Identification of Volterra Kernels of Nonlinear Van de Vusse Reactor

Hiroshi Kashiwagi and Li Rong

Abstract: Van de Vusse reactor is known as a highly nonlinear chemical process and has been considered by a number of researchers as a benchmark problem for nonlinear chemical process. Various identification methods for nonlinear system are also verified by applying these methods to Van de Vusse reactor. From the point of view of identification, only the Volterra kernel of second order has been obtained until now. In this paper, the authors show that Volterra kernels of nonlinear Van de Vusse reactor of up to 3rd order are obtained by use of M-sequence correlation method. A pseudo-random M-sequence is applied to Van de Vusse reactor as an input and its output is measured. Taking the crosscorrelation function between the input and the output, we obtain up to 3rd order Volterra kernels, which is the highest order Volterra kernel obtained until now for Van de Vusse reactor. Computer simulations show that when Van de Vusse chemical process is identified by use of up to 3rd order Volterra kernels, a good agreement is observed between the calculated output and the actual output.

Keywords: identification, Volterra kernel, nonlinear system, M-sequence, crosscorrelation

I. Introduction

Van de Vusse reactor is one of the highly nonlinear processes which have been used by many researchers as a benchmark for control problem; Van de Vusse[7], Kantor[3], Doyle V *et al*[2].

From the point of view of identification problem, Doyle V *et al*[2] obtained up to second order Volterra kernel, but no further research on the more precise identification has been reported until now.

Recently, one of the authors has developed a method for obtaining Volterra kernels of up to 3rd order of a nonlinear system by use of M-sequence correlation method[4]. In this method, a pseudo-random M-sequence is applied to a nonlinear process and the crosscorrelation function between the input and the output is measured. Then from the crosscorrelation function we can obtain up to 3rd order Volterra kernels.

This method of nonlinear system identification is applied to the highly nonlinear Van de Vusse reactor. Volterra kernels of Van de Vusse reactor of up to 3rd order are shown to be obtained by use of M-sequence correlation method.

II. Van de Vusse reactor

Van de Vusse reactor is known as a highly nonlinear process and quite frequently used as a benchmark test for various control strategies[2),3),7)].

In this reactor, a product A is to be converted to the desired product B, in an isothermal continuous stirred tank reactor $(CSTR)$, but the product B is degradated to product C.

In addition to this consecutive reaction, a high-order parallel reaction occurs and A is converted to by-product D. The reaction scheme is as follows

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$A + A \xrightarrow{k_3} D$$

where k_1, k_2, k_3 are the reaction rate constants, and the performance of the reactor is dependent on the relative values between these reaction rate constants.

When the concentration of product A and B is denoted by C_A and C_B, respectively, we have the following mass balance equation.

$$\begin{cases} \frac{dC_A}{dt} &= -k_1 C_A - k_3 C_A^2 + \frac{F}{V}(C_{Af} - C_A) \\ \frac{dC_B}{dt} &= k_1 C_A - k_2 C_B - \frac{F}{V} C_B \\ y &= C_B \end{cases} \tag{1}$$

where F is the inlet flow rate, and V is the volume of the $CSTR$. C_{Af} is the concentration of A in the inlet flow. y is the output of the process. We would like to know the dynamic characteristics from the inlet flow rate F to y, the concentration of product B.

Here, for simplicity, the process variables are normalized with respect to the operating point. That is, when we take the operating point as, $C_{A0} = 3.0mol/l$, $C_{B0} = 2.84mol/l$, $F_0/V = 55.7/h$, and kinetic parameters as $k_1 = 100/h$, $k_2 = 50/h$, $k_3 = 10l/mol/h$, $C_{Af} = 10mol/l$, $V = 1l$, we have

$$\begin{cases} \frac{dx_1}{dt} &= -100x_1 - 10x_1^2 + u(10 - x_1) \\ \frac{dx_2}{dt} &= 100x_1 - 50x_2 - u \cdot x_2 \\ y &= x_2 \end{cases} \tag{2}$$

where x_1 denotes the deviation variable for the concentration of A, and x_2 denotes that for B. u is the inlet flow rate around the operating point. The dynamic characteristics from u to y is to be obtained.

In order to know the nonlinear characteristics of this reactor, let us show the static characteristics between u and y. Fig.1

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shows the static output change with respect to the input u, which displays a nonlinear property that when the input u becomes greater than a certain value, the output begins to decrease. So the left of the peak and the right side have completely different behavior, showing high nonlinear characteristics.

For this Van de Vusse reactor, Doyle V[2] used the Carleman linearization method to obtain bilinear model, from which they obtained 2nd Volterra kernel.

Now we will show in the next section that 3rd Volterra kernel for this Van de Vusse reactor process can be obtained by use of M-sequence correlation method.

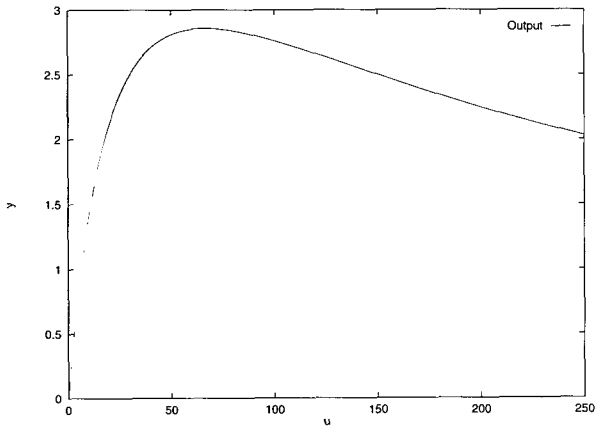

Fig. 1. Static input-output relationship.

III. The principle of identification of Volterra kernel by use of M-sequence[4]

Consider the identification of a nonlinear system which can be described as follows,

$$y(t) = \sum_{i=1}^{\infty} \int_0^{\infty} \int_0^{\infty} \cdots \int_0^{\infty} g_i(\tau_1, \tau_2, \cdots \tau_i) \times u(t-\tau_1)u(t-\tau_2)\cdots u(t-\tau_i) d\tau_1 d\tau_2 \cdots d\tau_i \quad (3)$$

where $u(t)$ is the input, and $y(t)$ is the output of the nonlinear system, and $g_i(\tau_1, \tau_2, ...\tau_i)$ is called Volterra kernel of i-th order. When $i = 1$, Eqn.(3) shows linear system.

In order to get the Volterra kernels $g_i(\tau_1, \tau_2, ...\tau_i)$, we use an M-sequance as an input to the nonlinear system. The crosscorrelation function $\phi_{uy}(\tau)$ between the input $u(t)$ and the output $y(t)$ can be written as,

$$\begin{aligned}\phi_{uy}(\tau) &= \overline{u(t-\tau)y(t)} \\ &= \sum_{i=1}^{\infty} \int_0^{\infty} \int_0^{\infty} \cdots \int_0^{\infty} g_i(\tau_1, \tau_2, \cdots \tau_i) \\ &\quad \times \overline{u(t-\tau)u(t-\tau_1)\cdots u(t-\tau_i)} d\tau_1 d\tau_2 \cdots d\tau_i \end{aligned} \quad (4)$$

where PPPP denotes time average. Usually the n-th moment of $u(t)$ is difficult to obtain. But when we use M-sequence, we can get n-th moment of $u(t)$ easily. Namely, the $(i+1)$th moment of the input M-sequence $u(t)$ can be written as

$$\overline{u(t-\tau)u(t-\tau_1)u(t-\tau_2)\cdots u(t-\tau_i)} = \begin{cases} 1 & \text{(for certain } \tau) \\ -1/N & \text{(otherwise)} \end{cases} \quad (5)$$

where N is the period of the M-sequence. When we use the M-sequence with the degree greater than 16, $1/N$ is in the order of 10^{-5}. So Eqn.(5) can be approximated as a set of impulses which appear at certain τ's.

Let us consider the case where we measure i-th Volterra kernel. Then for any integer $k_{i1}^{(j)}, k_{i2}^{(j)}, \cdots k_{i,i-1}^{(j)}$ (suppose $k_{i1}^{(j)} < k_{i2}^{(j)} < \cdots, k_{ii-1}^{(j)}$), there exists a unique $k_{ii}^{(j)}(mod\ N)$ such that

$$\begin{aligned} & u(t)u(t+k_{i1}^{(j)}\Delta t)u(t+k_{i2}^{(j)}\Delta t)\cdots u(t+k_{i,i-1}^{(j)}\Delta t) \\ = \ & u(t+k_{ii}^{(j)}\Delta t) \end{aligned} \quad (6)$$

where j is the number of a group $(k_{i1}, k_{i2}, \cdots, k_{i,i-1})$ for which Eqn.(6) holds and Δt is the time increment. This property is called "shift and add property" of the M-sequence (see Appendix). We assume that total number of those groups is m_i(that is, $j = 1, 2, \cdots, m_i$). Therefore Eqn.(5) becomes unity when

$$\tau_1 = \tau - k_{i1}^{(j)}\Delta t, \tau_2 = \tau - k_{i2}^{(j)}\Delta t, \cdots \tau_i = \tau - k_{ii}^{(j)}\Delta t \quad (7)$$

Therefore Eqn.(4) becomes

$$\phi_{uy}(\tau) \simeq \sum_{i=1}^{\infty} \sum_{j=1}^{m_i} g_i(\tau - k_{i1}^{(j)}\Delta t, \tau - k_{i2}^{(j)}\Delta t, \cdots \tau - k_{ii}^{(j)}\Delta t) \quad (8)$$

Since $g_i(\tau_1, \tau_2, \cdots \tau_i)$ is zero when any of τ_i is smaller than zero, each $g_i(\tau - k_{i1}^{(j)}\Delta t, \tau - k_{i2}^{(j)}\Delta t, \cdots \tau - k_{ii}^{(j)}\Delta t)$ in Eqn.(8) appear in the crosscorrelation function $\phi_{uy}(\tau)$ when $\tau > k_{ii}^{(j)}$.

In order to obtain the Volterra kernels from Eqn.(8), $k_{ii}^{(j)}$ in Eqn.(8) must be sufficiently apart from each other. For this to be realized, we have to select suitable M-sequences, which make the appearance of each cross-section of Volterra kernels sufficiently apart from each other. Some of the example of those usable M-sequences are the M-sequence having the generating characteristic polynomial $f(x) = 245165, 221321, 311171$ in octal notation with which we can obtain $g_2(\tau_1, \tau_2)$ for $\tau_2 - \tau_1$ from $1\Delta t$ to $20\Delta t$, $g_3(\tau_1, \tau_2, \tau_3)$ for $\tau_3 - \tau_1$ from $1\Delta t$ to $20\Delta t$ and for $\tau_3 - \tau_2$ from $1\Delta t$ to $19\Delta t$, from the observation of only one crosscorrelation function between the input and output.[4),5)]

When we measure Volterra kernels up to 3rd order, the crosscorrelation function $\phi_{uy}(\tau)$ becomes,

$$\begin{aligned} \phi_{uy}(\tau) &= \Delta t g_1(\tau) + F(\tau) \\ &+ 2(\Delta t)^2 \sum_{j=1}^{m_2} g_2(\tau - k_{21}^{(j)}\Delta t, \tau - k_{22}^{(j)}\Delta t) \\ &+ 6(\Delta t)^3 \sum_{j=1}^{m_3} g_3(\tau - k_{31}^{(j)}\Delta t, \tau - k_{32}^{(j)}\Delta t, \tau - k_{33}^{(j)}\Delta t) \end{aligned} \quad (9)$$

where

$$F(\tau) = (\Delta t)^3 g_3(\tau, \tau, \tau) + 3(\Delta t)^3 \sum_{q=1}^{m_1} g_3(\tau, q\Delta t, q\Delta t) \quad (10)$$

In general case, we have,

$$\begin{aligned}\phi_{uy}(\tau) &= \Delta t g_1(\tau) + F(\tau) \\ &+ \sum_{i=2}^{\infty} i!(\Delta t)^i \sum_{j=1}^{m_i} g_i(\tau - k_{i1}^{(j)}\Delta t, \tau - k_{i2}^{(j)}\Delta t, \\ &\qquad \cdots, \tau - k_{ii}^{(j)}\Delta t) \end{aligned} \tag{11}$$

Here the function $F(\tau)$ is the function of τ and sum of the odd order Volterra kernels when some of its arguments are equal. Since $F(\tau)$ appears together with $g_1(\tau)$ in a overlapped manner, $F(\tau)$ must be calculated from the odd order Volterra kernels and be subtracted from the measured $g_1(\tau)$ in order to obtain the accurate $g_1(\tau)$.

IV. Procedure for obtaining Volterra kernels

Eqn.(11) shows that the crosscorrelation function between the input M-sequence and the output contains all the crosssections of Volterra kernels, which are actually sliced crosssections of Volterra kernels along the diagonal direction.

Here the procedure for obtaining Volterra kernels from the crosscorrelation $\phi_{uy}(\tau)$ is briefly explained, as in the following steps.

1) Firstly we choose a suitable M-sequence for this purpose as is shown in section III, and carry out the experiment obtaining the crosscorrelation functin $\phi_{uy}(\tau)$.

2) Since $k_{ii}^{(j)}$'s in Eqn.(11) are obtained beforehand by computer search, we know a certain slice of Volterra kernel appear at a certain τ.

For example, $g_2(\tau - k_{12}^{(j)}\Delta t, \tau - k_{22}^{(j)}\Delta t)$ $(k_{12}^{(j)} < k_{22}^{(j)})$ appears in the range $k_{22}^{(j)}\Delta t < \tau < k_{22}^{(j)}\Delta t + 20\Delta t$, since Volterra kernels are zero when its arguments are negative. Note here that the suitable M-sequence is selected so as for other prominent kernel slices not to appear in this range. Now we obtain the second Volterra kernel slice as

$$\begin{aligned} g_2(\tau - k_{21}^{(j)}\Delta t, \tau - k_{22}^{(j)}\Delta t) &= \frac{N\phi_{uy}(\tau)}{2N(\Delta t)^2}, \\ (for\ \ k_{22}^{(j)}\Delta t < \tau < k_{22}^{(j)}\Delta t + 20\Delta t) & \end{aligned} \tag{12}$$

Therefore we can gather those kernel slices of $g_2(\tau_1, \tau_2)$ to construct $g_2(\tau_1, \tau_2)$, the second order Volterra kernel.

3) The third Volterra kernel is also obtained in the same way, by collecting kernel slices of $g_3(\tau_1, \tau_2, \tau_3)$ from the crosscorrelation function $\phi_{uy}(\tau)$.

$$\begin{aligned} g_3(\tau - k_{31}^{(j)}\Delta t, \tau - k_{32}^{(j)}\Delta t, \tau - k_{33}^{(j)}\Delta t) &= \frac{N\phi_{uy}(\tau)}{6N(\Delta t)^3}, \\ (for\ \ k_{33}^{(j)}\Delta t < \tau < k_{33}^{(j)}\Delta t + 19\Delta t) & \end{aligned} \tag{13}$$

4) The first order Volterra kernel is obtained from subtraction of the overlaping 3rd Volterra kernel as follows.

$$\begin{aligned} g_1(\tau) &= \frac{N\phi_{uy}(\tau)}{N\Delta t} \\ &-(\Delta t)^2(3\sum_{i=0}^{m} g_3(\tau, i\Delta t, i\Delta t) - 2g_3(\tau, \tau, \tau)) \end{aligned} \tag{14}$$

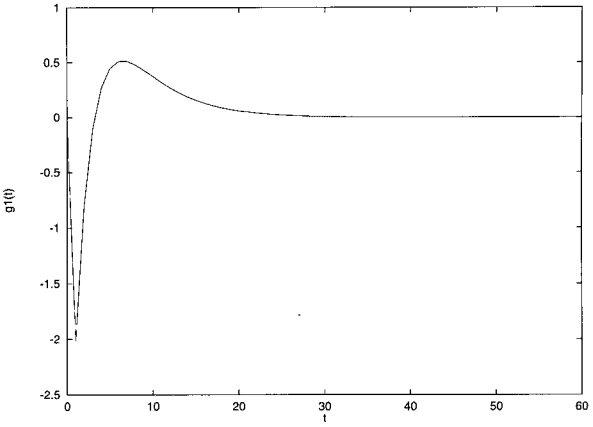

Fig. 2. Volterra kernel of first order $g_1(\tau)$

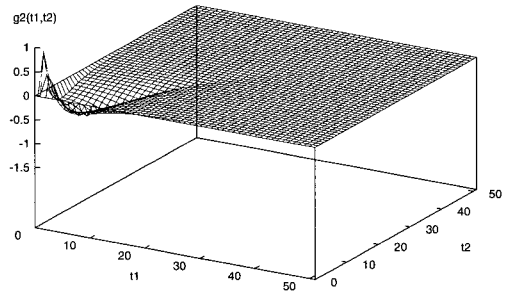

Fig. 3. Volterra kernel of second order $g_2(\tau_1, \tau_2)$

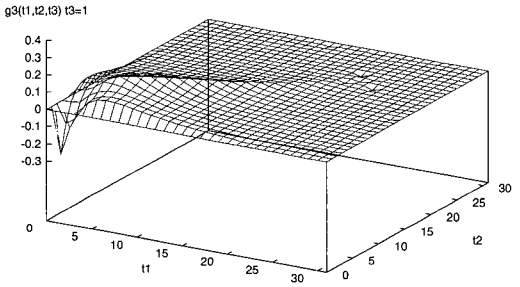

Fig. 4. Volterra kernel of third order $g_3(\tau_1, \tau_2, \tau_3)$ for $\tau_3 = 1\Delta t$

V. Identification of Van de Vusse reactor

The method of identification of Volterra kernels of nonlinear system by use of M-sequence correlation method is applied to nonlinear Van de Vusse reactor as shown in Eqn.(2).

16th degree M-sequence with the characteristic polynomial, $f(x) = 260577$, in octal notation, is used as the input $u(t)$. The first, second and third order Volterra kernels of the system are measured by calculating the crosscorrelation between the input and the output.

Fig.2 shows the first order Volterra kernel $g_1(\tau)$ thus mea-

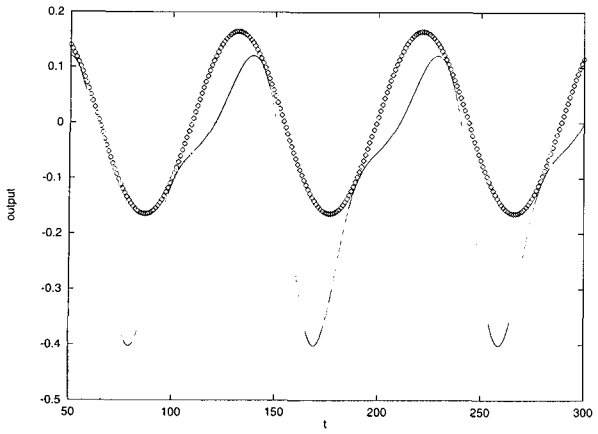

Fig. 5. Comparison of actual output with estimated one by use of only first order Volterra kernel.

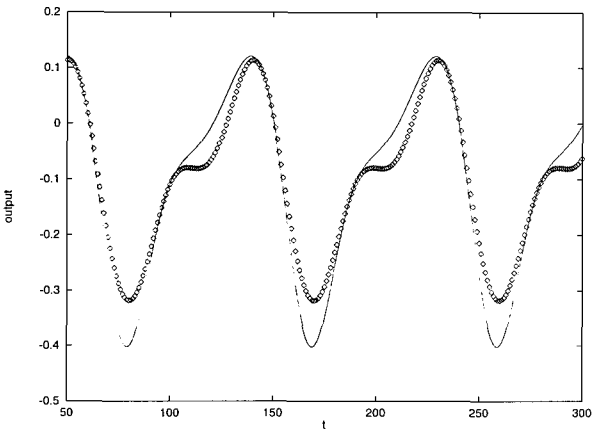

Fig. 6. Comparison of actual output with estimated one by use of up to second order Volterra kernels.

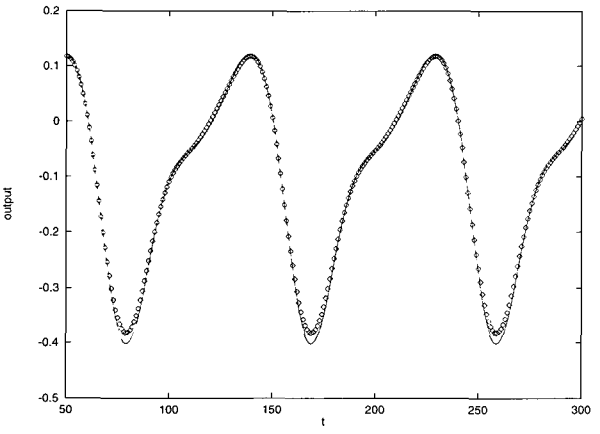

Fig. 7. Comparison of actual output with estimated one by use of up to third order Volterra kernels.

sured.

Fig.3 shows the second order Volterra kernel $g_2(\tau_1, \tau_2)$.

Fig.4 shows one of the crosssection of the third Volterra kernel $g_3(\tau_1, \tau_2, \tau_3)$, when $\tau_3 = 1\Delta t$.

By use of the measured Volterra kernels g_1, g_2, g_3, we calculate the output change for the input of $sin(0.07t)$, and compare with the actual output obtained from Eqn.(2).

Fig.5 shows the result of comparison of the actual output (solid line) with the output (diamond line) calculated by use of only first order Volterra kernel. We see there is a big difference between them.

Fig.6 shows the result of comparison of the actual output (solid line) with the output (diamond line) calculated by use of up to 2nd order Volterra kernels. We see the calculated output from up to second order Volterra kernels is closer to the actual output than in case of just first order Volterra kernel. But still we see some differences between them.

Fig.7 shows the result of comparison of the actual output (solid line) with the output (diamond line) calculated by use of up to 3rd order Volterra kernels, showing good agreement between them. From these results of simulation we can say that the use of up to 3rd order Volterra kernels for Van de Vusse reactor is very effective for describing the dynamic behavior of the reactor.

VI. Conclusions

The authors have presented here a method for obtaining up to 3rd order Volterra kernels of Van de Vusse reactor which is known as a highly nonlinear chemical process by use of M-sequence correlation method. From the result of simulation, we see that when the output is estimated by use of up to 3rd order measured Volterra kernels, the estimated output shows a good agreement with the actual output. It is expected that the use of up to 3rd order Volterra kernels for Van de Vusse reactor would be very effective as a benchmark problem for nonlinear chemical process for describing the dynamic characteristics of the reactor being used.

Appendix

M-sequence is one of the pseudorandom sequences, and is easily generated by a shift register with suitable feedback. M-sequence is widely used in control engineering as a simulation of actual noise, as a test signal for communication, as a signal for measuring a time delay and so on. Here we explain about two-level M-sequence.

M-sequence can be generated with an n-stage shift register circuit as shown in Fig.A.1. Each stage of the shift register contains 0 or 1, and each output is multiplied by a coefficient f_j (equal to 0 or 1) and added mod 2 and fed back. In the circuit, $\oplus$ denotes an exclusive OR circuit. The initial conditon of the shift register can be taken arbitrarily except for all zero. When the feedback coefficients f_j are suitably chosen, the generated sequence a_i has the maximum period $N = 2^n - 1$ and is called M-sequence. The sequence a_i is written as

$$a_{i+n} = \sum_{j=0}^{n-1} f_j a_{i+j} \qquad (mod\ 2) \tag{15}$$

Letting $f_n = 1$, we have

$$\sum_{j=0}^{n} f_j a_{i+j} = 0 \qquad (mod\ 2) \tag{16}$$

These expressions are called linear recurrence equations. When we introduce a delay operator x such as $a_{i+j} = x^j a_i$, Eqn.(16) becomes

$$\left(\sum_{j=0}^{n} f_j x^j\right) a_i = 0 \tag{17}$$

Here, the polynomial

$$f(x) = \sum_{j=0}^{n} f_j x^j \qquad (f_0 \neq 0, f_n = 1) \tag{18}$$

is called the characteristic polynomial. The coefficients f_j of the sequence a_i are 0 or 1, and the multiplication and addition between them obey mod 2 arithmetic. Therefore, the coefficients f_j of sequence a_i are considered to belong to Galoir Field $GF(2)$.

Usually we denote $f(x)$ by its coefficients in octal notation for simplicity. For example, when $f(x) = 1+x^4+x^5+x^6+x^8$, the coefficients becomes $\{f_j\} = 100011101$, which can be expressed as $f(x) = 435$ in octal notation.

The necessary and sufficient condition that the sequence a_i is an M-sequence is that the characteristic polynomial $f(x)$ is a primitive polynomial over $GF(2)$. A primitive polynomial is polynomial which divides $x^k - 1$ when $k = 2^n - 1$, but does not divide $x^k - 1$ when $0 < k < 2^n - 1$. Primitive polynomials over $GF(2)$ are found in Peterson[8] and Zierler and Brillhart[9].

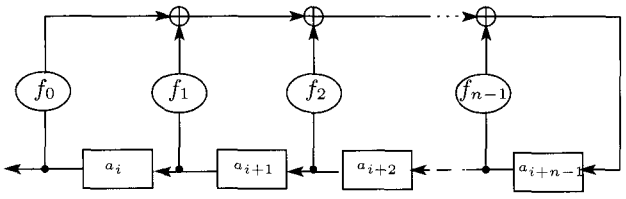

Fig.A.1FM-sequence generator

Among many properties of M-sequence, two properties related to this paper are stated as follows.

Property 1 : The modulo 2 sum of an M-sequence and a cyclic shift of itself is another M-sequence of the same order. In short, it represents some other cyclic shift of the original M-sequence. This property is called *shift and add property* of M-sequence. In general, there exists a unique υ such that

$$s_1 a_{i-1} + s_2 a_{i-2} + \cdots + s_n a_{i-n} = a_{i+\upsilon} \tag{19}$$

where $s_1, s_2, \cdots, s_n \in GF(2)$.

Property 2 : When $\{a_i\}$ ($a_i = 0$ or 1) is converted to $\{m_i\}$ ($m_i = 1$ or -1) by $m_i = 1 - 2a_i$, the auto-correlation function $\phi_{mm}(k)$ of an M-sequence is given by

$$\phi_{mm}(k) = \frac{1}{N} \sum_{i=0}^{N-1} a_{i-k} a_i = \begin{cases} 1 & (k = 0, N, 2N, \cdots) \\ -\dfrac{1}{N} & (\text{otherwise}) \end{cases} \tag{20}$$

If N is large, $\phi_{mm}(k)$ is approximately equal to a δ-function and the M-sequence becomes almost a white random signal.

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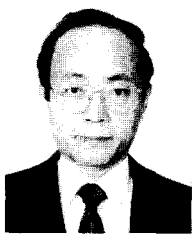

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