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Dynamic Predictive Modeling Under Measured and Unmeasured Continuous-Time Stochastic Input Behavior

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ABSTRACT: Many input variables of chemical processes have a continuous-time stochastic (CTS) behavior. The nature of these variables is a persistent, time-correlated variation that manifests as process variation as the variables deviate in time from their nominal levels. This work introduces methodologies in process identification for improving the modeling of process outputs by exploiting CTS input modeling under cases where the input is measured and unmeasured. In the measured input case, the output variable is measured offline, infrequently, and at a varying sampling rate. A method is proposed for estimating CTS parameters from the measured input by exploiting statistical properties of its CTS model. The proposed approach is evaluated based on both output accuracy and predictive ability several steps ahead of the current input measurement. Two parameter estimation techniques are proposed when the input is unmeasured. The first is a derivative-free approach that uses sample moments and analytical expressions for population moments to estimate the CTS model parameters. The second exploits the CTS input model and uses the analytical solution of the dynamic model to estimate these parameters. The predictive ability of the latter approach is evaluated in the same way as the measured input case. All of the data in this work were artificially generated under the probabilistic CTS model.

1. INTRODUCTION

The modeling of process variability is an important aspect of process identification.[1−5] Process variables often exhibit a nature that can be classified as continuous-time stochastic (CTS) behavior. Such behavior can be described as time-dependent correlated variation that can persist either above or below its nominal level, mean value, or set point for a period of time, although it has a stochastic or probabilistic nature. An example of this variation could be the flow rate from a control valve with a fixed opening. Although the opening is fixed, the flow rate changes because of CTS pressure changes upstream of the valve. A graphical illustration of CTS variation is shown in Figure 1 for the first-order dynamic response to a deterministic step change of a CTS input variable. If this input had only a deterministic nature, it would remain fixed after this step change, and the output would follow the deterministic response shown in Figure 1. The response of this system is shown for a CTS input for two values of variance ("sigma" in the plot). As shown, the greater the variance of the stochastic input, the greater the average deviation from the deterministic response. The CTS behavior for these two responses is evident in the random, but time-correlated, variation.

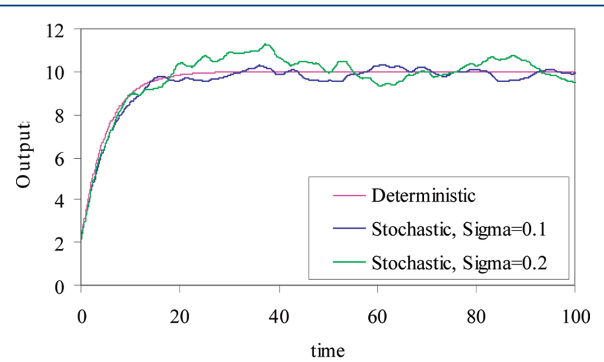

Figure 1. Dynamic response of a first-order system to a deterministic input change and CTS input changes at two different sigma values (0.1 and 0.2) or variance levels.

To further put this input behavior into a chemical process context, two examples are given: one with a measured input variable and one with an unmeasured input variable. A real data example of a measured process variable with CTS variability is shown in Figure 2. These data come from a pilot-scale distillation column for the separation of methanol and water. The variable is the accumulator level, and its set point and measured values over time are plotted in Figure 2. The variable level is time-continuous, and the CTS nature of this variable is evident in the continuous time-correlated pattern around the set point. This behavior is observed in values that are sequentially above the mean and below the mean (i.e., serially or time-correlated).

Our unmeasured process input example is an industrial starch dryer, for which the objective is to remove moisture from corn starch to a particular level. The starch is freely placed on the belt feeding the dryer. Variations in the inlet moisture content to the dryer depend on the belt speed; the amount of grain; the inlet moisture level of the grain; and the humidity of the room air, which is not controlled. The inlet moisture rate is

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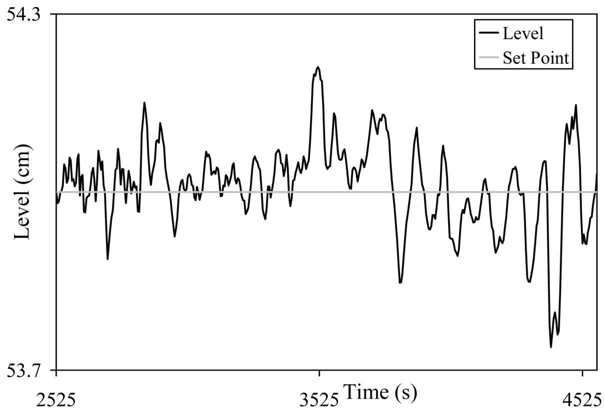

Figure 2. Accumulator level from a real distillation process showing CTS behavior.

not measured, and the variation of these variables causes variations in the inlet moisture rate that can be described as *process noise* or *variability*. This particular process was an actual industrial process that one of us (D.K.R.) experienced while working in industry. These variables changed gradually in a time-correlated manner that induced the unmeasured inlet moisture rate with CTS behavior. This was evident from CTS behavior of the outlet moisture content, which was inferred from the exhaust temperature of the dryer air. Therefore, the purpose of this article is to present a CTS modeling approach that can significantly improve output modeling by exploiting the modeling of CTS input behavior.

The scope of this article is single-input−single−output (SISO) processes and includes both measured and unmeasured CTS input cases. Recent work in treating stochastic behavior in chemical processes includes the significant contribution of Lima and Rawlings.[6] However, their scope and context were quite different from the scope and context of this work. Basically, their context was along the lines of filtering, and this treatment involves parameter estimation or system identification. Hence, in their context, the model structure and its parameters were known. The stochastic nature that they addressed was in the state variables. This work focuses on CTS time-varying input behavior under a certain probabilistic model. In their work, the input was deterministic. They considered multiple state variables, whereas this initial treatment considers single-input−single-output processes. Additionally, we treat the case of unmeasured input, which is not within their scope. Finally, from the estimated model of input behavior, we use predicted input values from the fitted model to predict output responses. Other recent related works include those of Giri and Bai,[7] Garnier and Wang,[8] and Vanbeylen.[9] However, none of those treatments address our scope, that is, continuous-time stochastic input variation.

In the measured input case, the output is taken to be measured offline, infrequently (a 1% rate of the input was used), and at a varying rate (a uniform distribution was used). After implementing the proposed method and estimating the model parameters on training data, testing results are presented for the model as a virtual (i.e., soft) sensor and in *k*-steps-ahead prediction (*k*SAP) with $k = 1$, 10, 20, and 50. These results are compared to the deterministic input results where the CTS behavior is not considered, the common practice. In the unmeasured input case, the dynamic process is required to be invertible, and the output is taken to be measured online and at a high frequency and constant rate. Although this is not a restrictive condition because the modeling context is continuous, it is made for convenience to illustrate the proposed method more easily. As in the other case, testing results are presented for *k*SAP with $k = 1$, 10, 20, and 50 and compared to deterministic input modeling results.

All of the data in this article were artificially generated based on the stochastic, dynamic, and static models given. The next section presents the process network used in this study, which is a SISO Wiener system. Section 3 presents the CTS model for the input and shows how it translates into CTS output behavior. Section 4 follows with details of the model identification methods. In section 5, we evaluate the proposed modeling approaches. The final section presents concluding remarks and discusses applications and future work.

2. PROCESS NETWORK

Continuous-time stochastic (CTS) modeling in this context addresses the development of CTS input models to obtain better predictive models for CTS output variables that depend on CTS inputs. From our review of the process identification literature, it appears that little to no work has been done on the CTS modeling of process inputs (i.e., CTS process identification). In model predictive control, the predictive model is used to determine future settings for the manipulated variable, which is an input, but the predictions are based on deterministic considerations.[10] In the virtual[11] (i.e., inferential or soft) sensor context when the inputs are not measured directly, the common practice is to use process settings for input variables (such as set points) or some other deterministic inference for input values over time. However, these approximations can significantly limit the accuracy of output predictions.

This work applies CTS input modeling under the Wiener block-oriented network. Although the Wiener system is quite simple, its ability to treat nonlinear static behavior and nonlinear dynamic behavior has allowed it to approximate real processes well, including pH neutralization, distillation, and reactions in continuous-stirred tank reactors (CSTRs).[12−17] Most applications of Wiener modeling in the literature have been discrete-time (DT) models,[18,19] but exceptions include the works of Greblicki[15,16] and Bhandari and Rollins.[14] Greblicki[15,16] introduced a nonparametric continuous-time (CT) approach with the dynamic block identified by impulse response methods. Bhandari and Rollins[14] proposed the continuous-time Wiener modeling method called the Wiener block-oriented exact solution technique (W-BEST). The method proposed in this article extends W-BEST to the treatment of an unmeasured input with CT stochastic input noise.

As illustrated herein, this application of the Wiener network provides very powerful and unique advantages in nonlinear dynamic modeling that offers an excellent basis to estimate CTS model parameters. The Wiener network is shown in Figure 3 for a single-input−single-output (SISO) process. In

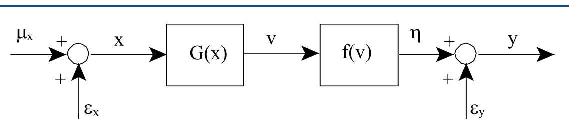

Figure 3. SISO description of a continuous-time stochastic process for x in a Wiener block-oriented network.

this figure, $x(t)$ is the CTS true input variable, $\mu_x(t)$ is the known and deterministic mean of $x(t)$, $\varepsilon_x(t)$ is the CTS process noise or deviation of $x(t)$ from $\mu_x(t)$, $v(t)$ is the unobservable output from the linear dynamic block $G(x)$, $\eta(t)$ is the unobservable CTS output from the nonlinear static block $f(v)$, $\varepsilon_y(t)$ is the stochastic output measurement error, and $y(t)$ is the measured CTS output.

As shown in the figure, when x is not measured, ε_x is needed to obtain x. With an invertible static block $f(v)$, this network can provide values for v by passing y through the inverse of this block, that is, from $v = f^{-1}(y)$. With the CTS model of ε_x, $\mu_x(t)$, and $G(x)$, one can obtain estimates for v and use these estimates, along with the values of v from $f^{-1}(y)$, under an estimation criterion such as least-squares to estimate the model parameters.

In the case where x is measured, ε_x values can be obtained directly from $\varepsilon_x = x - \mu_x$. Using the moment equations for ε_x, we derive an expression for an estimator of ε_x that depends on the CTS model parameters of ε_x, which we define as the vector $\boldsymbol{\theta}_{\text{sto}}$. The least-squares criterion is applied to the residuals to estimate $\boldsymbol{\theta}_{\text{sto}}$. This approach is called the CTS input method (CTSIM) because the inputs are used to obtain the values of ε_x and, thus, the estimation of $\boldsymbol{\theta}_{\text{sto}}$.

This work proposes two methods for CTS modeling of ε_x when x is not measured. Both methods need values for v and, thus, require $f(v)$ to be invertible. One is a derivative-free approach that relates the sample moments of v, using values obtained from $v = f^{-1}(y)$, to analytically derived expressions for v that depend on the CTS parameters of ε_x. This approach is called the CTS moment method (CTSMM). The least-squares criterion is applied to v moment residuals to estimate $\boldsymbol{\theta}_{\text{sto}}$. The other is a derivative-based approach and obtains estimates of ε_x using a finite-difference approximation scheme for the derivatives in $G(x)$. These estimates are used to estimate v, which leads to estimates of y using $f(v)$. The least-squares criterion is applied to the output (i.e., y) residuals to estimate $\boldsymbol{\theta}_{\text{sto}}$. This approach is called the CTS output method (CTSOM). These methods are presented in detail and evaluated in section 4, after the CTS models are presented in the next section. Using the fitted model, we also propose section 4 a scheme to predict the values of x and y continuously over the prediction horizon described as the time from the most recent measurement (input or output) to k sampling times in the future.

3. MODELS

The mathematical model for the scope of this work can be subdivided into the models for x, ε_x, v, and y. The purpose of this section is to describe the mathematical and probabilistic behavior and the assumptions for these variables. Because of their detailed CTS descriptions, subsections are dedicated to the models of ε_x and v.

3.1. Input and Output Measurement Models. With $\mu_x(t)$ as a deterministic function of time, eq 1 shows, mathematically, how the CTS nature of $x(t)$ comes from the CTS nature of $\varepsilon_x(t)$

$$x(t) = \mu_x(t) + \varepsilon_x(t) \tag{1}$$

For convenience, the measurement error in $x(t)$ [and, thus, also $\varepsilon_x(t)$] is assumed to be zero. Similarly, the measurement model for the output is given as

$$y(t) = \eta(t) + \varepsilon_y(t) \tag{2}$$

where $\varepsilon_y(t)$ is assumed to be independently distributed over time with a mean of zero and a variance of σ_y^2. The mean of $x(t)$, $\mu_x(t)$, is taken to be known. In practice, it could be the set point for some process variable in a control loop or the setting for some process equipment (e.g., the belt speed of a dryer or the amount a valve is open). Therefore, from measurements of $x(t)$, values for $\varepsilon_x(t)$ can be determined from

$$\varepsilon_x(t) = x(t) - \mu_x(t) \tag{3}$$

For the CTSIM, eq 3 is used to generate the values for $\varepsilon_x(t)$. Its CTS model is now given in detail.

3.2. CTS Model for $\varepsilon_x(t)$. A CTS process in this context is a time-continuous random function of a process variable. Thus, $\varepsilon_x(t)$ is a continuous random function of time.[20] The mean value function of $\varepsilon_x(t)$, $E[\varepsilon_x(t)]$, is the expected value of $\varepsilon_x(t)$ at time t. The covariance function of $\varepsilon_x(t)$ is defined as

$$\text{Cov}[\varepsilon_x(t_i), \varepsilon_x(t_j)] = E[\varepsilon_x(t_i), \varepsilon_x(t_j)] - E[\varepsilon_x(t_i)]E[\varepsilon_x(t_j)] \tag{4}$$

Note that both the expectation and covariance of the stochastic process are also continuous functions of time. At different time points, the mean value can be quite different and so can the covariance function. If the mean value function, $E[\varepsilon_x(t)]$, is constant and independent of t and its covariance function, $\text{Cov}[\varepsilon_x(t),\varepsilon_x(t + \delta)]$, depends only on δ, the distance between the two time points, the stochastic process is said to be weakly stationary. A stochastic process $\varepsilon_x(t)$ is said to be a Gaussian process if, for any given $k \geq 1$ and $t_1, ..., t_k$, the random vector $[\varepsilon_x(t_1), ..., \varepsilon_x(t_k)]$ is jointly normally distributed, a common and reasonable assumption for many stochastic chemical processes. The CTS model for $\varepsilon_x(t)$ in this work is a weakly stationary Gaussian process such that

$$E[\varepsilon_x(t)] = 0, \quad \forall\ t \tag{5}$$

$$\text{Cov}[\varepsilon_x(t_i), \varepsilon_x(t_k)] = \sigma^2 e^{-\alpha|t_k - t_i|} \tag{6}$$

for all i, k, where $t_k > t_i$, $\alpha > 0$, and σ^2 is the variance of $\varepsilon_x(t)$. This kind of covariance structure is common for chemical process variables, where the covariance between the two time points decreases as the interval increases. Therefore, $\varepsilon_x(t)$ has the property that it is nearly uncorrelated at different time points t_i and t_k that have a large δ and more correlated for a smaller δ. The speed of the correlation change depends on the parameter α. When α is large, the covariance decreases rapidly as the time interval increases. Note that

$$\text{Cov}[\varepsilon_x(t_i), \varepsilon_x(t_i)] = \sigma^2, \quad \forall\ i \tag{7}$$

and

$$\begin{aligned}\text{Cov}[\varepsilon_x(t_1), \varepsilon_x(t_2)] &= E[\varepsilon_x(t_1)\varepsilon_x(t_2)] - E[\varepsilon_x(t_1)]E[\varepsilon_x(t_2)] \\ &= E[\varepsilon_x(t_1)\varepsilon_x(t_2)] = \gamma_{t_1 t_2}\end{aligned} \tag{8}$$

through the use of eq 5. Later, we use eq 8 to propose an estimator for $\varepsilon_x(t)$.

3.3. CTS Model for $v(t)$. For simplicity, we present this work under a simple first-order linear dynamic system as given by eq 9 with reference to Figure 1

$$\tau \frac{dv(t)}{dt} + v(t) = x(t) = \mu_x(t) + \varepsilon_x(t) \tag{9}$$

Equation 9 is a stochastic differential equation (SDE). Under the assumption of steady state at $t = 0$; the use of deviation variables from the initial state; and with one input step change, namely

$$\mu_x(t) = \begin{cases} 0, & t \le 0 \\ \mu_x, & t > 0 \end{cases} \tag{10}$$

for simplicity, its analytical solution can be written as[21]

$$v(t) = \tau^{-1}e^{-t/\tau}\int_0^t e^{s/\tau}\varepsilon_x(s)ds + \mu_x(1 - e^{-t/\tau}) \tag{11}$$

The first two moments of the stochastic process $v(t)$ are

$$E[v(t)] = \mu_x(1 - e^{-t/\tau}) \tag{12}$$

$$\begin{aligned}\gamma_{v,t_1t_2} &= \mathrm{Cov}[v(t_1), v(t_2)] \\ &= \frac{\tau^{-2}\sigma^2}{\tau^{-2} - \alpha^2}[e^{-\alpha|\delta|} - \alpha\tau e^{-\alpha|\delta|} + (1 + \alpha\tau)e^{-(t_1+t_2)/\tau} \\ &\quad - e^{-(t_1/\tau)-\alpha t_2} - e^{-\alpha t_1-(t_2/\tau)}]\end{aligned} \tag{13}$$

such that

$$\begin{aligned}\mathrm{Cov}[v(t), v(t)] &= \mathrm{Var}[v(t)] = \sigma_{v,t}{}^2 \\ &= \frac{\tau^{-2}\sigma^2}{\tau^{-2} - \alpha^2}[1 - \alpha\tau + (1 + \alpha\tau)e^{-2t/\tau} \\ &\quad - 2e^{-[(1/\tau)+\alpha]t}]\end{aligned} \tag{14}$$

where $\delta = t_2 - t_1$. Note that all of these moments depend on time t (or t_1 and t_2) and that the output $v(t)$ is not weakly stationary. Thus, the correlation of the outputs at two different time points can be large even when the time difference is large for a certain set of parameters. From these analytical expressions for the moments of $v(t)$, we develop the CTSMM as mentioned above.

4. PARAMETER ESTIMATION AND PREDICTIVE MODELING METHODS

In this context of dynamic modeling, there are three sets of parameters: stochastic ($\boldsymbol{\theta}_{sto}$), including α, for example; dynamic ($\boldsymbol{\theta}_{dyn}$), including τ, for example; and static ($\boldsymbol{\theta}_{sta}$), including the parameters in $f(v)$. For a given modeling structure, the modeling objective is to obtain estimates of these three sets that provide the best fit to the response, namely, the smallest standard error in the predicted output. This section first presents the CTSIM, then the CTSOM, and finally the CTSMM.

4.1. CTSIM. The physically continuous input is taken to be measured discretely under a constant sampling rate. The development of this approach is based on this type of sampling for the input. More specifically, the proposed continuous-time stochastic input method (CTSIM) approximates the measured continuous input $x(t)$ as a piecewise input sequence as follows

$$x(t) \approx x_s(t) = \begin{cases} x_0, & t < 0 \\ x_1, & 0 \le t < \Delta t \\ x_2, & \Delta t \le t < 2\Delta t \\ \vdots & \\ x_m, & (m-1)\Delta t \le t < m\Delta t \end{cases} \tag{15}$$

where m is an integer representing the last sampling point in the measurement sequence. This sequence is the input to the Wiener network to produce a continuous-time solution for $y(t)$. For example, for the first-order dynamic system given by eq 9, the following solution is obtained

$$\begin{aligned}\tau\frac{dv_S(t)}{dt} + v_S(t) = x_S(t) &= x_1S(t) + (x_2-x_1)S(t - \Delta t) \\ &\quad + (x_3-x_2)S(t - 2\Delta t) + ... \\ &\quad + (x_m-x_{m-1})S[t - (m-1)\Delta t]\end{aligned} \tag{16}$$

where, with n as a positive integer, one can write

$$S(t - n\Delta t) = \begin{cases} 0, & t < n\Delta t \\ 1, & t \ge n\Delta t \end{cases} \tag{17}$$

and $v_S(0) = f^{-1}[y(0)]$. The solution to eq 16 is

$$\begin{aligned}v_S(t) &= v_S(0)e^{-t/\tau}S(t) + x_1(1 - e^{-t/\tau})S(t) \\ &\quad + (x_2-x_1)(1 - e^{-(t-\Delta t)/\tau})S(t - \Delta t) \\ &\quad + (x_3-x_2)(1 - e^{-(t-2\Delta t)/\tau})S(t - 2\Delta t) + ... \\ &\quad + (x_m-x_{m-1})(1 - e^{-[t-(m-1)\Delta t]/\tau})S \\ &\quad [t - (m-1)\Delta t]\end{aligned} \tag{18}$$

This equation gives an estimator of $y(t)$ as

$$\hat{y}(t) = f[v_S(t)] \tag{19}$$

Thus, to estimate θ_{dyn} and θ_{sta}, we propose

$$\mathrm{SSE}(\hat{\theta}_{dyn}, \hat{\theta}_{sta}): \quad \min_{\hat{\tau}>0} \sum_{i=1}^{n_{tr}} [y(i\Delta t) - \hat{y}(i\Delta t)]^2 \tag{20}$$

where n_{tr} is the number of sample points in the training data set.

To estimate θ_{sto}, an estimator must be formulated that depends on α. The first step is to obtain values for $\varepsilon_x(t)$ using eq 3. Assuming $t_2 > t_1$ and equating eq 6 to eq 8, we obtain

$$\gamma_{t_1t_2} = E[\varepsilon_x(t_1)\varepsilon_x(t_2)] = \sigma^2e^{-\alpha(t_2-t_1)} \tag{21}$$

With $\varepsilon_x(t_1)$ known

$$E[\varepsilon_x(t_1)\varepsilon_x(t_1)] = \sigma^2 \tag{22}$$

Now let

$$\hat{\gamma}_{t_1t_2} = \varepsilon_x(t_1)\hat{\varepsilon}_x(t_2) = \hat{\sigma}^2e^{-\hat{\alpha}(t_2-t_1)} \tag{23}$$

Solving eq 23 for $\hat{\varepsilon}_x(t_2)$ gives

$$\hat{\varepsilon}_x(t_2) = \frac{\hat{\sigma}^2e^{-\hat{\alpha}(t_2-t_1)}}{\varepsilon_x(t_1)} = \frac{[\varepsilon_x(t_1)]^2e^{-\hat{\alpha}(t_2-t_1)}}{\varepsilon_x(t_1)} = \varepsilon_x(t_1)e^{-\hat{\alpha}(t_2-t_1)} \tag{24}$$

with $\hat{\sigma}^2 = [\varepsilon_x(t_1)]^2$ by application of eq 22. Using eq 24, the objective function for estimating α is given as

$$\begin{aligned}&\mathrm{SSE}(\hat{\boldsymbol{\theta}}_{sto}): \\ &\min_{\hat{\alpha}>0}\sum_{i=1}^{n_{tr}}[\varepsilon_x(i\Delta t) - \hat{\varepsilon}_x(i\Delta t)]^2 = \min_{\hat{\alpha}>0} \\ &\sum_{i=1}^{n_{tr}}\{\varepsilon_x(i\Delta t) - \varepsilon_x[(i-1)\Delta t]e^{-\hat{\alpha}\Delta t}\}^2\end{aligned} \tag{25}$$

when measurement error is negligible. However, with significant measurement error, one can obtain multiple estimates at the same t and use

$$\mathrm{SSE}(\hat{\boldsymbol{\theta}}_{\mathrm{sto}}): \min_{\hat{\boldsymbol{\alpha}}>0} \sum_{j=1}^{n_{\mathrm{tr}}} \sum_{i=1}^{\min(n_p,j)} \{\boldsymbol{\varepsilon}(j\Delta t) - \boldsymbol{\varepsilon}[(j-i)\Delta t]\mathrm{e}^{-\hat{\boldsymbol{\alpha}} i\Delta t}\}^2 \tag{26}$$

where $n_p\Delta t$ is the farthest distance between two values of ε_x for any term in eq 26. Together with eq 20, these equations provide the parameter estimates for the vector $\boldsymbol{\theta} = (\boldsymbol{\theta}_{\mathrm{sto}}, \boldsymbol{\theta}_{\mathrm{dyn}}$, and $\boldsymbol{\theta}_{\mathrm{sta}})$ under the CTSIM.

4.2. CTSOM. The proposed continuous-time stochastic output method (CTSOM) estimates $\boldsymbol{\theta}_{\mathrm{dyn}}$ and $\boldsymbol{\theta}_{\mathrm{sta}}$ using the deterministic component of the input, namely, $\mu_x(t)$, given by the equation

$$\mu_x(t) = \begin{cases} \mu_0, & t < t_1 = 0 \\ \mu_1, & t_1 \le t < t_2 \\ \mu_2, & t_2 \le t < t_3 \\ \vdots \\ \mu_m, & t_m \le t \end{cases} \tag{27}$$

where t_i is the time of the ith input change and m is the total number of input changes. Using only the deterministic part of eq 9 with this input sequence gives

$$\tau\frac{\mathrm{d}v'_{\mathrm{D}}(t)}{\mathrm{d}t} + v'_{\mathrm{D}}(t) = (\mu_1-\mu_0)\mathbf{S}(t-t_1) + (\mu_2-\mu_1)\mathbf{S}(t-t_2) + (\mu_3-\mu_2)\mathbf{S}(t-t_3) + ... + (\mu_m-\mu_{m-1})\mathbf{S}(t-t_m) \tag{28}$$

where $v'_{\mathrm{D}}(t) = v_{\mathrm{D}}(t) - v_{\mathrm{D}}(0) = v_{\mathrm{D}}(t) - f^{-1}[y(0)]$. Note that, with the process in a pseudosteady state due to the CTS nature of the input, averages of several measurements can be used to approximate initial values.

The solution to eq 28 is

$$v_{\mathrm{D}}(t) = v_{\mathrm{D}}(0) + (\mu_1-\mu_0)(1-\mathrm{e}^{-(t-t_1)/\tau})\mathbf{S}(t-t_1) + (\mu_2-\mu_1)(1-\mathrm{e}^{-(t-t_2)/\tau})\mathbf{S}(t-t_2) + (\mu_3-\mu_2)(1-\mathrm{e}^{-(t-t_3)/\tau})\mathbf{S}(t-t_3) + ... + (\mu_m-\mu_{m-1})(1-\mathrm{e}^{-(t-t_m)/\tau})\mathbf{S}(t-t_m) \tag{29}$$

This equation gives a deterministic estimator, $y_{\mathrm{D}}(\mathrm{t})$, as

$$\hat{y}_{\mathrm{D}}(t) = f[v_{\mathrm{D}}(t)] \tag{30}$$

Thus, to estimate $\boldsymbol{\theta}_{\mathrm{dyn}}$ and $\boldsymbol{\theta}_{\mathrm{sta}}$, we propose

$$\mathrm{SSE}(\hat{\boldsymbol{\theta}}_{\mathrm{dyn}}, \hat{\boldsymbol{\theta}}_{\mathrm{sta}}): \min_{\hat{\boldsymbol{\tau}}>0} \sum_{i=1}^{n_{\mathrm{tr}}} [y(i\Delta t) - \hat{y}_{\mathrm{D}}(i\Delta t)]^2 \tag{31}$$

The first step in obtaining an estimate for α, is to obtain values for $\varepsilon_x(t)$ based on measurements that are denoted as $\tilde{\varepsilon}_x(t)$ These values are obtained by solving eq 9 for $\varepsilon_x(t)$ to give

$$\tilde{\varepsilon}_x(t) = \tau\frac{\mathrm{d}v(t)}{\mathrm{d}t} + v(t) - \mu_x(t) \tag{32}$$

where $v(t)$ is obtained from $f^{-1}[y(t)]$. Using a backward difference approximation for the derivative, eq 32 becomes

$$\tilde{\varepsilon}_x(t) = \tau\frac{v(t) - v(t-\Delta t)}{\Delta t} + v(t) - \mu_x(t) \tag{33}$$

With significant measurement error, one should use an effective averaging or smoothing method to obtain $\overline{v}(t)$ and replace $v(t)$ with $\overline{v}(t)$ in eq 33. By substitution of eq 33 into eq 24, the following estimator is proposed

$$\hat{\boldsymbol{\varepsilon}}_x(t) = \tilde{\boldsymbol{\varepsilon}}_x(t_1)\mathrm{e}^{-\hat{\boldsymbol{\alpha}}(t-t_1)} = \hat{\boldsymbol{\varepsilon}}_x(t) = \tilde{\boldsymbol{\varepsilon}}_{t_1}\mathrm{e}^{-\hat{\boldsymbol{\alpha}}(t-t_1)} \tag{34}$$

for $t > t_1$. Substituting eq 34 into eq 9 gives

$$\hat{\boldsymbol{\tau}}\frac{\mathrm{d}\hat{v}(t)}{\mathrm{d}t} + \hat{v}(t) = \boldsymbol{\mu}_x(t) + \tilde{\boldsymbol{\varepsilon}}_{t_1}\mathrm{e}^{-\hat{\boldsymbol{\alpha}}(t-t_1)} \tag{35}$$

Solving eq 35 gives a continuous-time estimator for $v(t)$ with $t > t_1$ as

$$\hat{v}(t) = v_{\mathrm{DD}}(t) + \frac{\tilde{\varepsilon}_{t_1}}{\hat{\tau}\hat{\alpha} - 1}[\mathrm{e}^{-(t-t_1)/\hat{\tau}} - \mathrm{e}^{-\hat{\alpha}(t-t_1)}]S(t-t_1) + v_{t_1}\mathrm{e}^{-(t-t_1)/\hat{\tau}}S(t-t_1) \tag{36}$$

where $v(t_1) = v_{t_1}$ and

$$v_{\mathrm{DD}}(t) = \mu(t_1)(1-\mathrm{e}^{-(t-t_1)/\tau})S(t-t_1) + [\mu(t_2) - \mu(t_1)](1-\mathrm{e}^{-(t-t_2)/\tau})S(t-t_2) + ... \tag{37}$$

Using eq 36, the objective function for estimating α is given as

$$\mathrm{SSE}(\hat{\boldsymbol{\theta}}_{\mathrm{sto}}): \min_{\hat{\boldsymbol{\alpha}}>0} \sum_{i=1}^{n_{\mathrm{tr}}} [\overline{v}(i\Delta t) - \hat{v}(i\Delta t)]^2 \tag{38}$$

Therefore, eqs 31 and 38 provide the parameter estimates for the full vector $\boldsymbol{\theta}$ under the CTSOM.

4.3. CTSMM. The final method to be proposed is the continuous-time stochastic moment method (CTSMM). The steps for estimating $\boldsymbol{\theta}$ under this method are as follows:

(1) Obtain estimates of $\boldsymbol{\theta}_{\mathrm{dyn}}$ and $\boldsymbol{\theta}_{\mathrm{sta}}$ under the procedure for the CTSOM. Recall that the CTSMM also requires $f(y)$ to be invertible.
(2) Derive the theoretical moment equations for $v(\mathrm{t})$.
(3) Derive the equations for the sample moments.
(4) Equate the sample moments to the theoretical moment equations in least-squares optimization to estimate $\boldsymbol{\theta}_{\mathrm{sto}}$.

Step 1 is given in section 4.2, and for the first-order process given by eq 9, step 2 is given in section 3.3. Thus, this section provides the details for steps 3 and 4 for applying the CTSMM in both Monte Carlo simulation (MCS) studies and process identification (PI) studies.

The general equation for the sample covariance of two sampled variables z_1 and z_2, with ordered measurements $z_{11}, z_{12}, ..., z_{1n}$, and $z_{21}, z_{22}, ..., z_{2n}$, respectively, is[21]

$$s_{z_1 z_2} = \sum_{i=1}^{n} (z_{1i} - \overline{z}_1)(z_{2i} - \overline{z}_2) \tag{39}$$

where

$$\overline{z}_j = n^{-1}\sum_{i=1}^{n} z_{ji}, \quad j = 1, 2 \tag{40}$$

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Note that $s_{z_i z_i} = s_{z_i}^2$, the sample variance calculated from the measurement of variable z_i.

Even after obtaining the "sampled" values for $v(t)$, calculating the sample variances is not as straightforward for a CTS process as revealed in the complexity of the true covariance expression given by eq 13, which shows the dependence on both times of the two variables. Thus, to obtain a sample covariance, multiple measurements for a variable must be obtained at a fixed time t at several time points. In actuality, this is impossible because only one measurement can be taken at a fixed time. We address this requirement by running multiple step tests of the same type, that is, same initial steady-state conditions and same input change, and assume that time points at the same distance from the steady state are equivalent. In an MCS study, one can actually go back to the same conditions and repeat the test as many times as desired. However, in a PI study, this is not possible because input changes follow sequentially in time. In a PI study, for every input change that is made, it takes at least one more change to return the process to the original steady state. Thus, PI studies have to have at least two different types of changes to obtain the replicated data needed to calculate a sample covariance at a fixed time from the initial steady state relative to another fixed time.

Before presenting the equations for the covariances in this context, several terms need to be defined. A *run* is defined as the time from an input change to the next one. Runs have the same *run type* if they have the same initial steady-state conditions and experience the same input change. Runs with the same run type are grouped together to gather the replicated data needed to calculate the sample moments. In addition, let n be the number of samples per run; m_k be the number of changes for run type k, $k = 1, ..., n_k$; n_k be the number of run types; t_i be the time of the ith sample after the first change, $i = 1, ..., nS_{mk}$, where

$$S_{mk} = \sum_{k=1}^{n_k} m_k \tag{41}$$

$v(t_i)$ be the value of $v(t)$ at t_i from inverting $y(t_i)$; t_i^* be the time of the ith sample from the most recent input change; and the true covariance for $v(t_1^*)$ and $v(t_2^*)$ for the kth run type be given as

$$\gamma_{k,t_1^* t_2^*} = \mathrm{Cov}[v_k(t_1^*), v_k(t_2^*)] \tag{42}$$

With these definitions, the sample covariance representing eq 23 is determined as

$$s_{k,t_1^* t_2^*} = \sum_{j=1}^{m_k} [v(t_{1jk}) - \bar{v}(t_{1jk})][v(t_{2jk}) - \bar{v}(t_{2jk})] \tag{43}$$

where $v(t_{ijk})$ is the value of $v(t)$ at time t_{ijk} from inverting $y(t_{ijk})$, t_{ijk} is the time of the ith sample on the jth run for the kth run type, and

$$\bar{v}(t_{ijk}) = m_k^{-1} \sum_{j=1}^{m_k} v(t_{ijk}) \tag{44}$$

For a distance $d > 0$, estimators for the two true moments for the kth run type are

$$\hat{\gamma}_{k,t_{i+d}^* t_i^*} = \frac{\hat{\tau}^{-2}\hat{\sigma}^2}{\hat{\tau}^{-2} - \hat{\alpha}^2}[\mathrm{e}^{-\hat{\alpha}(t_{i+d}^* - t_i^*)} - \hat{\alpha}\hat{\tau}\mathrm{e}^{-(t_{i+d}^* - t_i^*)/\hat{\tau}} + (1 + \hat{\alpha}\hat{\tau})\mathrm{e}^{-(t_{i+d}^* + t_i^*)/\hat{\tau}} - \mathrm{e}^{-(t_{i+d}^*/\hat{\tau}) - \hat{\alpha}t_i^*} - \mathrm{e}^{-\hat{\alpha}t_{i+d}^* - (t_i^*/\hat{\tau})}] \tag{45}$$

$$\hat{\sigma}_{k,t^*}{}^2 = \frac{\hat{\tau}^{-2}\hat{\sigma}^2}{\hat{\tau}^{-2} - \hat{\alpha}^2}[1 - \hat{\alpha}\hat{\tau} + (1 + \hat{\alpha}\hat{\tau})\mathrm{e}^{-2t_i^*/\hat{\tau}} - 2\mathrm{e}^{-[(1/\hat{\tau}) + \hat{\alpha}]t_i}] \tag{46}$$

Note that the ratio of $\hat{\gamma}_{k,t_{i+d}t_i}$ to $\hat{\sigma}_{k,t_i^*}{}^2$ is independent of $\hat{\sigma}^2$. We use this result to obtain $\hat{\alpha}$ by

$$\mathrm{SSE}(\hat{\alpha}): \quad \min_{\hat{\alpha}>0} \sum_{d=1}^{p} \sum_{i=1}^{n-d} \left(\frac{s_{1,t_{i+d}t_i}}{s_{1,t_i}{}^2} - \frac{\hat{\gamma}_{1,t_{i+d}t_i}}{\hat{\sigma}_{1,t_i^*}{}^2} \right)^2 \tag{47}$$

when $n_k = 1$, where p is the maximum number of lags considered. After obtaining $\hat{\alpha}$, we obtain $\hat{\sigma}^2$ by

$$\mathrm{SSE}(\hat{\sigma}^2): \quad \min_{\hat{\sigma}>0} \sum_{i=1}^{n} \left(\sigma_{1,t_i}{}^2 - \hat{\sigma}_{1,t_i^*}{}^2 \right)^2 \tag{48}$$

When $n_k > 1$, to obtain these estimates, the CTSMM uses

$$\mathrm{SSE}(\hat{\alpha}): \quad \min_{\hat{\alpha}>0} \sum_{k=1}^{n_k} \sum_{d=1}^{p} \sum_{i=1}^{n-d} \left(\frac{s_{k,t_{i+d}^* t_i^*}}{s_{k,t_i^*}{}^2} - \frac{\hat{\gamma}_{k,t_{i+d}^* t_i^*}}{\hat{\sigma}_{k,t_i^*}{}^2} \right)^2 \tag{49}$$

to obtain $\hat{\alpha}$ and

$$\mathrm{SSE}(\hat{\sigma}^2): \min_{\hat{\sigma}>0} \sum_{k}^{n_k} \sum_{i=1}^{n} \left(\sigma_{k,t_i^*}{}^2 - \hat{\sigma}_{k,t_i^*}{}^2 \right)^2 \tag{50}$$

to obtain $\hat{\sigma}^2$. Hence, eq 31 and the set of eqs 47−50 provide the parameter estimates for the full vector $\boldsymbol{\theta}$ under the CTSMM.

4.4. Evaluation. When the input is measured and the output is not measured online or is measured infrequently, the CTSIM can be used to develop a virtual (i.e., "soft") sensor by implementation of eq 19 after obtaining $\hat{\boldsymbol{\theta}}$. For predicting k-steps-ahead (kSA) of the most recent input measurement for CTSIM or kSA of the most recent output measurement for CTSOM and CTSMM after obtaining $\hat{\boldsymbol{\theta}}$, all three methods use the same prediction equation. This equation is a modified version of eq 36. More specifically, For $t = t_1 + k\Delta t$, eq 36 becomes

$$\hat{v}(t) = v_{\mathrm{DD}}(t_1 + k\Delta t) + \frac{\varepsilon_x(t_1)}{\hat{\tau}\hat{\alpha} - 1}(\mathrm{e}^{-k\Delta t/\hat{\tau}} - \mathrm{e}^{-\hat{\alpha}k\Delta t}) + v_{t_1}\mathrm{e}^{-k\Delta t/\hat{\tau}} \tag{51}$$

where t_1 is the current time; $v_{\mathrm{DD}}(t)$ is given by eq 37; and in the cases of CTSOM and CTSMM, $\varepsilon_x(t_1) = \tilde{\varepsilon}_{t_1}$.

One measure that we use to evaluate testing performance is the sum of squared prediction errors (SSPE), defined as

$$\mathrm{SSPE} = \sum_{i=1}^{M_{\mathrm{ts}}} (y_i - \hat{y}_i)^2 \tag{52}$$

where M_{ts} is the total number of time points in the test data set, y is the measured output, and $\hat{y}$ is the estimated or predicted output. SSPE results are obtained using the deterministic input $[\mu_x(t)]$ for comparative purposes. The proposed methods are compared on the basis of the deterministic input performance.

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Table 1. Base Case for the CTSMM in the Simulation Study[a]

	dynamic parameter τ	covariance parameter α	variance parameter σ
true value	5.00	0.600	0.500
mean of the estimates	5.35	0.635	0.495
standard error of the estimates	1.54	0.141	0.0293

[a] $n = 1000$, $m_1 = 10$, $p = 35$, and $\Delta t = 0.1$.

Table 2. Estimation Results for the Stochastic Model Parameters for the CTSMM for Different Values of m_k, the Number of Runs[a]

	m_1		
	10	15	20
mean of $\hat{\alpha}$	0.635	0.610	0.617
standard error of $\hat{\alpha}$	0.141	0.102	0.091
mean of $\hat{\sigma}$	0.495	0.491	0.493
standard error of $\hat{\sigma}$	0.029	0.022	0.019

[a] $\alpha = 0.6$ and $\sigma = 0.5$.

Thus, a relative SSPE (RSSPE) based on the following equation will also be used as a performance measure

$$\text{RSSPE} = \frac{\text{SSPE}(D)}{\text{SSPE}(k)} \tag{53}$$

where SSPE(D) is the SSPE result for the deterministic input sequence and SSPE(k) is the kSAP result for a proposed method. An RSSPE result significantly greater than 1 supports the usefulness of the proposed method over using just the deterministic input alone.

5. STUDIES

This section evaluates the three methods described in the previous section in four studies. In all studies, the data were artificially generated using a stationary Gaussian process generation algorithm described by Ripley[22] from parameters with values $\tau = 5$, $\alpha = 0.6$, and $\sigma = 0.5$, under the SISO first-order dynamic process given above. The first one (study 1) is a Monte Carlo Simulation (MCS) study in which a large number of data sets are generated under the same conditions to obtain accurate estimation measures of performance and the standard estimation error. The CTSMM was selected for this study

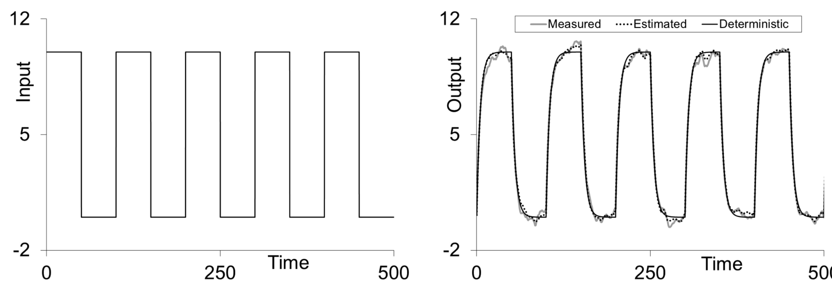

Figure 4. (Left) Sequence of set-point changes in the input for training and (right) output response for the training sequence for study 2.

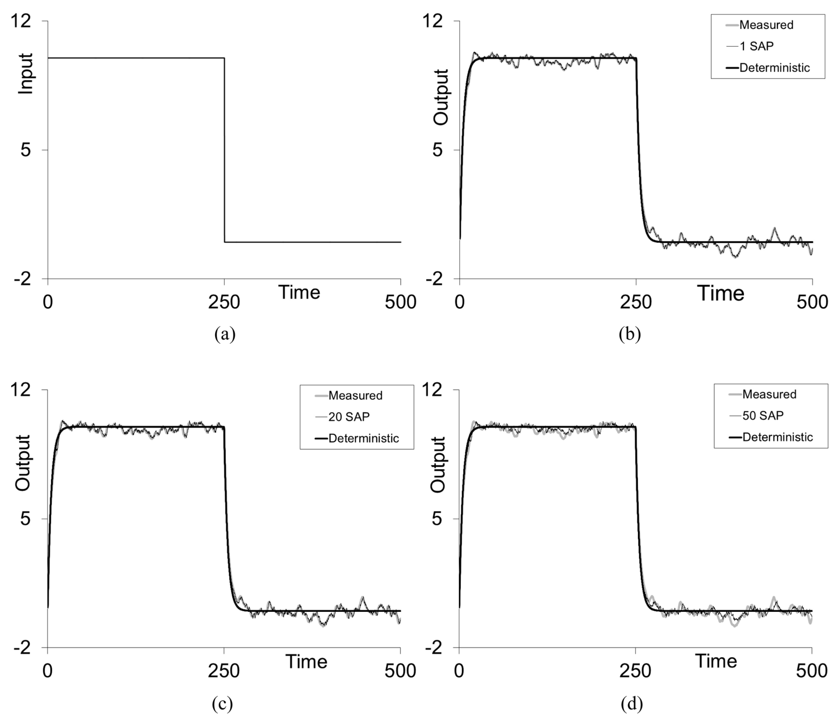

Figure 5. Study 2 test sequence results for (a) deterministic input, (b) 1SAP, (c) 20SAP, and (d) 50SAP.

because it is the only one that does not use a piecewise approximation to the input changes and has an exact theoretical solution. More specifically, the objective of this study was to obtain biases and standard errors for $\hat{\tau}$, $\hat{\alpha}$, and $\hat{\sigma}$ under the CSTMM. Output measurement error was not included in this study, as it would have had the effect of increasing the standard errors in proportion to the size of the standard error of the measured outputs and, thus, making it more difficult to isolate and evaluate the contribution due to the proposed estimation technique. Studies 2−4 are process identification (PI) studies that evaluate the proposed methods under sequential step tests. Study 2 is an evaluation of CTSMM without output measurement error [i.e., $\varepsilon_y(t) = 0$] and with $\nu(t) = y(t)$, for all t. Because the CTSMM is being evaluated, output measurement error is excluded for the same reason that it was excluded from study 1. Studies 3 and 4 apply the CTSIM and CTSOM, respectively, under more strenuous conditions in that the static model is nonlinear in the variables, the measurement noise is added, and the model parameters are estimated from about half the number of input changes as used in study 2.

5.1. Study 1. In study 1, we generated mathematically simulated values for $\varepsilon_x(t)$ and then integrated eq 9 numerically using the first-order implicit Euler method. The goal was to obtain an accurate solution to the true process. Using a sufficiently small step size, we were able to obtain an accurate solution using the Euler method. Hence, it was not necessary to use a continuous solution to obtain high accuracy. In this study, there was one run type (n_k = 1and k = 1) with a sampling time, Δt, equal to 0.1 time unit. One run consisted of n = 1000 samples for a total run time of 100 time units. In addition, the number of runs, m_k, was 10, with all input changes occurring at t = 0 and p = 35 (see eq 27). We repeated this simulation study 500 times so as to obtain highly accurate estimates of the average and standard errors of the estimated parameters, namely, $\hat{\tau}$, $\hat{\alpha}$, and $\hat{\sigma}$. Table 1 contains the results of this study. As shown, for this set of conditions, the means of the estimators were close to the true values with the standard errors as shown.

Table 2 illustrates the effect of m_k on the accuracies of $\hat{\alpha}$ and $\hat{\sigma}$. As expected, as m_k increased, the accuracies increased, as indicated by the reduction in the standard errors of the estimates. The results in Tables 1 and 2 support the CTSMM as a statistically sound approach in terms of estimator bias, standard error, and statistical consistency. More specifically, they show that these properties behave in a statistically sound manner for changes in sample size. However, the sample size should be chosen with care because data-collection costs increase as m_k increases.

Table 3. Test Sequence Performance Results for the CTSMM in Study 2

type	D	k = 10	k = 20	k = 50
SSPE	400.1	12.5	56.7	229.7
RSSPE	1.0	32.0	7.1	1.7

Study 1 demonstrated that the use of sample moments to estimate the model parameters can be accurate and have sound statistical properties. Other parameter estimation methods were applied in this study, and the details can be found in Zhai.[23] These include the methods of Bellach[24] and Chen and Kozin[25] for estimating τ and the method of Sorensen,[26] Pedersen's[27] maximum likelihood estimation (MLE), and Pedersen's[27] quasi-MLE for estimating α.

The objective of the next study was to demonstrate the application of the CTSMM in process identification where data collection is sequential over time. This study also evaluated the ability of CTSMM to obtain accurate estimates under a more limited amount of data in the form of sequential step tests and provided results for comparison with the other methods.

5.2. Study 2. Study 2 provides an illustration and evaluation of the CTSMM in model building (i.e., process identification) and testing in kSAP. This study used a series of 10 sequential step tests to obtain parameter estimates with n_k = 2, m_1 = m_2 = 5, n = 50, and Δt = 0.1 time unit. This deterministic training input sequence, in the form of set-point changes [i.e., $\mu_x(t) = x_{SP}(t)$], is shown in Figure 4. Application of eq 31 to estimate θ_{dyn} gave $\hat{\tau}$ = 0.4945, and with p = 15, application of eqs 48 and 49 produced $\hat{\alpha}$ = 0.514 and $\hat{\sigma}$ = 0.436, respectively. The values are well within one standard error of the true values for τ and α as determined in Table 1. The CTS output response, with $y(t) = \nu(t)$, is also shown in Figure 4, along with the fitted response.

For study 2, graphical results for k = 1, 20, and 50 in kSAP (i.e., application of eq 51) and for the deterministic case (ν_{DD} in eq 51) are shown in Figure 5 for the testing data. As shown, the kSAP responses follow the measured response much better than the deterministic response. This figure also shows how the CTSMM accuracy drops off as k increases. Quantitative results for SSPE and RSSPE are provided in Table 3. As shown in this table, the RSSPE results range from 32 for k = 10 to 1.7 for k = 50 and, thus, strongly support the usefulness of the CTSMM to provide a significant improvement in results over the deterministic results.

5.3. Study 3. The purpose of study 3 was to illustrate and evaluate the application of CTSOM in a process identification study. This study was more complex than study 2 in at least three ways. First, the static gain linear regression function was quadratic. Second, measurement noise (i.e., σ_y = 0.375) was

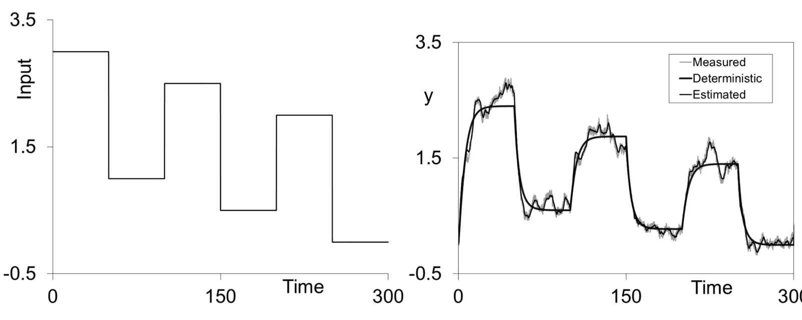

Figure 6. (Left) Deterministic training input sequence and (right) output responses for study 3.

added because it can have an additional adverse effect on accuracy because of the use of finite-difference approximations for derivatives (see eq 33). Third, the training sequence in this study used fewer input changes as well as a lower magnitude of changes to evaluate it against the CTSMM with much less information.

The training deterministic input sequence had six sequential step tests as shown in Figure 6. As shown, there were three run types ($n_k = 3$). The first run type was a step change of +3 units, the second run type was a step change of −2 units, and the third run type was a step change of +1.5 units. The first run type occurred once ($m_1 = 1$) at time $t = 0$, whereas the second run type occurred three times ($m_2 = 3$) at times $t = 50$, 150, and 250 units. The third run type occurred twice ($m_3 = 2$) at times $t = 100$ and 200 units. An input sequence of this type was chosen so as to have steady-state output (y) behavior at different input (x) levels, as needed to model nonlinear response behavior as shown in Figure 6 for the training data. The true static function is

$$y(t) = a_1 v(t) + a_2[v(t)]^2 \quad (54)$$

with $a_1 = 0.5$ and $a_2 = 0.1$.

The output responses to the training input sequence are also presented in Figure 6. The fitted model was obtained by following the procedure for the CTSOM given in section 4.2. Because there is output measurement error in this case, after $v(t)$ had been obtained by inverting $y(t)$, $\bar{v}(t)$ was calculated by averaging the 10 most recent values and used in eq 31 to estimate $\varepsilon(t)$. The $\boldsymbol{\theta}$ and $\hat{\boldsymbol{\theta}}$ values are reported in Table 4. As shown, these estimates are all close to their true values. Note that τ and α are well within one standard error of their true values for the standard errors given in Table 1. In Figure 6, the fitted response follows the CTS behavior of the measured output response quite well, as supported by an r_{fit} value (correlation of the measured and fitted output values) of 0.999.

Graphical results for the test sequence for study 3 are presented in Figure 7, and the SSPE and RSSPE results are listed in Table 5 for the deterministic case and for kSAP for $k = 1$, 10, 20, and 50. As shown, the kSAP responses follow the measured response quite well as compared to the deterministic response, which does not follow the CTS behavior. This figure also illustrates how the accuracy decreases as k increases. As shown in Table 5, the RSSPE ranged from 20.8 for $k = 1$ to 1.2 for $k = 50$

Table 4. Estimated and True Model Parameters for Study 3

	Steady-State Parameters		
a_1	0.5	$\hat{a}_1$	0.50
a_2	0.1	$\hat{a}_2$	0.10
	Dynamic Parameter		
τ	5	$\hat{\tau}$	4.85
	Stochastic Parameter		
α	0.6	$\hat{\alpha}$	0.70

Table 5. Test Sequence Performance Results for CTSOM in Study 3

type	D	$k = 1$	$k = 10$	$k = 20$	$k = 50$
SSPE	152.0	7.3	25.5	57.3	124.5
RSSPE	1.0	20.8	6.0	2.7	1.2

Table 6. Estimated and True Model Parameters for Study 4

	Steady-State Parameters		
a_1	0.5	$\hat{a}_1$	0.51
a_2	0.1	$\hat{a}_2$	0.10
	Dynamic Parameter		
τ	5	$\hat{\tau}$	4.85
	Stochastic Parameter		
α	0.6	$\hat{\alpha}$	0.69

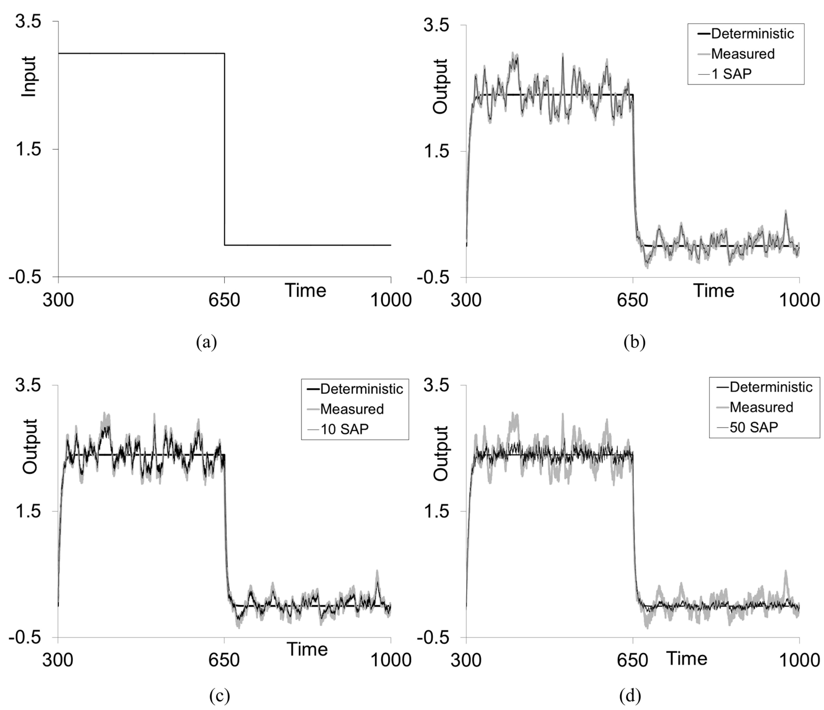

Figure 7. Graphical results for the test sequence in study 3: (a) deterministic input sequence, (b) 1SAP, (c) 10SAP, and (d) 50SAP.

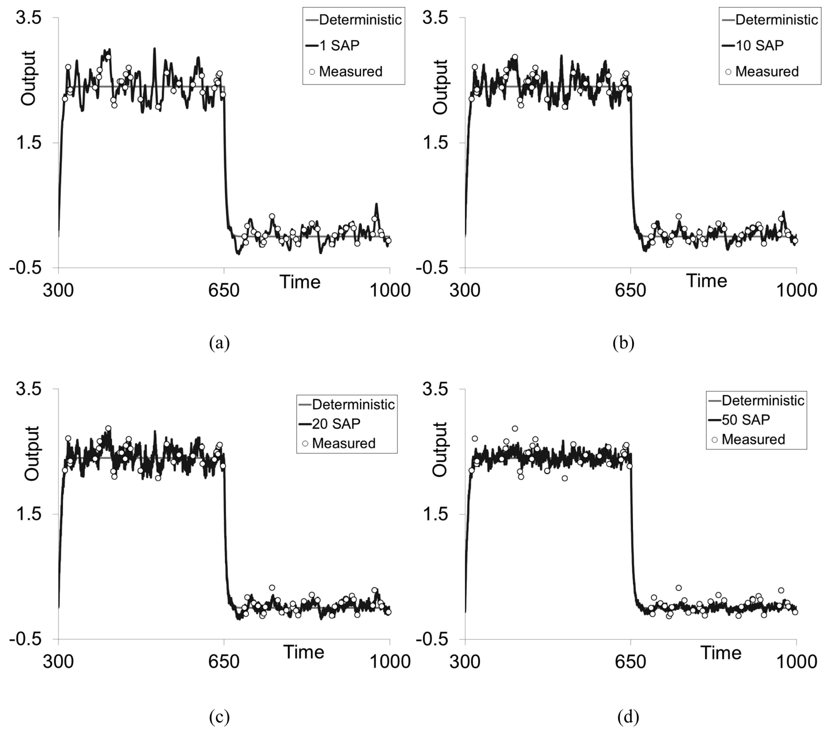

Figure 8. Graphical results for the test sequence in study 4: (a) 1SAP, (b) 10SAP, (c) 20SAP, and (d) 50SAP.

and, thus, with all of the values greater than 1, strongly supports the usefulness of CTSOM as compared to a deterministic approach.

5.4. Study 4. The purpose of study 4 was to illustrate and evaluate the application of CTSIM in a process identification study. This process and conditions for this study were exactly the same as for study 3 with a few changes. First, the input was measured at each time instant, and the output measuring rate was 1% of the input measuring rate. Furthermore, the outputs were measured at a nonconstant random rate that followed a uniform distribution. This output sampling rate was used to evaluate the ability of the proposed method to provide a good model when outputs are measured infrequently and at a nonconstant rate. The outputs were assumed to be measured offline.

The output responses to the training input sequence of Figure 6 are not shown for space considerations. The fitted model was obtained by following the procedure for the CTSIM given in section 4.1. The values $\boldsymbol{\theta}$ and $\hat{\boldsymbol{\theta}}$ are reported in Table 6. As shown, these estimates are all close to their true values. Note that τ and α are well within one standard error of their true values for the standard errors given in Table 1. The fitted response followed the CTS behavior of the measured output response quite well, with an r_{fit} value of 0.999.

Graphical results for the test sequence for study 4 are presented in Figure 8, and the SSPE and RSSPE results are listed in Table 7 for the deterministic case and for kSAP for k = 1, 10, 20, and 50. As shown, the kSAP responses follow the measured response quite well as compared to the deterministic response, which does not follow the CTS behavior. As in the previous studies, the prediction accuracy decreased as k increased. As shown in Table 7, the RSSPE ranged from 13.2 for k = 1 to 1.3 for k = 50 and, thus, with all of the values greater than 1, strongly supports the usefulness of CTSOM as compared to a deterministic approach. The RSSPE values in study 4 were slightly lower than those in study 3, likely because of the much lower number of outputs used in model building. In this study, we also evaluated eq 19, which would be used to develop a virtual sensor. These results were the same as the kSAP results in Table 7, thus strongly supporting the potential of this method in virtual sensor applications when online and frequent outputs are not available.

Table 7. Test Sequence Performance Results for CTSIM in Study 4

type	D	k = 1	k = 10	k = 20	k = 50
SSPE	0.79	0.06	0.17	0.37	0.61
RSSPE	1.0	13.2	4.6	2.1	1.3

6. CONCLUDING REMARKS

This article addressed the modeling of inputs to improve process modeling under continuous-time stochastic behavior. The basic idea is to exploit the probabilistic behavior of inputs that are time-correlated. This exploitation led here to the development of three methods. The first, the continuous-time stochastic input method (CTSIM), was developed for cases in which the inputs are measured with applications in the development of virtual sensors and predictive modeling. The other two approaches were developed for applications in which the inputs are not measured. The Wiener network with an invertible static nonlinear function provides the ability to obtain necessary intermediate values to estimate continuous-time stochastic model parameters. One approach, the continuous-time stochastic moment method (CTSMM), uses derived moment equations for the intermediate variable and equates them to sample moments to obtain parameter estimates. The other, the continuous-time stochastic output method (CTSOM), does not require sample moments but uses dynamic structures and, thus, relies on approximation methods to obtain accurate derivatives. This work showed that smoothing process variables using a filtering or averaging method can prove effective. In this article, a Monte Carlo simulation (MCS) study on the CTSMM provided standard errors that assisted in evaluating the other two parameter estimation methods, which were found to obtain accurate estimates under this evaluation.

The limitation of the CTSMM is that it is not easily suited for process identification studies, whereas the other two methods were developed to overcome this limitation. A key result of this work to overcome this limitation was the development of an estimator for the CTS input that depends on the CTS model parameters (i.e., eq 24). Future work in the evaluation, development, and application of these methods will include studies on real processes and extensions to multiple-input−multiple-output processes with measured and unmeasured inputs. Because most real processes exhibit continuous-time stochastic behavior, the development of methods that address this behavior can have a significant impact on improving inferential modeling (virtual sensors), predictive modeling, and predictive control.

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Notes

The authors declare no competing financial interest.

■ REFERENCES

(1) Nordsjo, A. E. Cramer−Rao Bounds for a Class of Systems Described by Wiener and Hammerstein Models. *Int. J. Control* **1997**, *68*, 1067.
(2) Nordsjo, A. E.; Wigren, T. On Estimation of Errors Caused by Non-Linear Undermodelling in System Identification. *Int. J. Control* **2002**, *75*, 1100.
(3) Schoukens, J.; Nemeth, J. G.; Crama, P.; Rolain, Y.; Pintelon, R. Fast Approximate Identification of Nonlinear Systems. *Automatica* **2003**, *39*, 1267.
(4) Vandersteen, G.; Rolain, Y.; Schoukens, J. Non-Parametric Estimation of the Frequency-Response Functions of the Linear Blocks of a Wiener-Hammerstein Model. *Automatica* **1997**, *33*, 1351.
(5) Bai, E.-W. Frequency Domain Identification of Hammerstein Models. *IEEE Trans. Autom. Control* **2003**, *48*, 530.
(6) Kadlec, P.; Gabrys, B.; Strandt, S. Data-driven Soft Sensors in the Process Industry. *Comput. Chem. Eng.* **2009**, *33*, 795−814.
(7) Lima, F. V.; Rawlings, J. B. Nonlinear Stochastic Modeling to Improve State Estimation in Process Monitoring and Control. *AIChE J.* **2011**, *57*, 996−1007.
(8) Giri, F., Bai, E.-W., Eds. *Block-Oriented Nonlinear System Identification*; Springer: Berlin, 2010.
(9) Garnier, H., Wang, L., Eds. *Identification of Continuous-Time Models from Sampled Data*; Springer: London, 2008.
(10) Vanbeylen, L. Nonlinear Dynamic Systems: Blind Identification of Block-Oriented Models, and Instability under Random Inputs. Ph.D. Thesis, Vrije Universiteit Brussel, Brussels, Belgium, 2011.
(11) Seborg, D. E.; Edgar, T.; Mellichamp, D. L.; Doyle, F. J. *Process Dynamics and Control*; Wiley: New York, 2011.
(12) Kalafatis, A.; Arifin, N.; Wang, L.; Cluett, W. R. A New Approach to the Identification of pH Process Based on the Wiener Model. *Chem. Eng. Sci.* **1995**, *50*, 3693.
(13) Huang, H.-P.; Lee, M.-W.; Tang, Y.-T. Identification of Wiener Models Using Relay Feedback Test. *J. Chem. Eng. Jpn.* **1998**, *31*, 604.
(14) Bhandari, N.; Rollins, D. K. Continuous-Time Multi-Input, Multi-Output Wiener Modeling Method. *Ind. Eng. Chem. Res.* **2003**, *42*, 5583.
(15) Greblicki, W. Nonparametric Identification of Wiener Systems. *IEEE Trans. Inf. Theory* **1992**, *38*, 1487.
(16) Greblicki, W. Nonparametric Approach to Wiener System Identification. *IEEE Trans. Circuits Syst. I* **1997**, *44*, 538.
(17) Wigren, T. Recursive Prediction Error Identification Using the Nonlinear Wiener Model. *Automatica* **1993**, *29*, 1011.
(18) Henson, M. A.; Seborg, D. E. *Nonlinear Process Control*; Prentice Hall PTR: Upper Saddle River, NJ, 1997.
(19) Rollins, D. K.; Bhandari, N.; Bassily, A. M.; Colver, G. M.; Chin, S.-T. A Continuous-Time Nonlinear Dynamic Predictive Modeling Method for Hammerstein Processes. *Ind. Eng. Chem. Res.* **2003**, *42*, 861.
(20) Ochi, M. K. *Applied Probability and Stochastic Processes in Engineering and Physical Sciences*; Wiley: New York, 1990.
(21) Devore, J. L. *Probability and Statistics for Engineering and the Sciences*; Duxbury Press: Pacific Grove, CA, 2003.
(22) Ripley, B. D. *Stochastic Simulation*; Wiley: New York, 1987.
(23) Zhai, D. Continuous-Time Block-Oriented Nonlinear Modeling with Complex Input Noise Structure. Ph.D. Dissertation, Iowa State University, Ames, IA, 2005.
(24) Bellach, B. Parameter Estimators in Linear Stochastic Differential Equations and Their Asymptotic Properties. *Math. Operationsforsch. Stat., Ser. Stat.* **1983**, *14*, 141.
(25) Chen, X.-K.; Kozin, F. Almost Sure Consistent Estimates of Parameters in Continuous Systems. *Control Theory Adv. Technol.* **1991**, *7*, 1.
(26) Sorensen, M. Estimating Functions for Discretely Observed Diffusions: A Review. In *Selected Proceedings of the Symposium on Estimating Functions*; Basawa, I. V., Godambe, V. P., Taylor, R. L., Eds.; Institute of Mathematical Statistics: Hayward, CA, 1997; Volume 32, pp 305−326.
(27) Pedersen, A. R. A New Approach to Maximum Likelihood Estimation for Stochastic Differential Equations Based on Discrete Observations. *Scand. J. Stat.* **1995**, *22*, 55.