) with respect to a single stripe is developed by the same procedure as for eqn. (S2).



Fig. A Step wise stripe by linear approximation

Fig. B Step wise stripes by palabola approximation