Estimation of the Transfer Function, Time Moments, and Model Parameters of a Flow Process

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Introduction

The usual approach to measuring the properties of a flow process is to impose an impulse on a concentration or any other measurable property of the flow considered, and to measure the resulting response of a sensor installed downstream, as shown in Figure 1 (Zwietering, 1959; Levenspiel and Bischoff, 1963; Pethö and Noble, 1982). A major problem in this approach is that a perfect impulse cannot be realized in practice. Further, the dynamics of the source that generates the impulse and of the sensor are included in the result, and the accuracy of the result is limited by disturbances such as sensor noise, especially in the tail end of the response (Skopp, 1984). To reduce the effects of disturbances, one would have to gather more data by repeating the experiment.

These problems are avoided in a random-input experiment where, at two locations along the direction of flow, the responses are measured to an upstream source of random variations; see Figure 2. In this experiment the two sensor responses are related precisely by the transfer function of the flow process considered, i.e., the flow process between the sensors (Levenspiel and Bischoff, 1963). The transfer function does not include the dynamics of the source and the sensors (Van Zee and Schurer, 1983). Further, the source may be artificial or natural and the source signal need not be known because it is not used. Finally, the duration of a random-input experiment can be increased arbitrarily to reduce the effects of disturbances. The use of a random input was earlier suggested by Lübbert (1982) and is common practice in cross-correlation techniques to measure velocities in pure plug flows (Beck, 1981; Bolon and Lacoume, 1983).

From the sensor responses the transfer function of the flow process can be derived by various methods, which we divide into parametric and nonparametric methods. The main result in this paper is the formulation of a parametric estimation method to obtain the transfer function, the time moments, and the parameters of the flow process, via an autoregressive, moving-average modeling technique. By simulations we compare the parametric method with some nonparametric methods described in the next section.

Nonparametric Methods

Let $h(k)$ be the impulse response (the time domain equivalent of the transfer function) of the flow process considered and let $u(k)$ and $y(k)$ be the first and the second sensor response or signal, respectively. The discrete-time argument k refers to the time $k \cdot \Delta$, with Δ the interval of the time discretization. If we assume that the source is installed upstream and that no production occurs in the flow process considered, then $h(k)$ is causal [$h(k) = 0$ for $k < 0$]. If we further assume that the flow process relates the sensor signals linearly, then we can use the convolution (Kailath, 1980),

$$y(k) = \sum_{\ell=0}^{\infty} h(\ell)u(k-\ell) \tag{1}$$

In principle, $h(k)$ can be obtained from $u(k)$ and $y(k)$, using Eq. 1. However, the deconvolution involved in solving Eq. 1 for $h(k)$ is numerically ill-conditioned. If one is only interested in the time moments of $h(k)$, then the method of moment differences (Aris, 1959; Bischoff, 1960) can be used. The time moments m_i of $h(k)$ are defined as (Paynter, 1957; Hwang and Shih, 1981):

$$m_i = \sum_{k=-\infty}^{\infty} h(k) \cdot (k \cdot \Delta)^i \tag{2}$$

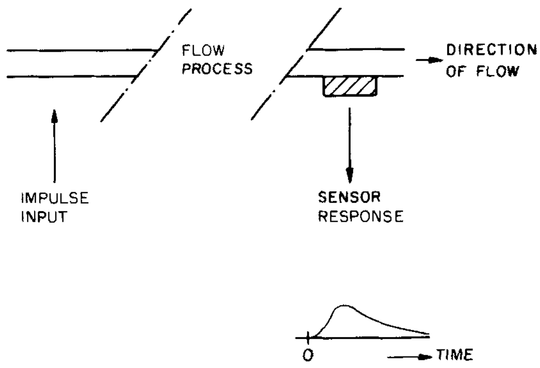

Figure 1. One-sensor experiment with impulse input.

Similarly, we can define the moments m_{iu} and m_{iy} of $u(k)$ and $y(k)$, respectively, by replacing $h(k)$ in Eq. 2 with $u(k)$ or $y(k)$. It can be shown (Aris, 1959) that

$$\frac{m_1}{m_0} = \frac{m_{1y}}{m_{0y}} - \frac{m_{1u}}{m_{0u}} \tag{3}$$

$$\left[\frac{m_2}{m_0} - \left(\frac{m_1}{m_0}\right)^2\right] = \left[\frac{m_{2y}}{m_{0y}} - \left(\frac{m_{1y}}{m_{0y}}\right)^2\right] - \left[\frac{m_{2u}}{m_{0u}} - \left(\frac{m_{1u}}{m_{0u}}\right)^2\right] \tag{4}$$

The normalized first moment and variance of $h(k)$, given by Eqs. 3 and 4, can be related to the parameters in various flow models, as will be discussed later. It should be noted that if numerical problems are to be avoided, m_{0u} and m_{0y} must be bounded and nonzero, so that for this method an impulse-type input experiment is more appropriate than a random-input experiment.

In the case of a random-input experiment one can use another nonparametric method based on the cross-covariance function $R_{yu}(k)$ of the sensor signals. Using the definition (Doob, 1953)

$$R_{yu}(k) = E\{y(\ell + k)u(\ell)\}, \tag{5}$$

where $E\{\cdot\}$ denotes the mathematical expectation, and Eq. 1, we obtain

$$R_{yu}(k) = \sum_{\ell=0}^{\infty} h(\ell) R_{uu}(k - \ell), \tag{6}$$

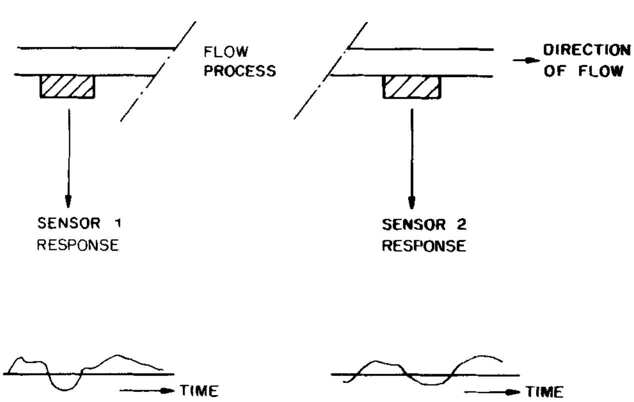

Figure 2. Two-sensor experiment with random input.

where $R_{uu}(k)$ is the autocovariance function of $u(k)$. Now we define the moments m_{iuu} and m_{iyu} of $R_{uu}(k)$ and $R_{yu}(k)$, respectively, by replacing $h(k)$ in Eq. 2 with $R_{uu}(k)$ or $R_{yu}(k)$. By the correspondence between Eqs. 1 and 6, the normalized first moment and variance of $h(k)$ can also be obtained using Eqs. 3 and 4 with m_{iu} and m_{iy} replaced by m_{iuu} and m_{iyu}, respectively. Note that $m_{1uu} = 0$, and that m_{0uu} and m_{0yu} are bounded and nonzero in the case of zero mean sensor signals.

A general disadvantage of nonparametric methods is that the errors in the estimates are larger than in the case of parametric estimation (Doob, 1953; Jenkins and Watts, 1968). The parametric method, described in the next section, is more accurate and yields not only the first- and second-order time moments of $h(k)$, but also $h(k)$ itself and thereby, in principle, any-order time moments of $h(k)$.

ARMA Parameter Estimation

A suitable parametrization of a discrete-time linear dynamic system is the autoregressive, moving-average (ARMA) form (Box and Jenkins, 1976; Eykhoff, 1979)

$$y(k) = \sum_{\ell=1}^{n} - a_\ell y(k - \ell) + \sum_{j=1}^{n} b_j u(k - j) \tag{7}$$

or, after z-transformation (Jury, 1964)

$$Y(z) = H(z) \cdot U(z) \tag{8}$$

with

$$H(z) = \frac{B(z)}{A(z)} \tag{9}$$

$$A(z) = 1 + \sum_{\ell=1}^{n} a_\ell z^{-\ell} \tag{10}$$

$$B(z) = \sum_{j=1}^{n} b_j z^{-j} \tag{11}$$

$H(z)$ is the transfer function of the flow process considered. The form of Eq. 7 is convenient to define the linear prediction error $e(k)$ of the model with given data $u(k), y(k)$ as

$$e(k) = y(k) + \sum_{\ell=1}^{n} a_\ell y(k - \ell) - \sum_{j=1}^{n} b_j u(k - j) \tag{12}$$

As $e(k)$ is a linear function of the parameters a_ℓ, b_j, parameter estimates can be obtained from the data by the standard linear least-squares solution, minimizing the criterion function (Box and Jenkins, 1976; Eykhoff, 1979; Swaanenburg et al., 1985):

$$J = \sum_{k=n}^{n+N-1} e^2(k) \tag{13}$$

The choice of the model order n is not critical, provided that it is sufficiently high to represent the dynamics of the system considered (Swaanenburg, 1985). High values of n are always safe, but require a large number of samples N, because the variance of the parameter estimates increases when n/N increases.

The advantages of the parametric approach described here are:

1. The solution of the linear least-squares problem is analytical and can be found from the data by means of existing, numerically robust algorithms (Swaanenburg et al., 1985).
2. The solution can be computed on-line by using a recursive form of the least-squares algorithm (Swaanenburg et al., 1985).
3. From the ARMA model parameters the related time moments and flow model parameters can be obtained.

From ARMA Parameters to Time Moments

To derive the time moments from the ARMA parameters one could first generate the impulse response with the aid of Eq. 7, yielding

$$\begin{aligned} h(k) &= 0 & k &< 1 \\ &= \sum_{\ell=1}^{k} - a_\ell h(k-\ell) + b_k & k &= 1, n \\ &= \sum_{\ell=1}^{n} - a_\ell h(k-\ell) & k &> n \end{aligned} \tag{14}$$

Then one could use Eq. 2 to obtain the time moments m_i of $h(k)$. The result of this approach is inherently approximate, due to the necessary truncation of the infinite sum Eq. 2 (Skopp, 1984) and the accumulation of round-off errors in using Eq. 14. A more elegant procedure to determine m_i from given ARMA parameters is to use an analytical relation, as derived below.

It was shown by Hwang and Shih (1981) that the time moments m_i can be derived from a given transfer function $H(z)$ by

$$m_i = (-\Delta)^i \left[\left(z \frac{d}{dz} \right)^i H(z) \right]_{z=1} \tag{15}$$

Applying Eq. 15 to the ARMA form of $H(z)$ as given in Eqs. 9, 10, and 11, we find

$$m_0 = H(1) \tag{16}$$

$$m_1 = -\Delta \cdot H'(1) \tag{17}$$

$$m_2 = \Delta^2 \cdot [H'(1) + H''(1)] \tag{18}$$

with

$$H(1) = \frac{B(1)}{A(1)} \tag{19}$$

$$H'(1) = \frac{B'(1)A(1) - B(1)A'(1)}{A^2(1)} \tag{20}$$

$$H''(1) = \frac{B''(1)A(1) + B'(1)A'(1) - B'(1)A'(1) - B(1)A''(1)}{A^2(1)} \tag{21}$$

$$- \frac{[B'(1)A(1) - B(1)A'(1)] \cdot 2A(1)A'(1)}{A^4(1)} \tag{22}$$

and with

$$A(1) = 1 + \sum_{\ell=1}^{n} a_\ell \quad B(1) = \sum_{j=1}^{n} b_j \tag{23}$$

$$A'(1) = \sum_{\ell=1}^{n} a_\ell \cdot (-\ell) \quad B'(1) = \sum_{j=1}^{n} b_j \cdot (-j) \tag{24}$$

$$A''(1) = \sum_{\ell=1}^{n} a_\ell \cdot (-\ell)(-\ell-1)$$

$$B''(1) = \sum_{j=1}^{n} b_j \cdot (-j)(-j-1) \tag{25}$$

The prime and double prime denote the first and second derivatives with respect to z. Thus we have derived an analytical relation between the ARMA parameters a_ℓ, b_j and the time moments m_i.

From Time Moments to Flow Model Parameters

When a mathematical-physical flow model is assumed to describe the flow process considered, one can obtain the flow model parameters, via the time moments, from the ARMA parameters. The main advantage of such an approach—as compared to direct estimation of the flow model parameters by a nonlinear estimation method—is that the ARMA model parameters are more easily obtained, namely, by linear least-squares estimation.

As an example of a flow model we consider the axial dispersive plug flow model described by the partial differential equation (Aris and Amundson, 1957; Levenspiel and Bischoff, 1963)

$$\frac{\partial c(x,t)}{\partial t} + v \frac{\partial c(x,t)}{\partial x} = D \frac{\partial^2 c(x,t)}{\partial x^2} \tag{26}$$

where $c(x, t)$ is the property measured by the sensors.

The transfer function relation between the Laplace-transformed responses $C(x, s)$ of the sensors at the axial locations x_1 and x_2 with distance L, can be obtained for various system boundary conditions (Aris and Amundson, 1957; Levenspiel and Bischoff, 1963; Gibilaro, 1978; Nauman, 1981, 1984). For example, in the case of open system boundaries we obtain

$$H_L(s) = \frac{C(x_2, s)}{C(x_1, s)} = \exp\left\{ \frac{v}{2D} \cdot L \cdot \left(1 - \sqrt{1 + \frac{4Ds}{v^2}} \right) \right\} \tag{27}$$

Back-transformation to the time domain yields the impulse response

$$h_L(t) = \frac{L}{2\sqrt{\pi D t^3}} \exp\left\{ -\frac{1}{4Dt}(L - vt)^2 \right\} \tag{28}$$

The time moments of Eq. 28 can be obtained from Eq. 27 (Himmelblau and Bischoff, 1968; Roffel and Rijnsdorp, 1982) by

$$m_i = (-1)^i \left[\frac{d^i H(s)}{ds^i} \right]_{s=0} \tag{29}$$

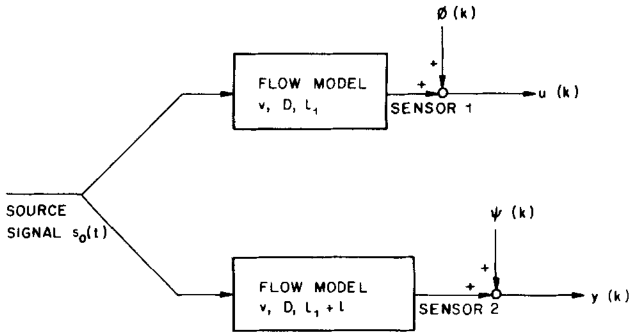

Figure 3. Simulated experiment.

Application of Eq. 29 to $H_L(s)$ yields

$$m_0 = 1 \tag{30}$$

$$\frac{m_1}{m_0} = \frac{L}{v} \tag{31}$$

$$\frac{m_2}{m_0} - \left(\frac{m_1}{m_0}\right)^2 = \frac{2LD}{v^3} \tag{32}$$

When Eqs. 31 and 32 are combined with Eqs. 16–25, the parameters v, D of the dispersive plug flow model, Eq. 26, can be derived from the estimated ARMA parameters a_ℓ, b_j.

Simulation Results

With the analytical solution $h_L(t)$ given in Eq. 28, an experiment has been simulated as shown in Figure 3. A signal $s_0(t)$ is used as a source signal for flow models describing sections of lengths L_1 and $L_1 + L$, the distances from the source to the first and the second sensor, respectively. The signals $u(k)$, $y(k)$ used for parameter estimation are the sensor signals corrupted with independent additive noise signals $\phi(k)$, $\psi(k)$. The sensor signals are obtained by convolution. For instance, $y(k)$ is obtained in the noise-free case as

$$y(k) = \int_0^{k \cdot \Delta} h_{L_1+L}(t) s_0(k \cdot \Delta - t)\, dt \tag{33}$$

with $s_0(t)$ piecewise constant, i.e., $s_0(t) = s_0(k \cdot \Delta)$ for $k \cdot \Delta \leq t < (k+1) \cdot \Delta$, and with $s_0(t) = 0$ for $t < 0$. The integration in Eq. 33 is performed numerically. The parameter values used are

$$L_1 = 1 \text{ m}$$
$$L = 1 \text{ m}$$
$$v = 0.08 \text{ m/s}$$
$$D = 0.01 \text{ m}^2\text{/s}$$
$$\Delta = 1 \text{ s}$$

Note that the average time delay is $L/v = 12.5$ s, i.e., not an integer number of sample intervals. The sensor noises $\phi(k)$ and $\psi(k)$ are defined as zero mean Gaussian white noises with standard deviation $\sigma = 0.02$, and the number of samples is $N = 256$. Figure 4 shows the simulated sensor signals in the case of an impulse-type input, which is defined as $s_0(t) = 1$ for $0 \leq t < 15$ and as $s_0(t) = 0$ elsewhere. In Table 1 the results of the method of moment differences applied to these sensor signals are given in the form of the velocity v and dispersion D obtained. In the noise-free case [$\phi(k) = 0$ and $\psi(k) = 0$ for all k] the results are very accurate, but when sensor noise is present the accuracy decreases, especially for D. Note that the accuracy cannot be improved by increasing M, the number of points used in the computation of m_{iu} and m_{iy}. Figure 5 shows the simulated sensor signals in the case of a random input, which is defined as a zero

Table 1. Estimation Results

Method	v, m/s	D, m²/s
True values	0.08	0.01
Moment differences:		
Noise-free	0.0800	0.00999
With noise, M = 60	0.0813	0.006
M = 80	0.0770	0.0124
M = 100	0.0732	0.0211
Covariance function moment differences:		
Noise-free, M = 50	0.0975	0.123
M = 100	0.0331	0.0374
M = 250	0.103	−0.108
Parametric:		
Noise-free, n = 8	0.0800	0.00997
n = 16	0.0800	0.00999
With noise, n = 8	0.0785	0.0102
n = 16	0.0791	0.0105

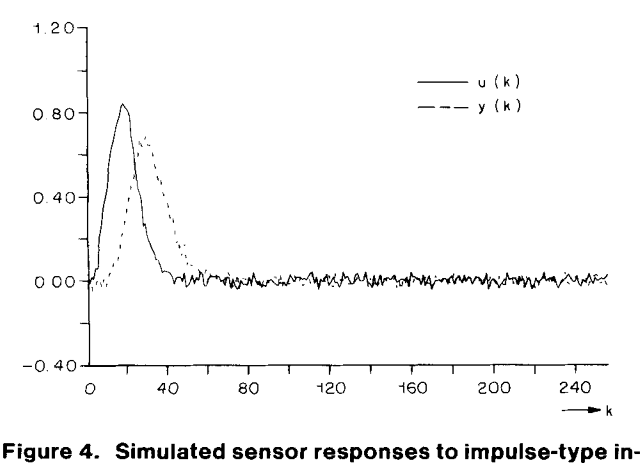

Figure 4. Simulated sensor responses to impulse-type input.

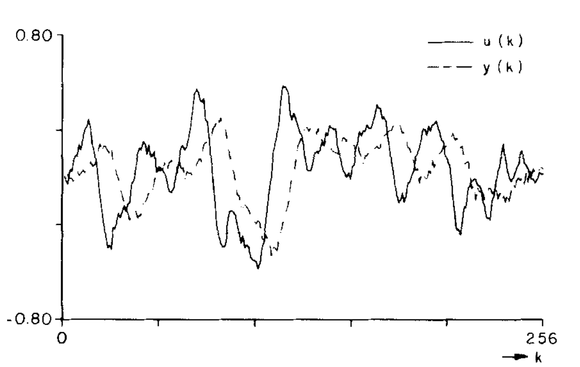

Figure 5. Simulated sensor responses to random input.

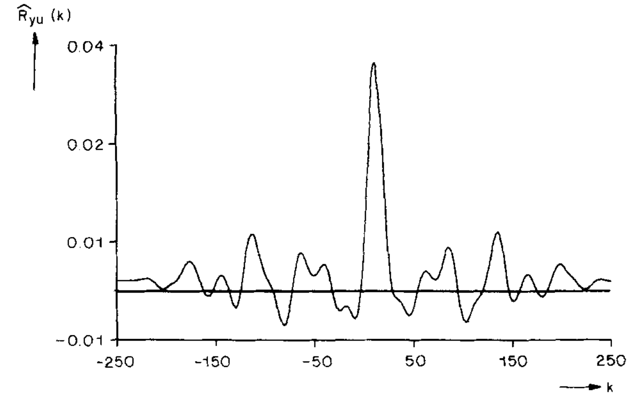

Figure 6. Cross-covariance function estimates.

mean Gaussian white noise with standard deviation $\sigma = 1$. For computing m_{iuu} and m_{iyu}, covariance function estimates should be available over an interval $k = [-M, M]$ with M sufficiently large to permit $\hat{R}_{uu}(M)$ and $\hat{R}_{yu}(M)$ to be converged to zero. However, even in the noise-free case, Figure 6, such a convergence does not occur, due to the estimation errors. When this lack of convergence is disregarded and the moments are computed for different values of M, the results in Table 1 are obtained. Since the estimation errors are already unacceptable in the noise-free case, the case with noise is not considered for this method.

When the same signals $u(k)$ and $y(k)$ are used in the parametric method with $n = 8$, 16, the results are very accurate in the noise-free case, as can be seen from Table 1 and Figure 7. When sensor noise is present, the results of the parametric method appear to be more accurate than the nonparametric results, as can be seen from Table 1. Moreover, in the case of parametric estimation the accuracy can be improved by increasing the number of samples N.

Notation

a_ℓ = autoregressive parameter in ARMA model
$A(z)$ = autoregressive polynomial in ARMA model
b_j = moving-average parameter in ARMA model
$B(z)$ = moving-average polynomial in ARMA model
$c(x, t)$ = concentration in dispersive plug flow model
$C(x, s)$ = Laplace transformation of $c(x, t)$
D = dispersion parameter of dispersive plug flow model
$e(k)$ = linear prediction error of ARMA model
$h(k)$ = discrete-time impulse response of the flow process

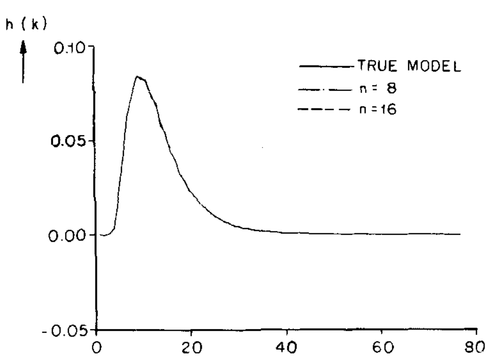

Figure 7. Parametric estimation results.

$h(t)$ = continuous-time impulse response of the flow process
$H(s)$ = continuous-time transfer function of the flow process
$H(z)$ = discrete-time transfer function of the flow process
J = least-squares criterion function
k, ℓ = discrete time
L = distance between sensors
L_1 = distance from source to sensor 1
m_i = time moments
M = interval parameter in moment calculation
n = order of ARMA model
N = number of samples in signals $u(k)$, $y(k)$
$R_{uu}(k)$ = autocovariance function of signal $u(k)$
$R_{yu}(k)$ = cross-covariance function of signals $y(k)$, $u(k)$
s = parameter of Laplace transformation
$s_0(t)$ = source signal in simulations
t = continuous time
$u(k)$ = signal from sensor 1
$U(z)$ = z-transformation of $u(k)$
v = velocity parameter of dispersive plug flow model
x = axial location in dispersive plug flow model
$y(k)$ = signal from sensor 2
$Y(z)$ = z-transformation of $y(k)$
z = parameter of z-transformation

Greek letters

Δ = interval of time discretization
σ = standard deviation
$\phi(k)$ = noise of sensor 1
$\psi(k)$ = noise of sensor 2

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