Real-Time Estimation of Dynamic Particle-Size Distributions in a Fluidized Bed: Theoretical Foundation

Significant noise (random error) is common in an on-line signal when measuring the particle size distribution in a fluidized bed. The application of optimal estimation theory to obtain a filtering algorithm that can rectify such measurements is detailed. Off-line simulation studies demonstrate that the filtering algorithm yields a measure of particle size distribution that is well-behaved, accurate, and able to track in real time as conditions change in the bed.

D. J. Cooper and D. E. Clough

Department of Chemical Engineering
University of Colorado
Boulder, CO 80309

SCOPE

Significant noise (random, unmodeled error) is common in an on-line signal when measuring the particle size distribution in a fluidized bed. The application of optimal estimation theory, which provides a mathematical basis for rectifying such measurements, is detailed. An optimal filtering algorithm is derived that tempers the noisy measurements with predictions from an idealized dynamic model to yield an accurate, well-behaved, real-time measure of particle size distribution. These qualities are desirable in a measure that is being monitored, and are necessary if the measure is to be used in computer control.

The theoretical development includes formulation of an idealized model that describes the mixing dynamics (including elutriation and attrition) in a fluidized bed, and the derivation of a filtering algorithm that combines predictions from this model with noisy measurements to yield the optimal estimates. Several off-line simulation studies are presented to illustrate the performance and capabilities of the filtering algorithm.

A general theoretical development is presented in this work. Although substantial detail has been included, the work is not intended to stand alone for those interested in implementation of this theory. Rather, for those versed in optimal estimation theory it is intended to provide a solid platform upon which they can build given the specifics of their application. For those unfamiliar with the theory it is intended to illustrate the capabilities of optimal estimation, and to introduce the methodology of application.

The general theoretical development enables others to adapt or extend the method. One example of a straightforward adaptation is to obtain an accurate, well-behaved measure of the elutriate stream particle size distribution. An extension of interest includes using a different idealized dynamic model that is specific to a particular application.

CONCLUSIONS AND SIGNIFICANCE

An optimal filtering algorithm is effective in producing accurate, well-behaved, real-time estimates of particle size distribution from measurements that are corrupted with random, unmodeled error (noise). Optimal estimation theory provides the mathematical basis for computing these estimates by combining the measurement data with predictions from an idealized dynamic model. Such estimates of particle size distribution are highly desirable if this parameter is being monitored during fluidized bed operation, and are necessary if it is being used in computer control applications.

Optimal estimation theory provides a specific framework for computing high-quality real-time estimates from noise measurements. Although not detailed in this work, the theory also provides for computing accurate, well-behaved, real-time estimates from measurements that are discrete in time, or available only after a significant time delay. The filtering algorithms for these situations are extensions of the general filtering algorithm developed here.

Probably the most important benefit from using optimal estimation theory is that a means is provided for the investigator to use actual measurement data, yet also include specific knowledge about the physical process to obtain a measure of improved accuracy. Such knowledge is included in the filtering algorithm via the idealized dynamic model. Thus, accurate, well-behaved, real-time estimates of particle size distribution can be obtained from measurements that are noisy, discrete in time, and/or delayed in time.

INTRODUCTION

Particle size distribution (PSD) is a fundamental parameter in fluidization. There are many instances, therefore, where current knowledge of PSD during fluidized bed operation would be desirable. This is especially so in situations where PSD is changing with time. The goal of this work is to detail a method for obtaining an on-line measaure of PSD in a fluidized bed. Further, the measure obtained is to be accurate, well-behaved, and in real time, tracking the overall distribution dynamics as conditions change. Such qualities are highly desirable in a measure that is being monitored, and they are necessary if the measure is to be used for computer control.

Our early investigations revealed that no instrument is commercially available that can yield a PSD measurement of the character described above. Even the best on-line instruments yield a PSD measurements that is corrupted with noise (random, unmodeled error). Error is introduced because instruments have accuracy limitations and can be affected by such things as an irregular particle shape. Also, sampling itself introduces error because it is a local phenomenon. Transportation of the particle sample from the process to the measuring instrument, even if it is only a few feet away, can significantly skew the resulting measurements. It is difficult to make sound operating decisions or develop control strategies based on such information.

Optimal estimation theory provides a mathematical basis for obtaining a well-behaved, accurate, real-time estimate from noisy measurements. An optimal filtering algorithm, derived from optimal estimation theory, can generate such estimates by minimizing an error criterion that, in effect, tempers the noise measurements with predictions from an idealized dynamic model.

In this paper we develop the theoretical basis for such a filtering algorithm and investigate some example applications through off-line computer studies. We have kept the presentation as general as possible so that others can adapt or extend the method to their specific applications.

Importance of Particle Size Distribution

PSD is of fundamental importance to the performance and operation of fluidized beds. For instance, for beds of uniform particle density with a distributed particle size, there is a range of velocities between the onset of fluidization for the finest particles and complete fluidization of the coarsest particles. The effect of a wider PSD is a wider range of velocities between beginning complete fluidization (Chen and Keairns, 1975; Vaid and Gupta, 1978). Also, for uniform particle density beds, segregation of particles occurs at low velocities above that needed for complete fluidization (Chen and Keairns, 1975; Nienow et al., 1978). The tendency toward segregation is a direct function of the PSD; in fact, Chen (1981) has published a theoretical model for predicting segregation due to size difference in fluidized beds.

Segregation generally decreases with increasing gas velocity, and at high gas velocities the bed approaches well-mixed behavior (Cranfield, 1978; Fan and Chang, 1979). For very wide PSD systems, however, Geldart et al. (1981) observed that segregation by size difference appears to be intrinsic to the system even at high velocities. Also, at these higher velocities the PSD of entrained particles approaches the PSD of the bed (George and Grace, 1981), and the PSD of elutriated particles can be related to the PSD of the bed via an elutriation constant (Levenspiel et al., 1968; Chen and Saxena, 1978; Weimer and Clough, 1980; Wen and Chen, 1982).

Zenz (1960) notes that PSD affects solids packing density, "powder viscosity," the tendency toward bridging or arching, the efficiency and loading of fines recovery facilities, and the operation of pneumatic conveyers. Many investigators believe that a wide PSD gives a better quality of fluidization, though others urge caution at making such generalizations (Geldart, 1972; Wen and Dutta, 1977). Gas-particle heat transfer rates (Kato and Wen, 1970) and particle-internals heat transfer rates (Priebe and Genetti, 1977; Henry, 1977) are affected by PSD. The efficiency of sulfur retention in fluidized bed coal combustors is affected by limestone or dolomite PSD (Rajan et al., 1978). The degree of reactivity in fluidized bed char gasifiers (Weimer and Clough, 1980) and in fluidized bed combustors (Horio and Wen, 1978; Baron et al., 1978) is influenced by PSD.

The literature supports the observation that PSD affects fluidization behavior, transport and kinetic properties in the bed, and process considerations for operation. Many factors affect PSD, including solids feed, discharge, elutriation, particle growth (e.g. deposition), and particle shrinkage (e.g. attrition, reaction). Elutriation, growth, shrinkage, and chemical reaction are all different for different particle sizes. Because PSD is so fundamental to the performance and operation of fluidized beds, it is an important parameter to be able to monitor and is a necessary parameter for the development of many control strategies capable of improving fluidized bed performance and operation.

Particle Size Distribution Measurement

There are many methods used to measure PSD; however, most of these are unsatisfactory when considering the requirements for real-time estimation and control (Davies, 1973; Cadle, 1975). The method required must be on-line and automatic, have a rapid response, and be able to measure over a wide particle size range with resonable accuracy. The device employed should be sturdy, require little maintenance, and be cost effective. Ideally it should be capable of measuring PSD under conditions of high particle concentration and velocity, and be so precise that the resolved PSD measurement is more than a Gaussian aproximation. Very few commercially available devices can yield a PSD measurement of the character and in the manner described above. Of the few devices that do meet these requirements, most employ either a light-scattering or a light-occultation (light-obscuration) method. Both of these optical measurement technqiues involve resolving the effect of an incident beam of light on a sample of particles.

Light-scattering theory is based on the assumption that particles in suspension will scatter an incident beam of light. The total measured scatter can be considered as the sum of the scattering by the individual particles. The amount of scattered light can be correlated with particle size, concentration, and refractive index, plus the wavelength and angle of incidence of the light beam. Devices have been developed that correlate PSD with forward-, backward-, and angle-scattered light.

Light occultation can be used with opaque or light absorbing particles. An incident beam of light is used to illuminate particles passing in front of a photodiode imaging system. The particles completely block the light, casting shadow images onto the photodiode imaging array. The individual particles are then sized by the number of photodiode elements that are occulted. Light occultation has some distinct advantages over light-scattering techniques. Light-occultation devices measure counts per particle size range (number of photodiode elements occulted). The raw signal is an actual distribution. Light-scattering devices correlate particle size with the amount of scattered light. Calibration will be for the specific particle refractive index. Even particle color will affect the calibration. These properties have little effect on light-occultation devices (Davies, 1974).

The theoretical development presented in this work is dependent on a PSD measurement, but it is reasonably independent of the device employed. We will assume that a value of PSD is available to the computer with negligible time delay after measurement, that the measurement can be represented as discrete values distributed across the domain of particle radius, and that the PSD measurement is virtually continuous in time. The case where the measurement is considered as discrete values in time will not be discussed, but such an implementation would be a straightforward extension of this work and the filtering theory is developed in detail in the literature (Bryson and Ho, 1975; Ray, 1981).

Distributed-Parameter Filtering

When the dynamic behavior of a process is described by a partial differential equation, such as the PSD in a fluidized process, the system is categorized as a distributed-parameter system. Other examples of such systems include chemical reactors, heat exchangers, underground coal and oil reservoirs, and solar collectors. Measurements on these systems often manifest significant uncertainties in the form of noise and bias, and the processes themselves are generally subject to random disturbances and nonideal behavior. These uncertainties must be addressed if the measurements are to be of use as parameters in process monitoring and control (Bryson and Ho, 1975). Optimal estimation theory provides a mathematical basis for deriving filtering algorithms that yield accurate, well-behaved estimates from noisy measurements.

A number of filtering algorithms have been developed and studied since Kalman (1960) and Kalman and Bucy (1961) introduced linear filtering theory. The structure of these algorithms varies depending on whether the system is continuous or discrete, linear or nonlinear, or lumped or distributed. The development of these algorithms is summarized in chronological order as follows: After Kalman (1960) and Kalman and Bucy (1961) introduced linear filtering theory for lumped systems, Bellman et al. (1966) and Detchmendy and Sridhar (1966) developed nonlinear filtering theory. Several survey papers (Aström and Eykhoff, 1971; Gustafsson, 1975) examined the theory and applications of linear and nonlinear lumped-parameter filters. These filters have been successfully applied in the aerospace and communications field. A number of researchers including Tzafestas and Nightingale (1968), Thau (1969), and Collins and Khatri (1969) introduced distributed filtering. Contributions of Meditch (1971) and Sakawa (1972) to the linear distributed filtering theory followed. In the late 1960s and early 1970s, nonlinear distributed filtering theory was developed (Seinfeld, 1969; Sherry and Shen, 1971; Seinfeld et al., 1971; Hwang et al., 1972; Padmanabhan and Colantuoni, 1974). The developments and applications of linear and nonlinear distributed-parameter filters during the last decade have been summarized in the works of Tzafestas (1978), Ray (1978), and Bencala and Seinfeld (1969).

In his summary work, Tzafestas (1978) outlines the procedures which must be followed when estimating parameters for any distributed-parameter system. These steps include:

1. Deriving an appropriate dynamic model that describes the physical system. This requires knowledge of the physical laws that govern the process, and the use of justifiable assumptions to obtain the simplest model that can adequately predict the response of the process to anticipated input changes.
2. Implementing a numerical solution technique for solving this model on-line and in real time.
3. Selecting and installing a measuring device.
4. Deriving the appropriate distributed-parameter filtering algorithm.
5. Implementing a numerical technique for solving the algorithm on-line and in real time.
6. Investigating the properties (accuracy, sensitivity, etc.) of the filtering algorithm experimentally.

There are many criteria that can be used in defining an optimal estimate. These criteria include the least-squares approach, the maximum-likelihood approach, the Bayesian approach, the orthogonal projection approach, and the innovations approach (Bryson and Ho, 1975; Tzafestas, 1978). All of these approaches yield filtering algorithms that are either identical or very similar in form. A comparison of the above is summarized by Tzafestas (1978).

In this work, we base our real-time PSD estimates on a least-squares minimization criterion. The least-squares approach is preferable for this application as it is deterministic and allows a stochastic optimal filtering problem to be solved while bypassing the requirement of a probabilistic treatment. Kailath (1974), in his survey work covering three decades of linear filtering theory, states that least-squares estimation is perhaps the most important criterion that has connections to and implications for a surprisingly large number of engineering problems. Also, both Bryson and Ho (1975) and Ray (1981), in their textbooks on advanced control, use a least-squares minimization approach in a substantial portion of their theoretical development.

Related Work

Investigators in other industries have faced a similar need of estimating size distributions, often for use in control strategy development. The measurement and control of PSD in grinding mills is one application that has received attention in the literature. Grinding mills are considered by some to be stable and thus require little control. A recent study in on-line PSD measurement, however, has shown that this is not the case (Atkins, 1975). In this study, the real-time behavior of particle size in a grinding mill circuit was investigated. Although the investigators observed significant particle-size dynamics, they noted that their overall error analysis was uncertain because the raw instrument signal proved too "noisy." No attempt was made to rectify the raw measurement signal. In a different investigation, dynamic models were used to deduce operating conditions and control strategies that would yield the most favorable PSD in a grinding mill (Cutting and Devenish, 1979). The use of dynamic models can prove valuable in measurement rectification; however, in this work the models were run off-line with no real-time plant measurements used.

Aerosol science is another area where PSD estimation methods have been published. Researchers have applied optimal estimation theory (Busigin et al., 1980) and least-squares minimization (Raabe, 1978) to obtain improved PSD estimates from noisy measurements. Again, these investigations were performed off-line, with the data first being collected and then mathematically analyzed. Optimal estimation theory has become so pervasive that lumped Kalman filters have been used to predict fish population behavior (Balchen, 1979), and distributed-parameter filters have been used to estimate insect population distributions (Hildebrand and Haddad, 1977) and air pollution concentration distributions (Omatu and Seinfeld, 1981). All three of the latter applications used a least-squares minimization criterion.

THEORETICAL DEVELOPMENT

Fluidized Bed Dynamic Model

An important part of any real-time estimation problem is modeling the process. Some early research of interest includes that of Levenspiel et al. (1968), who presented the governing equations for predicting the steady-state PSD in a solids processing fluidized bed. This was the first work that used a mass balance approach to account for solids feed, discharge, elutriation, particle growth, and particle shrinkage. The model assumed, however, that only the size of the particle changes during chemical reaction. Chen and Saxena (1978) extended this approach by deriving a steady-state model that not only considered the particle size distribution, but also the particle-conversion distribution (particle density distribution). This model is more descriptive of coal combustion and char gasification applications. Weimer and Clough (1980) further developed these concepts to account for the dynamic behavior of such systems.

In the continuous treatment of solids in a fluidized bed, a schematic of which is shown in Figure 1, fresh particles of known PSD, $P_0(r)$, are fed at a constant rate to a fluidized bed with a PSD, $P_b(r,t)$. They are discharged either by an overflow pipe or by entrainment via the fluidization gas. Considering the case where no reaction is occurring, and under the assumption of constant bed density and volume, the following general relation can be derived for spherical particles of radius R_i:

$$w\frac{\partial P_b(R_i,t)}{\partial t} = F_0P_0(R_i) - F_1(t)P_1(R_i,t) - F_2(t)P_2(R_i,t) + w\frac{\partial}{\partial r}\left\{P_b(R_i,t)\left(\frac{\partial r}{\partial t}\right)_{R_i}\right\} \quad (1)$$

with the requirement that at all times, the probability density function $P_b(r,t)$ be normalized such that:

$$\int_0^{R_{max}} P_b(r,t)dr = 1.0 \quad (2)$$

The form of the dynamic model can be recast by introducing an elutriation constant of the form:

$$K(r,t) = \frac{F_2(t)P_2(r,t)}{wP_b(r,t)} \quad (3)$$

by defining attrition kinetics (Levenspiel, 1968) in a form descriptive of a mechanism that assumes that tiny fragments are worn or abraded off the particles, are immediately carried overhead, and are not considered as part of the solids population, i.e.:

$$\left(\frac{\partial r}{\partial t}\right)_{R_i} = kR_i \quad (4)$$

and by specifying that the fluidization velocity is high enough (approximately three times minimum fluidization or greater) such that:

$$P_1(r,t) \approx P_b(r,t) \quad (5)$$

Substitution of Eqs. 3, 4, and 5 into Eq. 1 and rearranging yields a dimensionless fluidized bed dynamic model of the form:

$$\frac{\partial P_b(R_i,\tau)}{\partial \tau} = \alpha(R_i)\frac{\partial P_B(R_i,\tau)}{\partial r} + \beta(R_i,\tau)P_b(R_i,\tau) + \gamma(R_i) \quad (6)$$

where

$$\alpha(R_i) = \frac{wkR_i}{F_0} \quad (7)$$

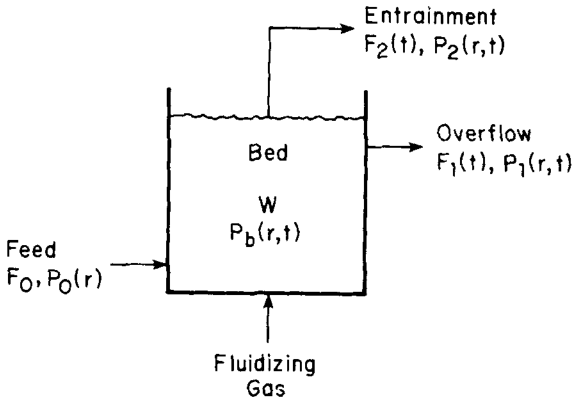

Figure 1. Fluidized bed, schematic diagram.

$$\beta(R_i,\tau) = \frac{w[k - K(R_i,\tau)] - F_1(\tau)}{F_0} \quad (8)$$

$$\gamma(R_i) = P_0(R_i) \quad (9)$$

and

$$\tau = \frac{tF_0}{w} \quad (10)$$

Discretizing the State Model

Real-time implementation of optimal distributed parameter filters requires the use of numerical techniques that yield both rapid and accurate solutions to the filter partial differential equations. Because such requirements can be difficult to achieve, simplifications are often made. One common approach is to discretize the state model partial differential equation and approximate it as a system of ordinary differential equations. Application of optimal estimation theory to the system of ordinary differential equations results in a system of lumped Kalman filters that approximate the linear distributed parameter filter. A system of lumped filters is easier to implement because the lumped filter differential equations can be readily solved in real time. Information relating to the correlated nature of the spatial noise is lost when such an approach is employed (Cooper et al., 1985), and this can affect filter performance. The lumping approximation can give satisfactory results in many cases, however. Computational burden is a very real consideration in real-time applications. We have therefore elected to use a lumped approximation in this work.

The general form for the dynamic state model for all $0 < r \leq R_{max}$ is:

$$\frac{\partial P_b(r,\tau)}{\partial \tau} = \alpha(r)\frac{\partial P_b(r,\tau)}{\partial r} + \beta(r,\tau)P_b(r,\tau) + \gamma(r) \quad (11)$$

The fluidized bed PSD, $P_b(r,\tau)$, which is continuous over particle radius, is approximated as a vector of N discrete states each at a specific radius, i.e.,

$$X(\tau) = \begin{bmatrix} P_b(R_1,\tau) \\ P_b(R_2,\tau) \\ \vdots \\ P_b(R_N,\tau) \end{bmatrix} \quad (12)$$

and the spatial derivative is approximated as:

$$\frac{\partial P_b(r,\tau)}{\partial r} = AX(\tau) \quad (13)$$

where A is a first derivative approximation operator such as a finite difference matrix or an orthogonal collocation matrix.

If α and $\beta(\tau)$ are appropriately defined spatially-discrete diagonal matrix representations and γ is an appropriately defined spatially-discrete vector representation for these coefficients, the state model partial differential equation can then be approximated as the system of ordinary differential equations:

$$\dot{X}(\tau) = \alpha AX(\tau) + \beta(\tau)X(\tau) + \gamma \quad (14)$$

Optimal Filtering Algorithm

Following the filter development used by most investigators (Meditch, 1971; Bryson and Ho, 1975; Tzafestas, 1978; Ray, 1981), the linear system to be filtered is expressed by the model:

$$\dot{X}(\tau) = \alpha AX(\tau) + \beta(\tau)X(\tau) + \gamma + U(\tau) \quad (15a)$$

$$Z(\tau) = MX(\tau) + V(\tau) \quad (15b)$$

$$X(\tau_0) = X_0 + U(\tau_0) \quad (15c)$$

Where $Z(\tau)$ is the measured output vector containing a measured value for each discrete radius size and M is a linear modeling matrix that describes the relationship between the true state and the measured output. $X(\tau)$ is the true initial state of the system and is unknown, but X_0 is an *a priori* estimate of it.

The variables $U(\tau)$ and $V(\tau)$ are noise vectors representing the uncertainties in the state model and the measured output model respectively. Both models are assumed to be such that the noise can be described as Gaussian-distributed, zero-mean, and white in time. The spatial discretization of the state model implies an added assumption that the model uncertainties are also white in space; that is, the spatially correlated nature of the uncertainties is assumed not to exist.

The model uncertainties then have covariance matrices of the form:

$$E[U(\tau_1)U^T(\tau_2)] = Q(\tau)\delta(\tau_1 - \tau_2) \quad (16a)$$

$$E[V(\tau_1)V^T(\tau_2)] = R(t)\delta(\tau_1 - \tau_2) \quad (16b)$$

and with a cross covariance of zero (uncorrelated), i.e.,

$$E[U(\tau_1)V^T(\tau_2)] = 0 \quad (17)$$

The *a priori* initial state estimate X_0 is also white in space with a covariance matrix of the form:

$$E[X_0X_0^T] = P_0 \quad (18)$$

Because $Q(\tau)$, $R(\tau)$, and P_0 are covariance matrices, they are positive, semidefinite, and symmetric.

The optimal real-time PSD estimate is obtained by minimizing the quadratic least-squares error criterion:

$$J = \frac{1}{2}[X(\tau_0) - X_0]^T P_0^{-1}[X(\tau_0) - X_0] + \frac{1}{2}\int_{\tau_0}^{\tau_f}[U(\tau)]^T Q^{-1}(\tau)[U(\tau)]d\tau + \frac{1}{2}\int_{\tau_0}^{\tau_f}[Z(\tau) - MX(\tau)]^T R^{-1}(\tau)[Z(\tau) - MX(\tau)]d\tau \quad (19)$$

where the first term in Eq. 19 minimizes the squared error of the initial state estimate, the second term minimizes the integral squared modeling error, and the third term minimizes the integral squared measurement error. For implementation, the matrices $Q(\tau)$, $R(\tau)$ and P_0 are chosen to allow a relative weighting among the three terms in the error criterion based on the investigator's confidence in the accuracy of the dynamic state model, the on-line measurement model, and the initial state estimate respectively.

The problem, to minimize J subject to the conditions expressed in Eq. 15, is treated via the calculus of variations by introducing a Lagrange multiplier and considering the augmented functional:

$$J_{aug} = J + \int_{\tau_0}^{\tau_f} \lambda^T(\tau)[\dot{X}(\tau) - \alpha AX(\tau) - \beta(\tau)X(\tau) - \gamma - U(\tau)]d\tau \quad (20)$$

Equation 20 yields the Euler-Lagrange equations:

$$\dot{X}(\tau) = \alpha AX(\tau) + \beta(\tau)X(\tau) + \gamma(\tau) + U(\tau) \quad (21a)$$

$$\dot{\lambda}(\tau) = -(\alpha A)^T\lambda(\tau) - \beta(\tau)\lambda(\tau) - M^T R^{-1}(\tau)[Z(\tau) - MX(\tau)] \quad (21b)$$

with the associated transversality conditions:

$$\lambda(\tau_0) = P_0^{-1}[X(\tau_0) - X_0] \quad (22a)$$

$$\lambda(\tau_f) = 0 \quad (22b)$$

Equations 21 and 22 have reduced the estimation problem to a two-point boundary value problem. Because the system is linear, the problem can be transformed into an initial value problem via a Riccati-type transformation. The transformation allows the definition of an initial condition that is "equivalent" to the terminal condition. The optimal real-time estimates can then be computed by integration forward in time. As suggested by the form of the first transversality condition, if a solution:

$$X(\tau) = X^*(\tau) + P(\tau)\lambda(\tau) \quad (23)$$

is assumed for the simultaneous Euler-Lagrange equations where $X^*(\tau)$ is the optimal (minimum least-squares error) estimate, then the following pair of linear, simultaneous filter equations can be derived.

$$\dot{X}^*(\tau) = \alpha AX^*(\tau) + \beta X^*(\tau) + \gamma + P(\tau)MR^{-1}(\tau)[Z(\tau) - MX^*(\tau)] \quad (24a)$$

$$\dot{P}(\tau) = \alpha AP(\tau) + P(\tau)(\alpha A)^T + 2\beta P(\tau) + Q(\tau) - P(\tau)M^T R^{-1}(\tau)MP(\tau) \quad (24b)$$

with initial conditions:

$$P(\tau_0) = P_0 \quad (24c)$$

$$X^*(\tau_0) = X_0 \quad (24d)$$

The simultaneous solution of these equations via integration forward in real time yields the optimal filtered PSD estimate $X^*(\tau)$. This estimate, based on information provided from the dynamic state model, the noisy measurements and the initial conditions, will be well-behaved and accurate. Results for several cases are presented in the following numerical examples.

NUMERICAL EXAMPLES

Before presenting the numerical examples, we note the following:

1. *Linear vs. nonlinear*. Up to this point, the dynamic state model has been presented as a linear differential equation with variable coefficients. The optimal filtering algorithm also has been developed for a linear system. Consider that:

$$F_1(\tau) = F_0 - F_2(\tau) \quad (25)$$

and $F_2(\tau)$ is made up of the component parts:

$$F_2(\tau) = (F_2 \text{ attrition}) + (F_2 \text{ elutriation}) \quad (26)$$

By assuming spherical particles, $F_2(\tau)$ can be expressed as (Levenspiel, 1968):

$$F_2(\tau) = 3kw + w\int_0^{R_{max}} K(r)P_b(r,\tau)dr \quad (27)$$

Substitution of Eqs. 25 and 27 into Eq. 8 yields a form for the state model coefficient:

$$\beta(r,\tau) = w\left[\frac{4k - K(r,\tau) + \int_0^{R_{max}} K(r,\tau)P_b(r,\tau)dr}{F_0}\right] - 1 \quad (28)$$

Because $P_b(r,\tau)$ appears in the coefficient $\beta(r,\tau)$, the dynamic state model is actually a nonlinear differential equation. Euler integration (forward indifference in time) is a very simple numerical technique that can be shown to be a successive linearization of this nonlinear term. Thus, Euler integration enables the use of linear filtering theory. Quasilinearization is another approach taken by some investigators. Quasilinearization has the advantage of being

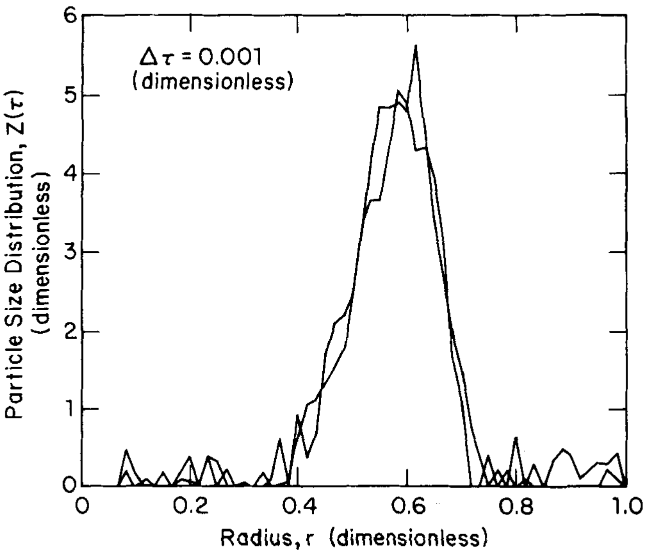

Figure 2. Illustration of noise in measurement.

independent of the numerical technique used, but it also requires further manipulation of the dynamic state model. In an effort to keep the presentation as illustrative as possible, Euler integration is used in the examples.

2. *Well-behaved vs. noisy.* A number of references have been made up to this point concerning the noisy nature of the measured signal compared to the well-behaved nature of the optimal estimate. In the examples, the measured values are simulated by adding random noise to the true system state (i.e., to the output of the dynamic state model). Figure 2 shows two PSD measurements actually used in the simulation for the first example. Note the change that can occur in measurements in only one Euler integration step ($\Delta\tau = 0.001$). In this same time period, the change in the optimal estimate is barely discernible when viewed on a similar plot.

3. *Initial conditions.* Illustrated in Figure 3 are the initial values used in all of the examples. The *a priori* estimate of the true state

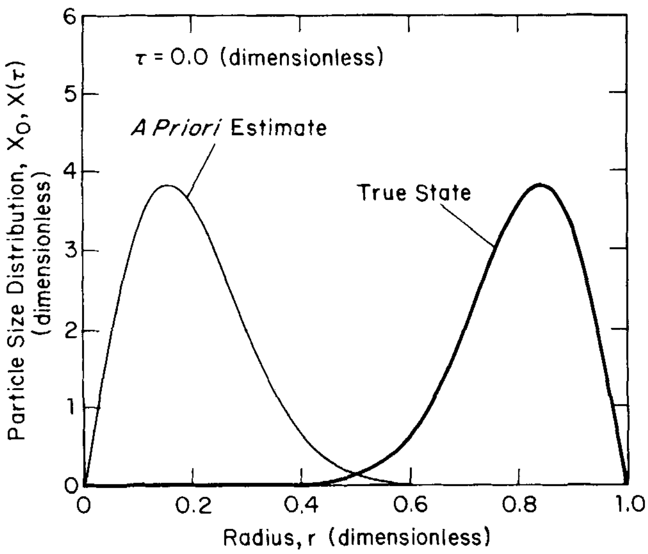

Figure 3. Initial conditions.

Table 1. Parameter Values and Relations Used in Examples 1-3

Parameter	Value/Relation	Units
Feed rate	$F_0 = 1.0$	$\frac{\text{mass}}{\text{time}}$
Attrition rate constant	$k = 0.75$	$\frac{1.0}{\text{time}}$
Elutriation rate constant	$K(r,\tau) = e^{-20.0r}$	$\frac{1.0}{\text{time}}$
Feed PSD	$P_0(r) = 40.0re^{-20.0r^2}$	—
Initial bed PSD	$P_b(r,\tau_0) = 40.0re^{-20.0r^2}$	—
Bed weight	$w = 5.0$	mass

initial condition is shown as a mirror image of the actual true state initial condition. This choice was made for two reasons. The first reason for using the same poor *a priori* estimate in all of the examples is so that the relative performance of the filtering algorithms can be compared. A second reason is to show that it is not necessary to have a good *a priori* estimate for the filter to converge. This fact lends credence to using optimal filtering in actual applications.

4. *Parameter values.* The parameter values and relations listed in Table 1 are used in all three examples and were chosen for illustration purposes. The units are left as arbitrary to reflect this. Although not actual experimental data, they are of reasonable form. These values were selected as they model a process undergoing significant dynamics. The filter's potential is demonstrated in that the algorithm is shown to be effective under these extreme conditions.

5. *Covariance (weighting) matrices.* The covariance matrices weight the individual terms in the quadratic least-squares error criterion, Eq. 19. Throughout the examples that follow, the spatial domain is discretized into 60 evenly distributed radius sizes. This means that $Q(\tau)$ and P_0 are 60 × 60 matrices. Because a lumped approach has been taken, all of the off-diagonal elements in these matrices are zero. It is the off-diagonal elements that provide the mathematical communication between neighboring locations in the spatial domain: the communication that is assumed not to exist when a lumped approach is employed.

The diagonal terms in these matrices can be defined by the relations:

$$Q_{\text{diag}}(r_n, r_n, \tau) = d_Q \tag{29}$$

$$P_{0\ \text{diag}}(r_n, r_n) = d_p \tag{30}$$

for $n = 1, \ldots, 60$. Different numbers of measurements are considered in the examples so the size of $R(t)$ will vary, though it will also be diagonal, i.e.,

$$R_{\text{diag}}(r_m, r_m, \tau) = d_R \tag{31}$$

for $m = 1, \ldots, M$, where M is the number of discrete measurements that span the spatial domain.

Example 1

A continuous PSD measurement is such that the discretized measurement vector $Z(\tau)$ contains a value for each of the 60 states (radius sizes) at every time step. For simplicity, consider that the measured values are in the same units as the states. M, the modeling matrix, is therefore a 60 × 60 identity matrix, i.e., a matrix with a diagonal of 1's and all off-diagonal terms of zero.

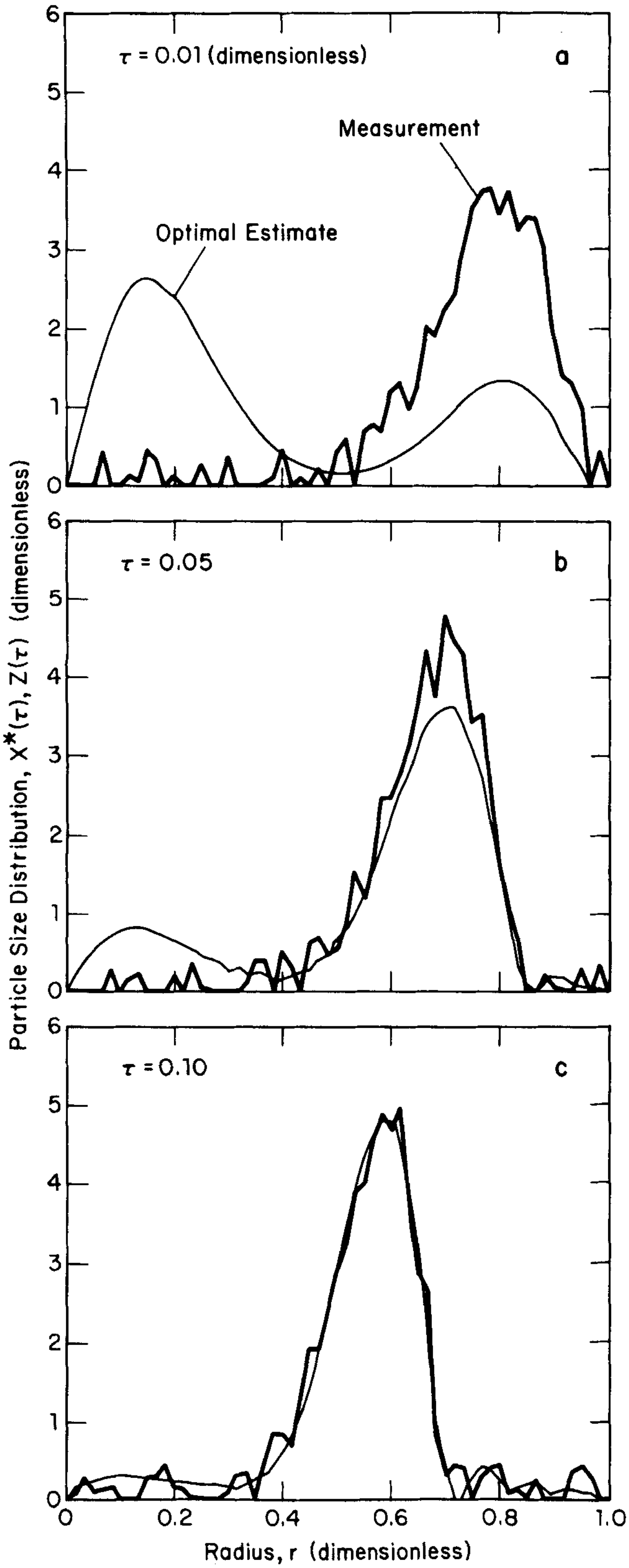

Figure 4. 60 measurements, good model: $d_Q = d_R = 0.01$; $d_P = 0.10$.

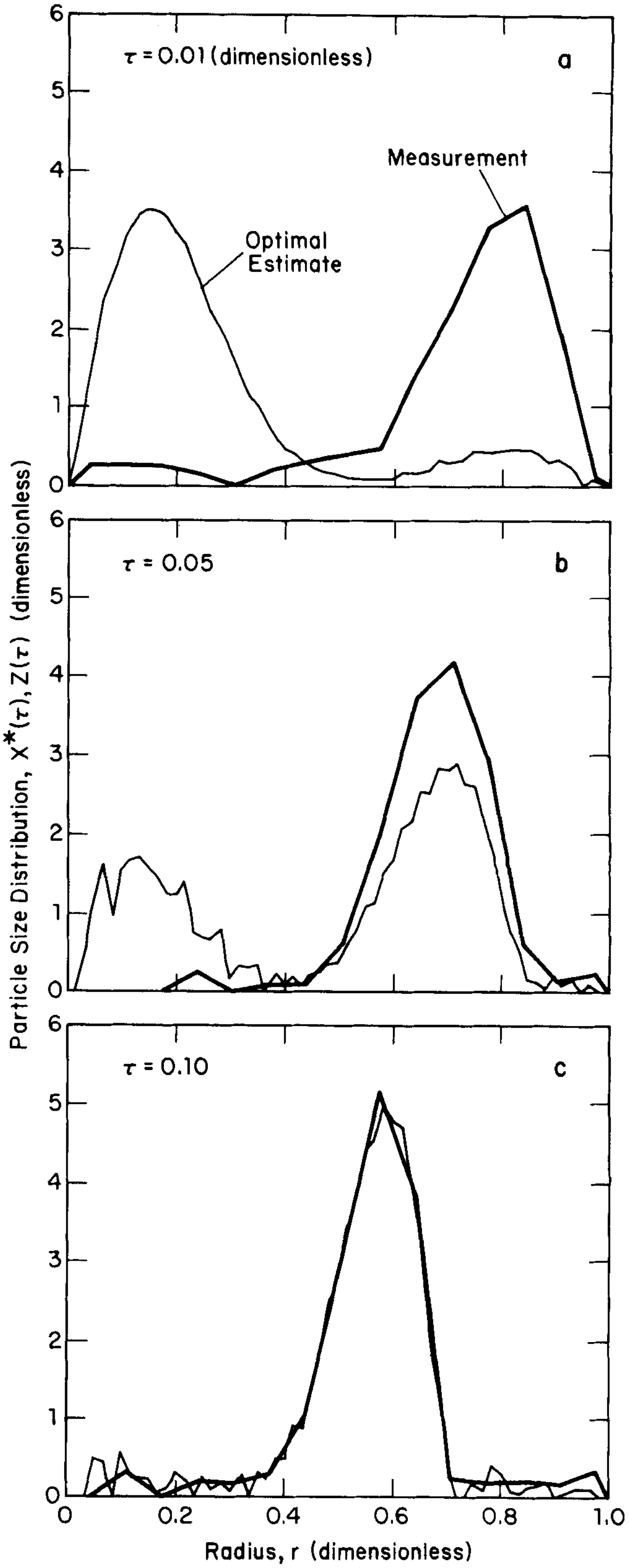

Figure 5. 15 measurements, good model: $d_Q = d_R = 0.01$; $d_P = 0.10$.

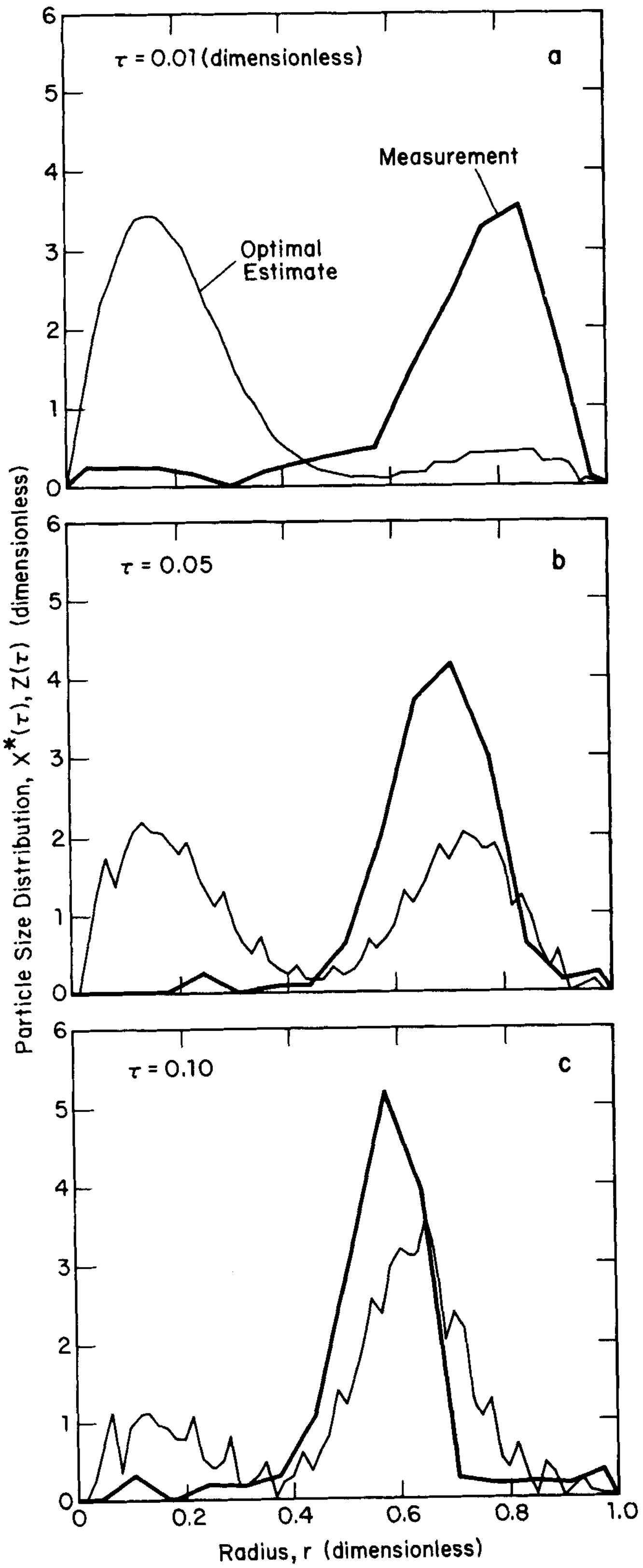

Figure 6. 15 measurements, bad model: $d_Q = d_R = 0.01$; $d_P = 0.10$.

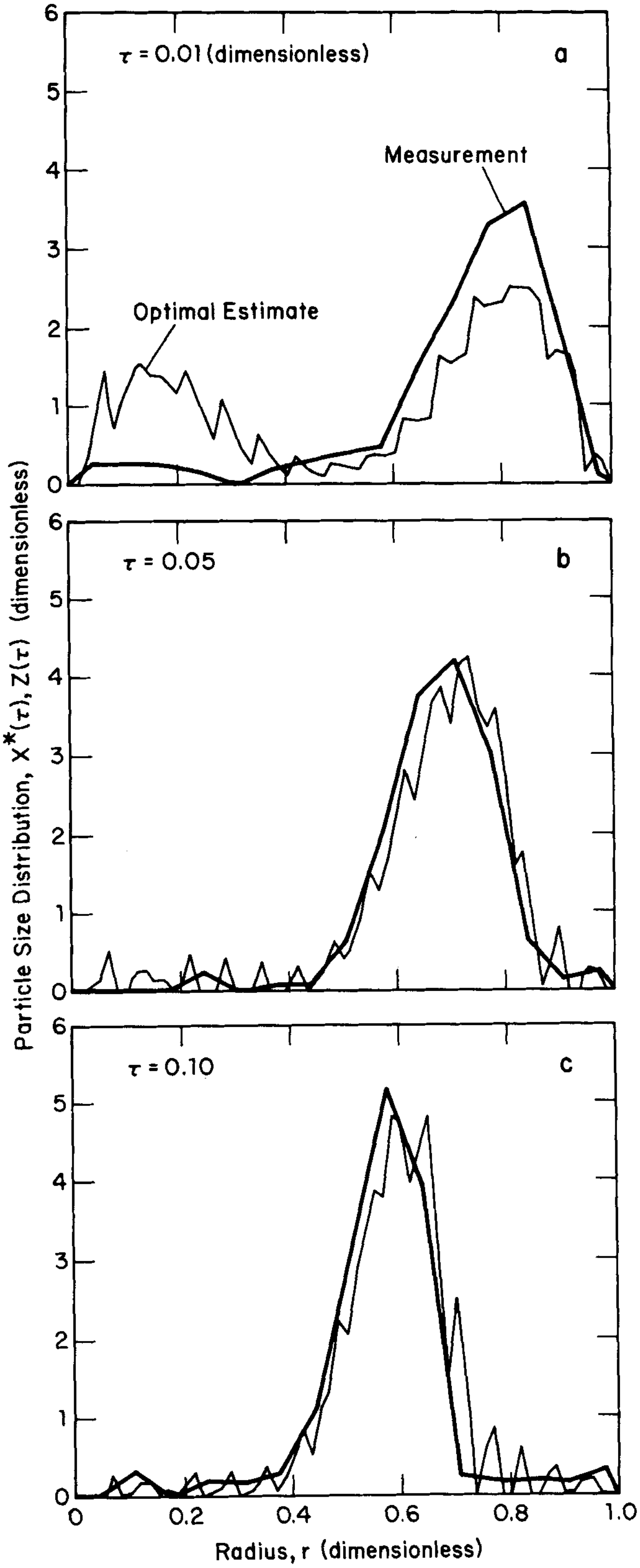

Figure 7. 15 measurements, bad model: $d_R = 0.001$; $d_Q = d_P = 0.10$.

The results presented are for the case where the state model predictions and the measured values are both considered to be reasonably accurate measures of the true state of the system. The *a priori* initial state estimate, however, is considered to be relatively poor. To reflect this, assign the values $d_R = d_Q = 0.01$ and $d_P = 0.01$ (larger values reflect a larger error).

Solution of Eq. 24 via Euler integration yields the optimal filtered estimate. The performance of the filtering algorithm over time can be seen in the results presented in Figure 4 for the dimensionless times $\tau = 0.01$, 0.05, and 0.10. In these figures the optimal estimate is shown to converge toward the noisy measurements, and it is virtually converged by time $\tau = 0.10$. Although not shown, the optimal estimate continues to track the measurements in a smooth, well-behaved manner for time $\tau > 0.10$.

Example 2

A continuous PSD measurement is such that the discretized measurement vector $Z(\tau)$ contains 15 values that span the 60 states at every time step. Each of the 15 PSD measurement values is such that it is the average of four states. The measured values are again in the same units as the states, M is therefore a 15×60 matrix with the form:

$$\mathbf{M} = \begin{bmatrix} 0.25 & 0.25 & 0.25 & 0.25 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.25 & 0.25 & 0.25 & 0.25 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0.25 & 0.25 & 0.25 & 0.25 \end{bmatrix} \quad (32)$$

The assumptions relating to the accuracy of the individual components of the error criterion are the same as in the previous example, thus $d_R = d_Q = 0.01$ and $d_P = 0.10$. Solution of the simultaneous filter equations via Euler integration yields the results shown in Figure 5 for the dimensionless times $\tau = 0.01$, 0.05, and 0.10. The optimal estimate shows distortion at the points where the measurement groups meet, but the optimal estimate still converges on the noisy measurements in a well-behaved fashion. The estimate is again virtually converged by time $\tau = 0.10$.

The distortion may be somewhat disconcerting to some, and the measured values may appear more well-behaved to them on the converged plot. Note, however, that the term "well-behaved" refers to the transition from one time period to the next. A distorted estimate is not the same as a wildly fluctuating one, as is illustrated in Figure 2. The distortions are amplified due to the very poor initial estimate that must be compensated for by the filtering algorithm. The distortions will smooth out somewhat as the optimal estimate remains converged on the measurements for a period of time. A less simplistic definition for M might also enable the filtering algorithm to yield smoother optimal estimates.

Example 3

Up to this point, the dynamic model that was used to derive the filtering algorithm was identical to the one being used to generate the noisy measurements. It is of little surprise, therefore, that the filters performed so well. In this final example, a somewhat more realistic and certainly more illustrative case is presented. Here, the case is considered where a bad model is used in the filtering algorithm.

The bad model is created in a very straightforward yet effective manner. It is the attrition rate that is responsible for the dynamics in these examples because the feed PSD is the same as the initial bed PSD (see Table 1). With a zero attrition, the bed PSD would not change. A bad model can be created by using a different attrition rate in the filtering algorithm than the one used in the model generating the noisy measurements.

In this example, a value of $k = 0.25$ is used in the filtering algorithm. The value of $k = 0.75$ continues to be used in the model generating the noisy measurements. This difference in the attrition rates has a dramatic effect, with the filtering algorithm substantially underestimating the true dynamics.

As in the previous examples, the values $d_R = d_Q = 0.01$ and $d_P = 0.10$ are used, implying that the dynamic model is equally accurate in predicting PSD behavior as the measurements. Figure 6 shows that the filter performance is quite unsatisfactory. The bad model causes the optimal estimate to lag behind the noisy measurements. By dimensionless time $\tau = 0.10$, the optimal estimate is far from being converged.

If the inadequacy of the dynamic model is acknowledged by assigning the value $d_Q = 0.10$ (i.e., large error in the model) and $d_R = 0.001$ (i.e., small error in the measurements relative to the model), the filter performance is substantially improved, as shown in Figure 7. The optimal estimate, though still lagging behind the measurements, is nearly converged by time $\tau = 0.10$.

CONCLUDING REMARKS

The application of optimal estimation theory to obtain a high-quality on-line measure of particle size distribution (PSD) in a fluidized bed has been presented. Optimal estimation theory provides a mathematical basis for obtaining an accurate, well-behaved measure of PSD in real time. These qualities are desirable in a measure of PSD if it is being monitored during process operation, and they are necessary if the measure is being used in computer control applications.

One comment often made by the newly initiated is that an approach such as time averaging of the noisy measurements is much easier to implement and seemingly as accurate. There are significant differences between the two approaches, however. One important difference is that time averaging can introduce a substantial lag in the tracking capabilities of the estimate because the average carries the weight of previous measurements. This lag can be reduced by "forgetting" older data, but this is a trade-off against reducing the noisiness. A large lag can result in a large estimate error during periods of substantial dynamics. Another difference is evident in the case where measurements are discrete in time (not developed in this work but a straightforward extension) or when a significant delay exists between the time of sampling and the time the measured value is available to the computer (a more challenging application). Optimal estimation theory provides a specific framework for computing the optimal real-time estimate in such cases.

Probably the most important benefit from using optimal estimation theory is that it provides a method for the investigator to build specific knowledge about the physical system into the filtering algorithm. This knowledge is included via the dynamic state model. Thus, the investigator can use actual data that is noisy, discrete in time, and/or delayed in time, yet obtain a measure that is accurate, continuous, well-behaved, and real-time.

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NOTATION

$\mathbf{A}$ = spatial-derivative discrete approximation, defined in Eq. 13
d_P = value for diagonal terms in $\mathbf{P}_0$ matrix, defined in Eq. 30
d_Q = value of diagonal terms in $\mathbf{Q}$ matrix, defined in Eq. 29
d_R = value of diagonal terms in $\mathbf{R}$ matrix, defined in Eq. 31
F_0 = feed rate of solids to fluidized bed, mass/time
F_1 = overflow discharge rate of solids from fluidized bed, mass/time
F_2 = entrainment rate of solids from fluidized bed, mass/time
J = quadratic least-squares error criterion, defined in Eq. 19
J_{aug} = augmented form of J, defined in Eq. 20
k = attrition rate constant, 1.0/time, defined in Eq. 4
K = elutriation constant, 1.0/time, defined in Eq. 3
$\mathbf{M}$ = linear modeling matrix, first used in Eq. 15b
M = number of discrete measurements spanning spatial domain
N = number of states (radius sizes) used in discrete approximation
$\mathbf{P}$ = state error covariance matrix, first used in Eq. 23
$\dot{\mathbf{P}}$ = first time-derivative of $\mathbf{P}$, defined in Eq. 24b
$\mathbf{P}_0$ = covariance matrix of $\mathbf{X}_0$, defined in Eq. 18
P_0 = feed PSD
P_1 = overflow discharge PSD
P_2 = entrainment PSD
P_b = fluidized bed PSD
$\mathbf{Q}$ = covariance matrix of $\mathbf{U}$, defined in Eq. 16a
r = dimensionless particle radius (independent spatial variable)
$\mathbf{R}$ = covariance matrix of $\mathbf{V}$, defined in Eq. 16b
R_i = any particle radius bounded by zero and R_{max}
R_{max} = maximum particle radius, dimensionless
t = time
$\mathbf{U}$ = noise vector representing uncertainty in the state model
$\mathbf{V}$ = noise vector representing uncertainty in the measurement model
w = weight of fluidized bed, mass
$\mathbf{X}$ = vector of N discrete fluidized bed PSD's, defined in Eq. 12
$\dot{\mathbf{X}}$ = first time-derivative of $\mathbf{X}$, defined in Eq. 14
$\mathbf{X}^*$ = optimal estimate of system state, first used in Eq. 23
$\dot{\mathbf{X}}^*$ = first time-derivative of $\mathbf{X}^*$, defined in Eq. 24a
$\mathbf{X}_0$ = *a priori* estimate of the system state at initial time
$\mathbf{Z}$ = vector of discretized PSD measurements, defined in Eq. 15b

Greek Letters

α = dynamic PSD model coefficient, defined in Eq. 7
$\boldsymbol{\alpha}$ = spatially discretized matrix representation of α
β = dynamic PSD model coefficient, defined in Eq. 8
$\boldsymbol{\beta}$ = spatially discretized matrix representation of β
δ = Dirac delta function
γ = dynamic PSD model coefficient, defined in Eq. 9
$\boldsymbol{\gamma}$ = spatially discretized vector representation of γ
λ = Lagrange multiplier vector, first used in Eq. 20
$\dot{\lambda}$ = first time-derivative of γ
τ = dimensionless time, defined in Eq. 10
τ_0 = dimensionless initial time
τ_f = dimensionless final time

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