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PROCESS MONITOR DESIGN FOR AN EXTRACTION COLUMN
AN APPLICATION OF ESTIMATION/DETECTION

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PREFACE

The work presented in this report represents some of the initial development of on-line material estimators and diversion detectors as well as code development. More thorough and sophisticated work has been accomplished in [16] and [21].

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ABSTRACT

The NRC Safeguards Program at LLL is directed toward developing a methodology for assessing the effectiveness of material control and accounting systems at processing/reprocessing facilities for special nuclear material. The methodology under development requires many types of mathematical models including performance models of safeguard components. Included in the class of safeguard components are real-time measurement systems which incorporate on-line estimators/detectors for the timely detection of material losses.

Performance modeling generally involves mathematical model development and simulation of the physical process being measured. This report discusses the development of material estimator designs for a liquid-liquid extraction column using a reprocessing application. These designs are applicable to any processing unit which can be adequately represented by linear or nonlinear models in state space form. Although this work is discussed in the context of a plutonium extraction column, it is representative of two classes of safeguard components which are generic to any fuel cycle involving chemical separations/purifications.

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I. INTRODUCTION

With the advent of the energy crisis, alternate means of developing fuel resources have been considered more seriously. Growth in the use of nuclear energy has progressed rapidly over the past decade necessitating the development of fuel fabrication and reprocessing plants. The need to account for and safeguard special nuclear materials (SNM) is obvious. Most current techniques employed in the accounting of SNM can be classified as off-line [1,2,3]; however, recent work has proposed the use of on-line techniques [4,5,6].

Off-line schemes of material accounting are usually based on the periodic calculation of a material balance closure which requires measured material flows and physical inventory [1]. Typically times between closures are quite long, and each closure may even require plant shutdown. Theft or loss is indicated if physical evidence of container tampering exists, the item is missing, or the material balance closure shows a specified threshold exceeded [2,3]. These techniques are not timely because a loss may not be determined for weeks or months, depending on the frequency of closure.

On-line material accounting and diversion detection techniques are characterized by dynamically measuring SNM quantities in critical plant processing units during actual operation. These techniques coupled with sensitive detectors offer a feasible approach to material accounting and detection [4,5,6]. A timely measurement with known accuracy is afforded which may eliminate plant shutdown.

In this report, we discuss the design of a real-time material accounting technique for a liquid-liquid extraction column containing SNM. Accountability of material is accomplished using on-line estimators. The estimators--an extended Kalman filter (EKF) and a linearized Kalman filter (LZKF)--are employed to generate state estimates of the chemical system. The diversion detector--a likelihood ratio device--uses the state estimate to decide whether or not diversion has occurred.

In Section II the development of the liquid-liquid extraction column model is discussed. The state space model developed consists of a system of nonlinear, stiff differential equations. In Section III the estimators are developed and compared. The diversion detector is designed in Section IV and implemented using the estimators. Simulation results are presented.

The following notation is used throughout the text: capital letters typically denote matrices, lower case denote vectors; R is a field; $x \sim X$ means x is distributed X ; $|\cdot|$ is the determinant of $\cdot$; A^T is the transpose of A ; $A:=B$ means A is defined by B ; and $\frac{\partial f(a)}{\partial a}$ is the Jacobian matrix of $f(a)$.

II. DYNAMIC MODEL OF A PULSED EXTRACTION COLUMN

In this section, we develop a model of a pulsed extraction column. The process of concern is nuclear fuel reprocessing using the Purex process, which primarily involves liquid-liquid extraction. After fuel rods are placed in nuclear reactors, they eventually deteriorate to the point where they must be replaced by new rods. Although the spent rods are no longer of use, they contain reusable nuclear material. Fuel reprocessing operations are concerned with salvaging this material for use in the manufacture of additional rods. Fuel pellets are obtained from the rods, chemically dissolved in nitric acid to form an aqueous solution of nitrates, and prepared for the separation process. In the Purex process, plutonium and uranium nitrates are complexed with tributylphosphate-then separated from other fission products by extraction with a suitable organic solvent. These SNM are then treated for final purification by absorption or ion exchange [4].

Liquid-liquid extraction is an operation in which immiscible solutions are brought into contact, and a transfer of solutes (here U and Pu) occurs in a direction (aqueous to organic or organic to aqueous) determined by equilibrium relationships. The liquid-liquid, pulsed extraction column is a chemical processing unit used to bring two immiscible phases (aqueous and organic) into better than usual contact, enhancing the transfer of mass between them by the hydraulic pulsation of the liquid through holes in plates spaced throughout the column. The basic principle involved in this transfer is the fact that complexed nitrates of uranium and plutonium in higher oxidation states are readily soluble in certain organic liquids

(here 15% tributylphosphate (TBP) in kerosene). The nitrates of the remaining fission products are insoluble in the organic liquid; therefore, enabling separation. A representation of a three-stage, four species (U, Pu, HNO_3 , salts) liquid-liquid extraction column is shown in Figure 1.

Development of the dynamic equations governing the physical operation of the column follows under the assumptions that: (i) the dominant rate factor is that of mass transfer, not chemical rate kinetics; and (ii) the heat capacity of the material is not a function of temperature. Writing the mass balance equations for the organic phase concentrations $c_i^o(j)$ of the i-th species at the j-th stage yields

$$\frac{d}{dt} c_i^o(j) = \frac{1}{V_j^o} [v_{j-1} c_i^o(j-1) - v_j c_i^o(j) + K(c_i^*(j) - c_i^o(j))] \quad (2.1)$$

where

V_j^o is the organic phase volume at the j-th stage

v_j is the organic phase flow rate at the j-th stage

K is a rate constant

and $c_i^*(j)$ the ideal equilibrium organic phase concentration. Similarly, the mass balance for the aqueous phase concentration $c_i^a(j)$ of the i-th species at the j-th stage is given by

$$\frac{d}{dt} c_i^a(j) = \frac{1}{V_j^a} [L_{j+1} c_i^a(j+1) - L_j c_i^a(j) - K(c_i^*(j) + c_i^o(j)) + \delta_{kj} F_a c_i^f(k)] \quad (2.2)$$

where

V_j^a is the aqueous phase volume at the j-th stage

L_j is the aqueous phase flow rate at the j-th stage

Figure 1. Extraction Column Model

F_a is the aqueous phase feed flow rate

$c_i^f(k)$ is the aqueous phase feed concentration occurring at the k-th stage

δ_{kj} is the Kronecker delta.

The ideal organic phase concentration of the i-th species at the j-th stage is given by

$$c_i^*(j) = k_i(j)c_i^a(j)(S^2(j) + S(j)\delta_{i3}) \quad (2.3)$$

where

$k_i(j)$ is the distribution coefficient of the i-th species at the j-th stage and $S(j)$ is given by (if the Richardson [7] relationships are used)

$$S(j) = \frac{1}{4 \left(\sum_{k=1}^3 k_k(j)c_k^a(j) \right)} \left[(k_3c_3^a(j) + 1)^2 + 29.2 \left(\sum_{k=1}^3 k_k(j) \right) x_{TBP} \right]^{1/2} - (k_3(j)c_3^a(j) + 1) \quad (2.4)$$

x_{TBP} is the mass fraction of tributylphosphate in hydrocarbon solvent.

The distribution coefficient $k_i(j)$ is the ratio of the concentration of the i-th species at the j-th stage in the organic and aqueous phases and is given for the four species (1 for U^{+6} , 2 for Pu^{+4} , 3 for H^+ , 4 for salts) as:

$$k_1(j) = t_1(T)Z_j y_1(x_{TBP})$$

$$k_2(j) = t_2(T)Z_j y_1(x_{TBP}) [0.2 + 0.55 x_{TBP}^{1.25} + 0.0074 \sum_j^2] \quad (2.5)$$

$$h_3(j) = t_3(T) y_2(x_{TBP}) [0.135 \sum_j 0.82 + 0.0052 \sum_j 3.44]$$

$$h_4(j) = 0$$

where

$$t_e(T) = \exp(\alpha_e(1000./T - 3.3539)), \quad e = 1, \dots, 3$$

$$\alpha_1 = 2.5, \quad \alpha_2 = -0.2, \quad \text{and} \quad \alpha_3 = 0.34,$$

$$\sum_j = 2c_1^a(j) + 2c_2^a(j) + c_3^a(j),$$

$$z_j = 3.7 \sum_j 1.57 + 1.4 \sum_j 3.9 + 0.011 \sum_j 7.3,$$

$$y_1(x_{TBP}) = 4.0 x_{TRP}^{-0.17} - 3.0$$

and

$$y_2(x_{TBP}) = 1.0 - 0.54 \exp(-15.0 x_{TBP})$$

Also writing the energy balance relations for the temperatures $T(j)$ at the j -th stage,

$$\frac{d}{dt} T(j) = [1/(v_j^0 + v_j^a)] [v_{j-1} T(j-1) + z_{j+1} T(j+1) - (v_j + z_j) T(j) + \delta_{j,k} F_a T^f(k)] \quad (2.6)$$

assuming uniform and constant heat capacities of the solutions.

After some minor manipulations, it is possible to obtain the state space representation of the 4-species, 3-stage extraction column consisting of 27 states. The state model takes the following general form

$$\frac{d}{dt} x_t = f(x_t) + g(u_t) \quad (2.7)$$

where x_t is an n vector, $f(\cdot)$ and $g(\cdot)$ are n -vector functions. For this model the expression (2.7) can be simplified to

$$\begin{aligned} f(x_t) &= Fx_t + f_d(x_t) \\ g(u_t) &= Gu_t \end{aligned} \quad (2.8)$$

where $F \in \mathbb{R}^{n \times n}$, $G \in \mathbb{R}^{n \times m}$, and u_t is an m vector.

By defining the state vector as

$$\begin{aligned} x^T := & [c_1^0(2) \dots c_4^0(2) \mid \dots \mid c_1^0(4) \dots c_4^0(4) \mid c_1^a(2) \dots \\ & c_4^a(2) \mid \dots \mid c_1^a(4) \dots c_4^a(4) \mid T(2) \dots T(4)]^T, \end{aligned}$$

we obtain the following linear parts of (2.8)

$$F = \begin{bmatrix} \overline{F_{11}} & \overline{0} & \overline{0} \\ \overline{F_{21}} & \overline{F_{22}} & \overline{0} \\ \overline{0} & \overline{0} & \overline{F_{33}} \end{bmatrix},$$

where

$$F_{11} = \begin{bmatrix} -(\kappa_{12} + v_{22})I & 0 & 0 \\ v_{23}I & -(\kappa_{13} + v_{33})I & 0 \\ 0 & v_{34}I & -(\kappa_{14} + v_{44})I \end{bmatrix},$$

$$F_{21} = \text{diag}(\kappa_{2i}I), \quad i = 2, 3, 4,$$

$$F_{22} = \begin{bmatrix} -\lambda_{22}I & \lambda_{32}I & 0 \\ 0 & -\lambda_{33}I & \lambda_{43}I \\ 0 & 0 & -\lambda_{44}I \end{bmatrix}$$

$$F_{33} = \begin{bmatrix} -(v_2 + l_2) a_2 & l_3 a_2 & 0 \\ v_2 a_3 & -(v_3 + l_3) a_3 & l_4 a_3 \\ 0 & v_3 a_4 & -(v_4 + l_4) a_4 \end{bmatrix}$$

and

$$I \in \mathbb{R}^{4 \times 4}$$

$$\kappa_{1j} = K/V_j^0$$

$$\kappa_{2j} = K/V_j^a$$

$$v_{ij} = v_i/V_j^0$$

$$\lambda_{ij} = l_i/V_j^a$$

$$a_i = 1/V_j^0 + v_i^a$$

Also the nonlinear part of $f(x_t)$ is given by

$$f_d^T(x_t) = [\kappa_{12} c^{*T}(2) \kappa_{13} c^{*T}(3) \kappa_{14} c^{*T}(4) \kappa_{22} c^{*T}(2) \kappa_{23} c^{*T}(3) \kappa_{24} c^{*T}(4)]^T \quad (2.11)$$

for

$$c^{*T}(j) := [c_1^*(j) \dots c_4^*(j)]^T$$

Defining the input vector u as

$$u^T := [c_1^0(1) \dots c_4^0(1) | c_1^f(2) \dots c_4^f(2) | c_1^a(5) \dots c_4^a(5) | T(1) T^f(3) T(5)] \quad (2.12)$$

yields

$$G = \begin{bmatrix} -v_{12}^1 & 0 & 0 & | & & \\ 0 & 0 & 0 & | & & \\ 0 & 0 & 0 & | & & \\ 0 & 0 & 0 & | & 0 & \\ 0 & \beta I & 0 & | & & \\ 0 & 0 & \lambda_{54} I & | & & \\ \hline & 0 & & | & v_{12}^{\alpha_2} & 0 \\ & & & | & 0 & F_a \\ & & & | & & \lambda_{54}^{\alpha_4} \end{bmatrix}$$

Simulation[†] of the three-stage extraction column was accomplished using the DYNOSYL process simulator [8] under the conditions in Table I. Typical product outputs for plutonium and uranium (gm/liter) in both the organic and aqueous phases are shown in Figure 2. Note that for each species, we show the normal plant operation and a diversion of the SNM. The diversion

[†] We chose to simulate the 3-stage, 4-species column in order to keep computer time to a minimum. More stages cause no increase in complexity, but execution time increases.

TABLE 1. SIMULATION PARAMETERS

TIME (HOURS)	0.0 - 10.0	($\Delta T = 0.02$)
NO. OF STAGES/SPECIES/STATES	3 / 4 / 27	
FEED STAGE	3	
FEED CONCENTRATION		
U (GM/%)	200.0	
P _U (GM/%)	7.0	
HNO ₃ (MOLES/%)	2.9	
SALTS (MOLES/%)	0.0	
TBP CONCENTRATION (IN HYDROCARBON)	15%	
RATE CONSTANT	100.0	
TEMPERATURE (°C)	25.0	
PHASE VOLUMES (LITERS)	2.0	
FLOW RATES (L/M)		
FEED	6.0	
AQUEOUS SOLVENT	4.33	
ORGANIC SOLVENT	10.33

Figure 2. Simulated Output Streams for Three Stage Extraction Column with Fixed % Diversions from the Feed Stream

scenario depicted in this figure, is that an upstream theft has occurred causing the input feed flow rate of the column to decrease the annotated percentage.

Effect of the feed change (theft) on the column concentrations is depicted in the figure. Note that the given percentage is related to the time rate of theft, e.g., a 8% diversion of the feed stream corresponds to a decrease of Pu in the organic output of

$$0.08 (6.4/\text{min}) (6.2 \text{ gm/l}) = 3 \text{ gm/min.}$$

Other diversion levels are calculated similarly and depicted in the figure.

This completes the deterministic description of the three-stage extraction column in state space form. Expansion to more stages would be straightforward. The design of on-line estimators for material accounting or diversion detection follows.

III. MATERIAL ESTIMATOR DESIGN

The requirements for accurate material accounting and timely diversion detection which do not require plant shutdown, initiated design efforts on material estimators [4,5]. In this section we develop on-line techniques to estimate the amount of SNM in process using Kalman estimators [5].

Kalman filtering theory applied to models characterized by linear, ordinary, differential equations has been very successful, but when systems of concern are modeled by nonlinear differential equations success has not been as prevalent. Most chemical processes are practically modeled by these nonlinear equations which evolve directly from partial differential equations models discretized over the space coordinates [6]. In this section we will develop the extended and linearized Kalman filters for some classes of Material Control and Accounting (MC&A) components which can be represented by nonlinear differential equations. The EKF is based on a first order Taylor series approximation expanded about the current state estimate, while the linearized filter is expanded about a reference or perturbation trajectory. The linearized filter has the advantage that it possesses the desirable features of a linear filter---off-line precomputation of parameters and the performance capabilities (in some cases) of the EKF. Both filters require a model of the process and measurement before they can be constructed.

In order to account for parameter uncertainty or modeling errors, we include a white, Gaussian process noise source in equation (2.7), i.e.,

$$\dot{x}_t = f(x_t) + g(u_t) + w_t \quad (3.1)$$

where x_t , w_t are n -vectors, $f(\cdot)$, $g(\cdot)$ are n vector functions, and $w_t \sim N(0, Q_t)$.

We assume a discrete measurement scheme, modeling instruments and corresponding accuracies as

$$z_k = h(x_k) + v_k \quad (3.2)$$

where z_k , v_k are p -vector, $h(\cdot)$ is a p -vector function and $v_k \sim N(0, R_k)$.

Recall that the Kalman filter obtains $\hat{x}_{k|k-1} = E\{x_k | \text{past data}\}$, the (minimum variance) estimate of the state x_k^+ at time k based on $k-1$ measurements.

In order to linearize (3.1) we first generate a deterministic reference trajectory (x_t^*, u_t^*) . In practice the reference trajectory is obtained by: (1) developing a mathematical model of the unit, (2) simulating this model, and (3) using the simulation to generate (x_t^*, u_t^*) ; thus

$$\dot{x}_t^* = f(x_t^*) + g(u_t^*). \quad (3.3)$$

Consider deviations from this reference trajectory

$$\delta x_t := x_t - x_t^* \quad (3.4)$$

$$\delta u_t := u_t - u_t^* \quad (3.5)$$

By differentiating (3.4) and substituting (3.1) and (3.3) we obtain the deviation or perturbation trajectory as

$$\dot{\delta x}_t = (f(x_t) - f(x_t^*)) + (g(u_t) - g(u_t^*)) + w_t \quad (3.6)$$

⁺ The state of chemical process can be the concentration or temperature, etc.

Now expanding $f(x_t)$, $g(u_t)$ in a Taylor series about the reference, we have

$$f(x_t) = f(x_t^*) + \frac{\partial f(x_t^*)}{\partial x_t^*} \delta x_t + \text{h.o.t.}$$

$$g(u_t) = g(u_t^*) + \frac{\partial g(u_t^*)}{\partial u_t^*} \delta u_t + \text{h.o.t.} \quad (3.7)$$

Neglecting the higher order terms in (3.7) and substituting in (3.6) we obtain

$$\delta \dot{x}_t = \frac{\partial f(x_t^*)}{\partial x_t^*} \delta x_t + \frac{\partial g(u_t^*)}{\partial u_t^*} \delta u_t + w_t$$

which is in the form of (3.1) and depicted in Figure 3. Similarly for the discrete measurement scheme, applying

$$h(x_k) = h(x_k^*) + \frac{\partial h(x_k^*)}{\partial x_k^*} \delta x_k, \quad (3.8)$$

to the measurement deviation

$$\delta z_k := z_k - z_k^* = z_k - h(x_k^*), \quad (3.9)$$

we obtain

$$\delta z_k = \frac{\partial h(x_k^*)}{\partial x_k^*} \delta x_k + v_k$$

Summarizing, we have linearized a deterministic model using a first order Taylor series approximation for $f(\cdot)$, $g(\cdot)$, $h(\cdot)$ and developed a linearized perturbation model valid for small δx_t given by

[†] The state of chemical process can be the concentration or temperature, etc.

$$x_t^* = \int_0^t [f(x_\tau^*) + g(u_\tau^*)] d\tau \quad (\text{REFERENCE})$$

$$\delta x_t = \int_0^t \left[\frac{\partial f(x_\tau^*)}{\partial x_\tau} \delta x + \frac{\partial g(u_\tau^*)}{\partial u_\tau} \delta u_\tau \right] d\tau \quad (\text{PERTURBATION})$$

FIGURE 3: LINEARIZED DETERMINISTIC SYSTEM

$$\begin{aligned}\dot{\delta x}_t &= F(x_t^*) \delta x_t + G(u_t^*) \delta u_t + w_t \\ z_k &= H(x_k^*) \delta x_k + v_k\end{aligned}\quad (3.10)$$

where $F(\cdot)$, $G(\cdot)$, $H(\cdot)$ are the obvious Jacobians.

The linearized Kalman filter can be derived in a number of ways. Here we choose to present the standard linear algorithm and then modify it to obtain the desired results. For the linearized model, we can apply the standard linear Kalman estimator algorithm [9], which yields

Prediction:

$$\begin{aligned}\dot{\delta \hat{x}}_t &= F(x_t^*) \delta \hat{x}_t + G(u_t^*) \delta u_t^*, \quad t_k \leq t \leq t_{k+1}^+ \\ \delta \hat{\pi}_t &= F(x_t^*) \delta \hat{\pi}_t + \delta \hat{\pi}_t^T F^T(x_t^*) + Q_t\end{aligned}\quad (3.11)$$

Innovation:

$$\begin{aligned}\delta e_{k+1} &= \delta z_{k+1} - H(x_{k+1}^*) \delta \hat{x}_{k+1|k} \\ R_{k+1}^e &= H(x_{k+1}^*) \delta \hat{\pi}_{k+1|k} H^T(x_{k+1}^*) + R_{k+1}\end{aligned}\quad (3.12)$$

Correction:

$$\begin{aligned}K_{k+1} &= \delta \hat{\pi}_{k+1|k} H^T(x_{k+1}^*) \left(R_{k+1}^e \right)^{-1} \\ \delta \hat{x}_{k+1|k+1} &= \delta \hat{x}_{k+1|k} + K_{k+1} \delta e_{k+1} \\ \delta \hat{\pi}_{k+1|k+1} &= \left[I - K_{k+1} H^T(x_{k+1}^*) \right] \delta \hat{\pi}_{k+1|k}\end{aligned}\quad (3.13)$$

[†] We will use $t_k := k$ interchangeably throughout.

where

$$\delta\tilde{\pi} := \text{Cov}(\delta\tilde{x}_{k+1}|k), \quad \delta\tilde{x}_{k+1}|k := \delta x_{k+1} - \delta\hat{x}_{k+1}|k \quad \text{and} \quad \delta x_0 \sim N(\delta\hat{x}_0|0, \delta\hat{\pi}_0|0)$$

This algorithm is not implemented because we want $\hat{x}$ not $\delta\hat{x}$; however, once $\delta\hat{x}$ is known $\hat{x}$ can be found from (x^* is known)

$$\delta\hat{x}_{k+1}|k = \hat{x}_{k+1}|k - x_{k+1}^* \quad (3.14)$$

In fact, it is clear that $\tilde{\pi}_{k+1}|k = \delta\tilde{\pi}_{k+1}|k$, since

$$\delta\tilde{x}_{k+1}|k = \delta x_{k+1} - \delta\hat{x}_{k+1} = x_{k+1} - \hat{x}_{k+1}|k =: \tilde{x}_{k+1}|k \quad (3.15)$$

and of course, $\tilde{\pi}_{k+1}|k := \text{Cov}(\tilde{x}_{k+1}|k)$. Thus, we can merely substitute $\tilde{\pi}$ for $\delta\tilde{\pi}$ in the above equations.

If we substitute (3.14) and (3.3) into (3.11), we obtain

$$\hat{x}_t^* = f(x_t^*) + F(x_t^*) (\hat{x}_t - x_t^*) + g(u_t^*) + G(u_t^*) (u_t - u_t^*) \quad (3.16)$$

The innovations can be found by substituting (3.9) and (3.14) into (3.12), i.e.,

$$e_{k+1} = z_{k+1} - h(x_{k+1}^*) - H(x_{k+1}^*) (\hat{x}_{k+1}|k - x_{k+1}^*)^\dagger \quad (3.17)$$

Finally, the correction equations are found by substituting (3.14) into (3.13)

$$\hat{x}_{k+1}|k+1 = \hat{x}_{k+1}|k + K_k e_k \quad (3.18)$$

[†] Note that $e_{k+1}^* := z_{k+1}^* - h(x_{k+1}^*) = 0$ which implies $\delta e_{k+1} = e_{k+1}$.

These equations are usually implemented rather than those of (3.11) - (3.13) in order to obtain the linearized Kalman filter state estimates since $\hat{x}$ rather than $\delta\hat{x}$ is desired. The algorithm is summarized in Table II. The relationship between these implementations is shown in Figure 4 where $t_k := k$.

If, instead of using the reference trajectory, we choose to linearize about each new estimate as it becomes available, i.e., $x_{k+1}^* = \hat{x}_{k+1|k}^+$, then the EKF algorithm results.

The reason for choosing the estimate to linearize is to use a better reference trajectory as soon as one is available. As a consequence, large initial estimation errors are not allowed to propagate through time; thus, the linearity assumptions are less likely to be violated. So, if we initially linearize about $x_k^* = \hat{x}_{k|k}$, then clearly,

$$\delta\hat{x}_{k+1|k} = \delta\hat{x}_{k|k} = 0$$

or we can say that

$$\delta\hat{x}_{\alpha|k} = 0 \quad k \leq \alpha \leq k+1 \quad \forall k \quad (3.19)$$

i.e., between observations the best estimate of the state is the reference state (from (3.14) using (3.19)) and therefore

$$\dot{\hat{x}}_{\alpha|k} = f(\hat{x}_{\alpha|k}) + g(u_{\alpha}) \quad k \leq \alpha \leq k+1$$

[†] We also choose $u_t^* = u_t$, i.e., we linearize about $(\hat{x}_t, u_t)$.

TABLE II. SUMMARY OF CONTINUOUS-DISCRETE LINEARIZED KALMAN FILTER

State Estimate: $\hat{x}_t = f(x_t^*) + F(x_t^*) (\hat{x}_t - x_t^*) + g(u_t^*) + G(u_t^*) (u_t - u_t^*)$

Error Covariance: $\hat{\pi}_t = F(x_t^*) \hat{\pi}_t + \hat{\pi}_t F^T(x_t^*) + Q_t$

Innovations: $e_{k+1} = z_{k+1} - h(x_{k+1}^*) - H(x_{k+1}^*) [\hat{x}_{k+1|k} - x_{k+1}^*]$

Innovations Covariance: $R_{k+1|k}^e = H(x_{k+1}^*) \hat{\pi}_{k+1|k} H^T(x_{k+1}^*) + R_{k+1}$

Kalman Gain: $K_{k+1} = \hat{\pi}_{k|k-1} H^T(x_k^*) (R_{k|k-1}^e)^{-1}$

State Update: $\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1} e_{k+1}$

Covariance Update: $\hat{\pi}_{k+1|k+1} = (I - K_{k+1} H(x_{k+1}^*)) \hat{\pi}_{k+1|k}$

FIGURE 4. LINEARIZED KALMAN FILTER IMPLEMENTATION

Now using the predicted estimate, $x_k^* = \hat{x}_{k+1|k}$ as our relinearization point, we obtain

$$\delta \hat{x}_{k+1|k+1} = \hat{x}_{k+1|k+1} - \hat{x}_{k+1|k} \quad (3.20)$$

Thus, substituting (3.19), (3.20) and for δz_{k+1} in (3.13) we obtain

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1} \epsilon_{k+1} \quad (3.21)$$

and $\epsilon_{k+1} = z_{k+1} - h(\hat{x}_{k+1|k})$,

$$\hat{x}_{t_{k+1}|t_k} = \hat{x}_{t_k|t_k} + \int_{t_k}^{t_{k+1}} \left[f(\hat{x}_a|t_k) + g(u_a) \right] da$$

These equations with the corresponding error covariance and gain propagation have become known as the extended Kalman filter (EKF) and are used widely with great success to perform state estimation for nonlinear systems. The EKF equations are summarized in Table III.

In order to implement the algorithm it is necessary to specify the system Jacobian matrix. Because of the model structure (2.8) the Jacobian can be decomposed as

$$J = J_{LIN} + J_{NLIN}, \quad (3.22)$$

where the linear part is $J_{LIN} := F$ of (2.8) and

TABLE III. SUMMARY OF CONTINUOUS - DISCRETE EXTENDED KALMAN FILTER

Prediction:

$$\hat{x}_{k+1|k} = \hat{x}_{k|k} + \int_k^{k+1} [f(\hat{x}_{\alpha|k}) + g(\hat{x}_{\alpha|k}, u)] d\alpha$$

$$\tilde{\pi}_{k+1|k} = \int_k^{k+1} [F(\hat{x}_{k|k})\tilde{\pi}_{\alpha|k} + \tilde{\pi}_{\alpha|k}F^T(\hat{x}_{k|k}) + Q_{\alpha}] d\alpha$$

Innovation:

$$e_{k+1} = z_{k+1} - h(\hat{x}_{k+1|k})$$

$$R_{k+1|k}^e = H(\hat{x}_{k+1|k})\tilde{\pi}_{k+1|k}H^T(\hat{x}_{k+1|k}) + R_{k+1}$$

Correction:

$$K_{k+1} = \tilde{\pi}_{k+1|k}H^T(\hat{x}_{k+1|k})(R_{k+1|k}^e)^{-1}$$

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1}e_{k+1}$$

$$\begin{aligned} \tilde{\pi}_{k+1|k+1} &= [I - K_{k+1}H(\hat{x}_{k+1|k})]\tilde{\pi}_{k+1|k}[I - K_{k+1}H(\hat{x}_{k+1|k})]^T \\ &\quad + K_{k+1}R_{k+1}K_{k+1}^T \end{aligned}$$

where

$$F(\hat{x}_{k|k}) := \left. \frac{\partial (f(x) + g(x, u))}{\partial x} \right|_{x=\hat{x}_{k|k}}, \quad H(\hat{x}_{k|k}) = \left. \frac{\partial (h(x))}{\partial x} \right|_{x=\hat{x}_{k|k}}$$

and

$$\tilde{\pi}_{k+1|k} := \text{Cov}(\tilde{x}_{k+1|k}) \text{ for } \tilde{x}_{k+1|k} := x_{k+1} - \hat{x}_{k+1|k}$$

$$x_0 \sim N(\hat{x}_{0|0}, \tilde{\pi}_{0|0})$$

$$J_{NLIN} = \begin{bmatrix} 0 & J_1^0 & J_2^0 & J_3^0 & 0 & 0 \\ 0 & J_1^a & J_2^a & J_3^a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ at } j\text{-th stage,}$$

$$J_j^a = - \left(\frac{v_j^a}{v_j^0} \right) J_j^0$$

and

$$J_j^0 = \left[\frac{\partial f(c_i^0(j))}{\partial c_k^0(j)} \right]_{ik} = \left[\frac{\partial k_i(j)}{\partial c_k^0(j)} c_i^0(j) + k_i(j) \delta_{i,k} \right]$$

$$\bullet (\delta_{i,3} S(j) + S^2(j)) + k_i(j) c_i^0(j)$$

$$\bullet \left(\delta_{i,3} + 2 S(j) \right) \frac{\partial S(j)}{\partial c_k^0(j)}$$

The required partial derivatives can be calculated from

$$\frac{\partial k_1(j)}{\partial c_k^0(j)} = t_1(T) \frac{\partial Z_j}{\partial c_k^0(j)} y_1(x_{TBP})$$

$$\frac{\partial k_2(j)}{\partial c_k^0(j)} = t_2(T) y_1(x_{TBP}) \left\{ \frac{\partial Z_j}{\partial c_k^0(j)} [0.2 + 0.55 x_{TBP}^{1.25} + 0.0074 \sum_j^2] + 0.03 Z_j \sum_j \right\}$$

$$\frac{\partial k_3(j)}{\partial c_k^0(j)} = 2 t_3(T) y_2(x_{TBP}) \left\{ 0.11 \sum_j^{-0.18} + 0.018 \sum_j^{2.44} \right\} \quad (3.23)$$

where $\sum_j$ is given in (2.5) and

$$\frac{\partial Z_j}{\partial c_k^0(j)} = [5.81 \sum_j^{0.57} + 5.46 \sum_j^{2.9} + 0.08 \sum_j^{6.3}] \frac{\partial \sum_j}{\partial c_k^0(j)}$$

Also,

$$\begin{aligned} \frac{\partial S(j)}{\partial c_k^0(j)} &= \left[-\frac{3.65 x_{TBP}}{\psi(j)r(j)} + \frac{(k_3(j)c_3^0(j) + 1) - r(j)}{4\psi(j)^2} \right] \\ &\left[k_k(j) + c^{0T}(j) \frac{\partial k(j)}{\partial c_k^0(j)} \right] + 1/4 \psi(j)k_3(j)\delta_{k3} \\ &+ c_3^0(j) \frac{\partial k_3(j)}{\partial c_3^0(j)} [k_3(j)c_3^0(j) + 1)r(j)^{-1} - 1] \end{aligned} \quad (3.24)$$

where

$$c^{0T}(j) = [c_1^0(j) \dots c_4^0(j)]^T, k^T(j) = [k_1(j) \dots k_4(j)]^T$$

$$\psi(j) = k_1(j)c_1^0(j) + k_2(j)c_2^0(j) + k_3c_3^0(j)$$

$$r(j) = [(k_3(j)c_3^0(j) + 1)^2 - 29.2\psi(j)x_{TBP}]^{1/2}$$

Process measurements for the extraction column are sparse because not much commercial instrumentation exists. However, some recent experimental work [10] has shown that the various concentrations can be measured directly from the final stage output streams. For purposes of this study, we assumed that the class of measurement instrumentation used to obtain

various concentrations could be typified by gamma ray spectrometers (unity gain) with measurement errors ranging between 0.1% to 1% (see [10] - [13]). The measured state variables are the organic and aqueous phase output concentrations and the phase temperature - 11 total measurements. Thus, we have modeled the linear measurement relation

$$z_k = Hx_k + v_k$$

where $\text{Cov}(v_k) = R_k \delta_{j,k}$

$$H = \left[\begin{array}{c|c|c} \begin{array}{c} 0_{11,8} \\ \hline \frac{I_4}{0_{7,4}} \end{array} & \begin{array}{c} 0_{11,8} \\ \hline -\frac{0_{4,4}}{I_4} \\ \hline 0_{3,4} \end{array} & \begin{array}{c} -\frac{0_{8,3}}{I_3} \end{array} \end{array} \right] \quad (3.25)$$

Organic Aqueous Temperatures

Typical noisy simulations of the product output (U^{+6} and Pu^{+4}) are shown in Figure 5 for normal plant operating conditions. Here we chose to simulate a 1% measurement error to be conservative. Thus, the corresponding noise covariance matrix is

$$R = \text{diag} \left\{ 2.25 \times 10^{-2}, 10^{-6}, 10^{-6}, 10^{-6}, 10^{-6}, 10^{-6}, 10^{-6}, 1.6 \times 10^{-1}, 10^{-3}, 10^{-4}, 10^{-4} \right\} (\text{gm/liter})^2$$

Note also that these simulations include process noise inputs (see (3.1)) with corresponding covariance

$$Q = \text{diag} (\sigma_i^2), i \in \underline{16} \text{ and } \sigma_i^2 = 10^{-6} (\text{gm/liter})^2$$

Figure 5. Noisy Product Measurements with Fixed % Diversions from the Feed Stream

Note also that each figure includes a specified signal level. If one were interested in constructing an estimator (if necessary) for accounting or a decision device for detection, the signal-to-noise (SNR) ratio is of prime concern. We define this ratio as

$$SNR_i := \frac{(\text{measurement output signal level})^2}{(\text{measurement noise variance})} = (H^T x_i^T x_i H) R^{-1} \quad (3.26)$$

Since R is diagonal, and with the given structure of H , each signal is decoupled from each other, we obtain for each selected state i

$$SNR_i = \frac{x_i^2}{r_i} \quad (3.27)$$

and

$$SNR_i(\text{db}) = 10 \log SNR_i$$

One should also note the large signal levels for diversion are discernible visually indicating that a good measurement instrument eliminates the need for signal processing algorithms when signal levels are high; however, this is not the case for low SNR (~ 10 db). We implemented the EKF and LZKF algorithms and processed the simulated data in Figure 5 to investigate the performance of both estimators.

To compare performance of the EKF to the LZKF, runs were made using DYNREST [14] under various conditions (normal and diversion) at the stated noise levels of Figure 5. Typical runs of the EKF for normal unit operation are shown in Figure 6 with the product outputs "reconstructed" from the noisy data of Figure 5. These estimates appear to track the true

Figure 6. EKF Runs Reconstructing Column Product

states (see Figure 2) quite well. In fact, the steady state variance of the error associated with the product states as predicted by the filter is

$$\hat{\sigma}_{ii}^{\text{EKF}} = \{ 2.5 \times 10^{-6}, 3 \times 10^{-4}, 10^{-4}, 10^{-6} \}, \quad i = 9, 10, 16, 17 \quad (\text{gm/l})^2$$

Some typical runs of the LZKF were performed over the same measurement data. The first set of runs used a near perfect reference trajectory, i.e., the simulated process model and measurement system outputs were contaminated respectively with a $\{w\}$ and $\{v\}$ of variance 10^{-10} . Using this reference trajectory, we see (Figure 7) that the LZKF appears to perform quite well - almost identical to the EKF. This result is expected due to the perfect reference. The predicted error variance for this run was

$$\hat{\sigma}_i^{\text{LZKF}(1)} = \{ 1.2 \times 10^{-2}, 8.2 \times 10^{-5}, 1.3 \times 10^{-3}, 3.9 \times 10^{-4} \}, \quad i = 9, 10, 16, 17 \quad (\text{gm/l})^2$$

Similar runs were accomplished using as reference trajectory the steady state value of the states, i.e., a constant reference. Obviously, this run is more realistic, since a good steady state value of the process output is known quite well. As expected, the state estimates during the transient phase of operation is poor, caused by the fact that the constant reference is not a good model during this period; however, as the process reaches steady state, the LZKF estimator appears to track quite well (see Figure 8). The predicted error variance for this run was

Figure 7. LZKF Runs Reconstructing Column Product
(...with ~ Perfect Reference Trajectory)

Figure 8. LZKF(2) Runs Reconstructing Column Product with Constant Reference Trajectory

$$\hat{\pi}_i^{\text{LZKF}(2)} = \{ 9 \times 10^{-4}, 1 \times 10^{-6}, 1.1 \times 10^{-3}, 1.8 \times 10^{-6} \}, \quad i = 9, 10, \\ 16, 17 \quad (\text{gm/g})^2$$

It is of interest to compare the two LZKF runs with constant reference trajectories. We see that some of the tracking inaccuracies during the transient phase can be decreased by "opening" the bandwidth of the filter (adjusting Q), i.e., the wider bandwidth selected (Figure 9) appears to track better in transient phase than that of Figure 8. However, in steady state there is more uncertainty indicated by the lack of smoothness. In Figures 10 and 11, we show the respective innovations for both runs. Note that LZKF(3) tracking appears better than LZKF(2) because generally the innovations are smaller initially (peaks during transient) and appear less biased.

Table IV summarizes the respective error variances for these runs. As expected, the EKF appears to perform slightly better than the LZKF filters.

The final comparison of the EKF and the LZKF(1) is their signal enhancement capability when used as part of an estimator-correlator [15] for diversion detection. Many different detectors can be built; however, simple construction results when the inputs are independent and uncorrelated. If we view the EKF and LZKF(1) filters merely as "whitening" filters[†] which have as input the correlated measurements $\{z_k\}$ and as output the uncorrelated innovations $\{\epsilon_k\}$, we would like to measure how well they perform. For this comparison, we define the following SNR,

[†] Here we mean a device producing an independent sequence.

Figure 9. LZKF(3) Runs Reconstructing Column Product with Constant Reference Trajectory

Figure 10. LZKF(2) Innovations for Column Products with Constant Reference Trajectory

Figure 11. LZKF(3) Innovations for Column Products with Constant Reference Trajectory

TABLE IV. FILTER PERFORMANCE COMPARISON

	<u>EKF</u>	<u>LZKF(1)</u>	<u>LZKF(2)</u>	<u>LZKF(3)</u>
$\tilde{\pi}_9$	2.5×10^{-6}	1.2×10^{-2}	9×10^{-4}	1.2×10^{-2}
$\tilde{\pi}_{10}$	$3. \times 10^{-4}$	8.2×10^{-5}	$1. \times 10^{-6}$	8.2×10^{-5}
$\tilde{\pi}_{16}$	$1. \times 10^{-4}$	1.3×10^{-3}	1.1×10^{-3}	2×10^{-3}
$\tilde{\pi}_{17}$	$1. \times 10^{-6}$	3.9×10^{-4}	1.8×10^{-6}	1.34×10^{-7}

$$SNR_{\epsilon} := E \left\{ \epsilon^T \epsilon \right\} [R^{\epsilon}]^{-1}$$

or since the $\{\epsilon_k\}$ are independent

$$SNR_{\epsilon}^i := E \left\{ \epsilon_i^2 \right\} / r_i^{\epsilon} \quad (3.28)$$

Typical operation of these filters in a safeguards application is concerned with the ability of the filter to track the diversion of SNM that has not been modeled. A complete discussion of this problem is beyond the scope of this report (see Candy, et al. [16] for details). However, it is important to note that the filter can be "tuned" to track diversions rapidly (timeliness) at the cost of accuracy (state detection) or it can be "detuned" to enhance the model mismatch between estimator model and diversion scenario, thereby increasing the SNR_{ϵ} (innovations detector). In this report, we chose to investigate the latter. The simulations of these filters for a 6% diversion of SNM from the feed are depicted in Figures 12 and 13. As expected, we see the innovations become biased at the diversion time indicating a model mismatch. The filter performances appear reasonably close with the EKF better. Table III shows the calculated SNR_{ϵ} .

It appears that the EKF performs better than the LZKF in most cases; however, the tradeoff is increased computational complexity. In the next section we use these "whitening" filters to implement an on-line diversion detector.

Figure 12. EKF Innovation Signal Enhancement for 6% Diversion Run

Figure 13. LZKF(1) Innovation Signal Enhancement for 6% Diversion Run

TABLE III. COMPARISON OF EKF AND LZKF FOR INNOVATIONS SIGNAL ENHANCEMENT

	<u>EKF</u>	<u>LKZF(1)</u>
SNR (db)		
ϵ_1	0.45 (-3.5)	0.3 (-5.3)
ϵ_2	4.8 (6.85)	0.047 (-13)
ϵ_8	87.8 (19.4)	55.9 (17.4)
ϵ_9	10.0 (1.0)	0.65 (-1.8)

IV. DIVERSION DETECTOR DESIGN

The requirements for accurate and timely diversion detectors which may not require plant shutdown initiated design efforts on material estimators [4,5]. In this section we develop an on-line technique to detect diversion. The design philosophy is based on robustness; therefore, techniques to model specific diversion schemes are not considered [5].

We must depend on the measurement sequence $\{z_k\}$ to extract state information; therefore, a detector must be based on the measurements directly. Consider the following binary decision problem of choosing between two hypothesis

$$H_1: z_k = h(x_k) + v_k \quad (4.1)$$

$$H_0: z_k = h(\bar{x}_k) + v_k$$

where $\bar{x}_k$ is a nominal (deterministic) reference trajectory. Note that accepting H_1 corresponds to a diversion while accepting H_0 corresponds to normal plant operation.

We choose a likelihood ratio detector because of its optimality properties and performance [17]. Recall that the likelihood ratio of $Z(N) := \{z_1, \dots, z_N\}$ is

$$L(Z(N)) := \frac{p(Z(N)|H_1)}{p(Z(N)|H_0)} \quad \begin{array}{l} \text{accept } H_1 \\ > \\ \text{accept } H_0 \end{array} \quad (4.2)$$

where T is defined as the threshold of the test. Applying Bayes' rule [18] to $L(Z(k))$ yields

$$L(Z(k)) = L(Z(k-1)) \frac{p(z_k|Z(k-1), H_1)}{p(z_k|Z(k-1), H_0)},$$

and taking logarithms gives the recursion

$$\Lambda(k) = \Lambda(k-1) + \ln p(z_k|Z(k-1), H_1) - \ln p(z_k|Z(k-1), H_0) \quad (4.3)$$

where $\Lambda(k) := \ln L(Z(k))$. The reason for this formulation rather than (4.2) is that we desire a decision to be made (if possible) as each measurement becomes available. The basis of such a formulation is the Wald test [19].

In order to construct the detector, the conditional densities in (4.3) must be specified. Clearly, under H_0 we have

$$p(z_k|Z(k-1), H_0) = (2\pi)^{-p/2} |R_k|^{-1/2} \exp \left\{ -1/2 (z_k - h(\bar{x}_k))^T R_k^{-1} (z_k - h(\bar{x}_k)) \right\}, \quad (4.4)$$

since $v_k \sim N(0, R_k)$.

Unfortunately the density $p(z_k|Z(k-1), H_1)$ is not easily determined; however, using a pseudo Bayes approximation--i.e., assume the required density is Gaussian--it is possible to derive approximate expressions [15]. Thus, we need only specify the first two moments,

$$E \{ z_k | Z(k-1), H_1 \} = E \{ h(x_k) | Z(k-1) \} =: \hat{h}(x_k)^+$$

⁺ The crucial point to note is that we do not have $h(x_k)$ available to construct H_1 (and never will for diversion); therefore, we must estimate it with $\hat{h}(x_k)$.

and

$$\text{Cov}(z_k | Z(k-1), H_1) = E \left\{ \tilde{h}(x_k) \tilde{h}^T(x_k) | Z(k-1), H_1 \right\} + R_k \quad (4.5)$$

where

$$\tilde{h}(x_k) := h(x_k) - \hat{h}(x_k)$$

These statistics can be expressed in terms of the innovations sequence $\{\epsilon_k\}$. This sequence is zero mean, Gaussian with covariance [20].

$$R_e(k|k-1) := \text{Cov}(\epsilon_k | Z(k-1), H_1) = \text{Cov}(z_k | Z(k-1), H_1) \quad (4.6)$$

The detector can be constructed using the innovations as

$$\begin{aligned} \Lambda(k) = & \Lambda(k-1) + \ln |R_e(k|k-1)|^{-1/2} - \ln |R_k|^{-1/2} - 1/2 \epsilon_k^T R_e^{-1}(k|k-1) \epsilon_k \\ & + 1/2 (z_k - h(\bar{x}_k))^T R_k^{-1} (z_k - h(\bar{x}_k)) \end{aligned} \quad (4.7)$$

Examining this relation it is apparent that the innovation and its corresponding covariance must be specified, we use the EKF and LZKF of the previous section for this purpose.

The implementation of the reference detector is straightforward, once the estimator has been developed. Note that the estimator is included for two purposes. First, for use in a possible "dynamic" material accounting scheme and secondly, to enhance the SNR employed by the reference detector. For example, if we consider the SNR at the output of the estimator, we define

$$SNR = E(\hat{x}^T \hat{x}) \bar{\pi}^{-1} \quad (4.8)$$

or assuming that the states are uncorrelated

$$SNR_i = \frac{E(\hat{x}_i^2)}{\bar{\pi}_i} \quad (4.9)$$

For this measure to be meaningful, we must be assured that the filter is tracking the true value (x) and therefore the error covariance $\bar{\pi}$ predicted by the filter is accurate. For normal runs, Table V shows the filter signal enhancement compared to the original measured signals.

The SNR of (4.9) is only a valid measure of filter performance under the above mentioned conditions. Consider the operation of the reference detector. During normal plant operation, we expect the filter to track the reconstructed states very well in steady state. Therefore, the sequential detector should indicate a no decision (select another sample) or select H_0 (the reference) as more samples are available. During a diversion scenario, we expect the detector to select H_1 , since the reference trajectory is no longer valid and eventually (depending on filter bandwidth)[†] start to track the diversion. Note that no attempt is being made here to do an exhaustive study of diversion detector performance. The input SNR simulated are quite large for practical interpretation of these results. We merely indicate a few interesting facts.

[†] See Candy et al. [16] for a complete discussion of these tradeoffs.

TABLE V. SNR COMPARISON OF MEASUREMENT DATA AND KALMAN FILTERS

	<u>Z (db)</u>	<u>EKF (db)</u>	<u>LZKF(1) (db)</u>	<u>LZKF(3) (db)</u>
SNR ₁	4×10^4 (46)	3.6×10^8 (85)	7.5×10^4 (49)	7.5×10^4 (49)
SNR ₂ [†]	29×10^4 (45)	9.6×10^1 (20)	3.5×10^2 (26)	3.5×10^2 (26)
SNR ₈	4.5×10^4 (47)	7.3×10^7 (79)	5.6×10^6 (67.5)	3.6×10^6 (65.6)
SNR ₉	1.5×10^4 (42)	1.5×10^7 (72)	3.8×10^4 (46)	1.1×10^8 (80.5)

where the measurement $SNR := x_i^2 / r_i$ and the filter $SNR := E\hat{x}_i^2 / \hat{r}_i$

[†] The reason for the large tracking error here is unknown. It appears to be an oversight in tuning the filters. LZKF(2) enhanced the signal at 45 db (see Table IV).

The reference detector was applied to the simulated feed diversion scenario to briefly study the feasibility of such a device. Feed flow diversions of 2%, 4%, 6%, and 8% were simulated and supplied as input to the sequential reference detector using the EKF for signal enhancement. For this simulation, we define the input SNR of interest as

$$SNR_{in} := (H \Delta x \Delta x^T H^T) R^{-1}$$

where $H \Delta x$ is the actual measured change from steady state caused by the diversion (see Figure 2); or component-wise due to the diagonal structure above we have

$$SNR_i := \Delta x_i^2 / r_i \quad i = \underline{11}$$

Calculation of the above SNR reveals that the input is highly dominated by the eighth measurement (Pu in aqueous phase); therefore, we will use

$$SNR_8 \approx SNR = \Delta x_8^2 / r_8$$

as our measure of input signal-to-noise. Figure 14 reveals the performance of the reference detector (with EKF) for the above mentioned diversion. Note that only the decision function is depicted to indicate the change when a diversion occurs. In all but the 2% case did the function change significantly during the diversion. This change implies that for given thresholds the detector would decide that a diversion took place except for the data record length used in the 2% diversion simulation.

Figure 14. Simulated Reference Detector Runs for Feed Flow Diversion Using an EKF

Finally, we compare the performance degradation of replacing the EKF by LZKF(1) and LZKF(3) in the reference detector. Here we choose an arbitrary threshold of .10. Figure 15 shows the respective decision function for a 6% feed diversion. We note in all cases the diversion was detected at the given threshold; however, the detection times varied. These times are given in Table VI for comparative purposes. Again we see that the detector with the EKF responds more quickly as expected. This completes the discussion of the diversion detector feasibility study.

Figure 15. Reference Detector Runs for 6% Feed Diversion Using EKF and LZKF Signal Enhancement

TABLE VI. DETECTION RESPONSE TIME FOR EKF AND LZKF SIGNAL ENHANCERS

Detection Response Time (Hours)	
EKF	0.7
LZKF(1)	0.98

V. SUMMARY

In this report we have developed a simplified dynamic model for a three-stage extraction column, simulated its operation under normal and abnormal conditions using DYNOSYL [8], and applied it in a safeguards feasibility study. On-line dynamic estimators were implemented using DYNEST [14] and used to enhance various signal-to-noise ratios for material accounting as well as diversion detection studies. Simulation runs were accomplished with high SNR (~ 45 db) in order to study the performance of the extended and linearized Kalman filters. The EKF performance appeared superior to various LZKF; however, the degradation in detection performance using the LZKF did not appear intolerable.

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