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Nonlinear Filters for State Estimation of UV Flash Processes

Tobias K. S. Ritschel and John Bagterp Jørgensen

Abstract—We describe four algorithms for state estimation of stochastic differential-algebraic equations. We consider the extended Kalman filter, the unscented Kalman filter, the particle filter, and the ensemble Kalman filter. The differential-algebraic equations that we consider are in a semi-explicit index-1 form. Models of dynamic UV flash processes are in such a form. The UV flash is relevant to rigorous models of many chemical phase equilibrium processes because it is a mathematical representation of the second law of thermodynamics. State estimation is relevant to model predictive control, model identification, fault detection, monitoring, and prediction. State estimation of UV flash processes is therefore important to safe and economical operation of processes such as flash separation, distillation, multiphase flow in pipelines, and oil production. We compare the accuracy and efficiency of the four filters using a numerical example that involves a UV flash separation process. Furthermore, we demonstrate that the filters can be used as soft sensors that estimate the vapor-liquid composition of the separation process based on temperature and pressure measurements.

I. INTRODUCTION

State estimation is concerned with the reconstruction of state variables based on measurements and a model of the relevant process. State estimation is important to model predictive control, model identification, monitoring, prediction, and fault detection of chemical processes [1]. State estimation has been applied to many chemical processes including stirred tank reactors [2]–[4], batch reactors [5]–[8], plug-flow reactors [9], [10], fermentation [11], [12], distillation columns [13]–[15], oil and gas flow in pipes [16], and oil production [17]. Many chemical processes involve thermodynamic equilibrium between fluid phases. The phase equilibrium conditions are derived from the second law of thermodynamics, i.e. the entropy of a closed system is maximal when it is at equilibrium. The UV flash is a key component in rigorous models of dynamic phase equilibrium processes. The UV flash has been used to model flash separation [18]–[20], distillation [21], and computational fluid dynamical processes [22], [23]. It is possible to formulate the UV flash problem as an equality-constrained optimization problem [24]. The optimization variables are temperature, pressure, and vapor-liquid composition (in moles). The optimization problem involves constraints on the internal energy, \( U \), the volume, \( V \), and the total amount of moles of each chemical component, \( n \). The solution to the optimization problem maximizes entropy while satisfying the equality constraints.

The corresponding phase equilibrium conditions are the first-order optimality conditions of the optimization problem. Therefore, the phase equilibrium conditions are a set of algebraic equations. Consequently, it is natural to model dynamic phase equilibrium processes with differential-algebraic equations (DAEs). Dynamic optimization algorithms for UV flash processes have recently been developed [25], but state estimation in such systems has not been addressed yet.

Many processes are nonlinear. There exist a number of state estimation algorithms (filters) for nonlinear systems, e.g. the extended Kalman filter (EKF), the unscented Kalman filter (UKF), the particle filter (PF), and the ensemble Kalman filter (EnKF) [26]. The EKF linearizes the nonlinear model and applies the original Kalman filter equations. This linearization can cause the EKF to be imprecise for highly nonlinear systems. The UKF uses deterministic samples to improve the accuracy compared to the EKF. However, the UKF can also suffer from limited accuracy for severely nonlinear systems. The PF uses a set of random samples to approximate the distribution of the states. It can therefore be more precise than the EKF and the UKF. The number of samples in the UKF is fixed whereas the number of samples in the PF is a tuning parameter. The EnKF is a specific particle filter that uses the Kalman filter equations. It has gained attention in oceanography and oil reservoir characterization [27]–[29] where large-scale models are common. There exist alternatives to the above filters, e.g. moving-horizon estimation [30], and algorithms based on neural networks [31]. State estimation algorithms were originally developed for stochastic difference and stochastic differential equations. However, it is natural to model many processes with DAEs. That is because algebraic equations often arise when a fast process is approximated as a quasi-steady-state process. For instance, it is common to assume that systems reach thermodynamic phase equilibrium instantaneously. Recently, authors have developed the EKF [32]–[34], the UKF [35]–[39], PFs [40], [41], and the EnKF [42] for DAE models.

In this work, we present the EKF, the UKF, the PF, and the EnKF for state estimation of dynamic UV flash processes. We model the UV flash processes with semi-explicit index-1 stochastic DAEs. We compare the accuracy of the four filters with a numerical example that involves flash separation of a hydrocarbon mixture. In the example, the states are estimated based on temperature and pressure measurements. Furthermore, we demonstrate that such state estimates can be used for soft-sensing of the vapor-liquid composition of the mixture.

This paper is structured as follows. We describe the semi-explicit index-1 stochastic DAE form that we consider in
Section II. In Section III, we describe the numerical solution of stochastic DAEs in such a form. In Section IV, we describe the EKF, and in Section V, we describe the UKF. We describe the PF in Section VI and the EnKF in Section VII. In Section VIII we describe the model of the UV flash separation process, and in Section IX, we present the numerical example. We present conclusions in Section X.

II. STOCHASTIC SEMI-EXPLICIT INDEX-1 DAE SYSTEMS

In this work, we consider stochastic DAEs in the form
\[ G(x(t), y(t), z(t)) = 0, \]
\[ dx(t) = F(y(t), u(t))dt + \sigma(y(t), u(t))d\omega(t). \]

\(x(t)\) is a vector of state variables, \(y(t)\) is a vector of algebraic variables, and \(z(t)\) is a vector of adjoint algebraic variables. The algebraic equations (1a) are formulated such that they can represent phase equilibrium conditions. The stochastic differential equations (1b) are formulated such that they can represent conservation equations. We assume knowledge of the manipulated inputs, \(u(t)\), and the initial distribution of the states, \(x(t_0) \sim N(x_0, P_0)\). \(\omega(t)\) is a standard Wiener process, i.e., its incremental covariance is \(Idt\). It is possible to solve the algebraic equations (1a) for \(y(t)\) and \(z(t)\) when \(x(t)\) is specified. We obtain measurements, \(y^m(t_k)\), of the outputs, \(z^m(t_k)\), at discrete times, \(t_k\):
\[ z^m(t_k) = H(y(t_k)), \]
\[ y^m(t_k) = z^m(t_k) + v(t_k). \]

The measurement noise, \(v_k = v(t_k)\), follows a normal distribution, i.e., \(v_k \sim N(0, T_k)\).

III. NUMERICAL SIMULATION

In order to solve the stochastic DAE (1), we discretize the stochastic differential equations with a semi-implicit scheme. We discretize the deterministic and stochastic part with Euler’s implicit and explicit method, respectively. We split the time interval between the \(k\)’th and the \(k + 1\)’th measurement into \(N_t\) time steps. For each time step, we solve the residual equations, \(R_{k,n+1} = 0\), for \(w_{k,n+1} = [x_{k,n+1}; y_{k,n+1}; z_{k,n+1}]\) where the residual function is
\[ R_{k,n+1} = R_{k,n+1}(w_{k,n+1}) = R_{k,n+1}(x_{k,n+1}, y_{k,n+1}, z_{k,n+1}) = R_{k,n+1}(x_{k,n+1}, y_{k,n+1}, z_{k,n+1}; x_{k,n}, y_{k,n}, u_k) = D_{k,n+1} \begin{bmatrix} x_{k,n+1}; y_{k,n+1}; x_{k,n}, y_{k,n}, u_k \end{bmatrix}, \]
and
\[ D_{k,n+1} = D_{k,n+1}(x_{k,n+1}, y_{k,n+1}; x_{k,n}, y_{k,n}, u_k) = x_{k,n+1} - F(y_{k,n+1}, u_k)\Delta t_{k,n} - \sigma(y_{k,n}, u_k)\Delta \omega_{k,n} - x_{k,n}. \]

The increments, \(\Delta w_{k,n}\), are sampled from \(N(0, I\Delta t_{k,n})\). We use Newton’s method to solve the residual equations:
\[ w_{k+1}^{l} = w_{k,n+1}^{l} + \Delta w_{k,n+1}^{l}. \]

We compute the Newton step by solving
\[ M\Delta w_{k,n+1}^{l} = -R_{k,n+1}(w_{k,n+1}^{l}). \]

The iteration matrix is
\[ M \approx \frac{\partial R_{k,n+1}}{\partial u_{k,n+1}} = \begin{bmatrix} I & -\frac{\partial F}{\partial y} & \frac{\partial F}{\partial z} & 0 \end{bmatrix}. \]

A. Efficient solution of the linear system

We exploit the structure of the Jacobian matrix in (7) to solve the linear system (6) efficiently. We compute \(\Delta x_{k,n+1}^{l}\) directly by
\[ \Delta x_{k,n+1}^{l} = \left( \frac{\partial F}{\partial y} \Delta t_{k,n} \right) \Delta y_{k,n+1}^{l} - D_{k,n+1}, \]
and we compute \(\Delta y_{k,n+1}^{l}\) and \(\Delta z_{k,n+1}^{l}\) by solving the reduced linear system,
\[ \tilde{M} \begin{bmatrix} \Delta y_{k,n+1}^{l} \\ \Delta z_{k,n+1}^{l} \end{bmatrix} = \frac{\partial G}{\partial x} D_{k,n+1} - G(x_{k,n+1}, y_{k,n+1}, z_{k,n+1}). \]

The reduced iteration matrix is
\[ \tilde{M} \approx \begin{bmatrix} \frac{\partial G}{\partial y} & \frac{\partial G}{\partial z} \end{bmatrix} \left( \frac{\partial F}{\partial y} \Delta t_{k,n} \frac{\partial G}{\partial y} \right). \]

\(\tilde{M}\) is smaller than \(M\) and is therefore cheaper to factorize.

IV. THE EXTENDED KALMAN FILTER

In this section, we describe the extended Kalman filter. We initialize the filter with the mean and covariance of the initial states:
\[ \hat{x}_{0|0} = x_0, \]
\[ P_{0|0} = P_0. \]

The initial estimates of the algebraic and adjoint algebraic variables satisfy the algebraic equations:
\[ G(\hat{x}_{0|0}, \hat{y}_{0|0}, \hat{z}_{0|0}) = 0. \]

A. Measurement-update

The one-step ahead prediction of the outputs, the measurements, and the covariance matrix are
\[ \hat{z}_{k|k-1} = H(\hat{y}_{k|k-1}), \]
\[ \hat{y}_{k|k-1} = \hat{z}_{k|k-1}, \]
\[ T_{k|k-1} = C_k P_{k|k-1} C_k^T + T_k, \]
where \(T_k\) is the measurement noise covariance matrix, and
\[ C_k = \frac{\partial H}{\partial y}(\hat{y}_{k|k-1}) = \frac{\partial H}{\partial y}(\hat{y}_{k|k-1}) \frac{\partial \hat{y}_{k|k-1}}{\partial \hat{x}_{k|k-1}}. \]

We compute the sensitivities of the algebraic and adjoint algebraic variables by solving
\[ \begin{bmatrix} \frac{\partial G}{\partial y} & \frac{\partial G}{\partial z} \end{bmatrix} \begin{bmatrix} \frac{\partial \hat{y}_{k|k-1}}{\partial \hat{x}_{k|k-1}} \\ \frac{\partial z_{k|k-1}}{\partial \hat{x}_{k|k-1}} \end{bmatrix} = -\frac{\partial G}{\partial x}. \]
The innovation is
\[ e_k = y_k - \hat{y}_k|k-1, \quad (16) \]
and the Kalman filter gain matrix is
\[ K_{fx,k} = P_{k|k-1}C_k' T_{k|k-1}^{-1}. \quad (17) \]
We compute the filtered state and its approximate covariance matrix by
\[ \hat{x}_k|k = \hat{x}_k|k-1 + K_{fx,k} e_k, \quad (18a) \]
\[ P_{k|k} = P_{k|k-1} - K_{fx,k} T_{k|k-1} K_{fx,k}'. \quad (18b) \]
The corresponding estimates of the algebraic and adjoint algebraic variables satisfy
\[ G(\hat{x}_k|k, \hat{y}_k|k, \hat{z}_k|k) = 0. \quad (19) \]
We compute the corresponding covariance matrices by
\[ P_{x,k|k} = \Phi_{yx}(t_k, t_k) P_{k|k} \Phi_{yx}(t_k, t_k)', \quad (20a) \]
\[ P_{z,k|k} = \Phi_{zx}(t_k, t_k) P_{k|k} \Phi_{zx}(t_k, t_k)', \quad (20b) \]
We compute the sensitivities, \( \Phi_{yx}(t_k, t_k) = \frac{\partial \hat{y}_k(t)}{\partial \hat{x}_k|k} \) and
\( \Phi_{zx}(t_k, t_k) = \frac{\partial \hat{z}_k(t)}{\partial \hat{x}_k|k} \), by solving
\[ \begin{bmatrix} \frac{\partial G}{\partial x} \\ \frac{\partial G}{\partial y} \\ \frac{\partial G}{\partial z} \end{bmatrix} \begin{bmatrix} \Phi_{yx}(t_k, t_k) \\ \Phi_{zx}(t_k, t_k) \end{bmatrix} = -\frac{\partial G}{\partial x}. \quad (21) \]
\[ B. \ \text{Time-update} \]
In between measurement \( k \) and \( k+1 \), we propagate the mean by solving the DAE,
\[ \begin{align*}
\dot{x}_k(t_k) &= \hat{x}_k|k, \\
G(\hat{x}_k(t), \hat{y}_k(t), \hat{z}_k(t)) &= 0, \\
\frac{d \hat{x}_k(t)}{dt} &= F(\hat{y}_k(t), u(t)),
\end{align*} \quad (22) \]
for \( t \in [t_k; t_{k+1}] \). The sensitivities, \( \Phi_{xx}(t, s) = \frac{\partial \hat{x}_k(t)}{\partial \hat{x}_k|k} \), \( \Phi_{yx}(t, s) = \frac{\partial \hat{y}_k(t)}{\partial \hat{x}_k|k} \), and \( \Phi_{zx}(t, s) = \frac{\partial \hat{z}_k(t)}{\partial \hat{x}_k|k} \), satisfy
\[ \begin{align*}
\Phi_{xx}(s, s) &= I, \\
\frac{\partial G}{\partial x} \Phi_{xx}(t, s) + \frac{\partial G}{\partial y} \Phi_{yx}(t, s) + \frac{\partial G}{\partial z} \Phi_{zx}(t, s) &= 0, \\
\frac{d \Phi_{xx}(t, s)}{dt} &= \frac{\partial F}{\partial y} \Phi_{yx}(t, s).
\end{align*} \quad (23) \]
The covariance matrix is given in terms of the sensitivities, [33]:
\[ \begin{align*}
P_k(t) &= \Phi_{xx}(t, t_k) P_{k|k} \Phi_{xx}(t, t_k)', \\
&+ \int_{t_k}^{t} \Phi_{xx}(t, s) \sigma(\hat{y}_k(s), u(s)) \sigma(\hat{y}_k(s), u(s))' \Phi_{xx}(t, s)' ds.
\end{align*} \quad (24) \]
C. Numerical solution of the time-update equations
We discretize (22) with Euler's implicit method. For each of the \( N_k \) time steps, we solve the residual equations,
\[ \begin{bmatrix} D_{k,n+1} \hat{x}_{k,n+1} \hat{y}_{k,n+1} \hat{z}_{k,n+1} \end{bmatrix} = 0, \quad (25) \]
where \( D_{k,n+1} = D_{k,n+1} \hat{x}_{k,n+1} \hat{y}_{k,n+1} \hat{z}_{k,n+1} \hat{u}_{k} \) is
\[ D_{k,n+1} = \hat{x}_{k,n+1} - F(\hat{y}_{k,n+1}, \hat{t}_k) \Delta t_k - \hat{x}_{k,n}, \quad (26) \]
and \( \hat{x}_{k,0} = \hat{x}_{k,k} \). We compute the sensitivities by solving
\[ \begin{bmatrix} 1 \\ -\frac{\partial F}{\partial y} \Delta t_k \\ \frac{\partial F}{\partial y} \end{bmatrix} \begin{bmatrix} \Phi_{xx}(t_k, t_k, t_k) \\ \Phi_{yx}(t_k, t_k, t_k) \\ \Phi_{zx}(t_k, t_k, t_k) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \quad (27) \]
We exploit the structure of the system matrix in (27) as we described in Section III-A. We approximate the integral in (24) with a left rectangle rule:
\[ P_{k,n+1} = \Phi_{xx}(t_k, t_k) \tau_k, \quad (28a) \]
\[ \tau_k = P_{k,n} + \sigma(\hat{y}_{k,n}, u_k) \sigma(\hat{y}_{k,n}, u_k)' \Delta t_k, \quad (28b) \]
\[ P_{k,0} = P_{k,k} \]
and the one-step ahead estimates are \( \hat{x}_{k+1|k} = \hat{x}_{k,N_k} \), \( \hat{y}_{k+1|k} = \hat{y}_{k,N_k} \), and \( \hat{z}_{k+1|k} = \hat{z}_{k,N_k} \). The covariance matrix is \( P_{k+1|k} = P_{k,N_k} \).

V. THE UNSCENTED KALMAN FILTER
The initial state estimate and the covariance matrix are
\[ \begin{align*}
\hat{x}_{0|1} &= x_0, \\
P_{0|1} &= P_0.
\end{align*} \quad (29) \]
A. Measurement-update
We compute \( 2n_x + 1 \) samples of the states by
\[ \begin{align*}
\hat{x}_{i+1|k-1} &= \hat{x}_{k|k-1}, \\
\hat{x}_{i+1|k-1} &= \hat{x}_{k|k-1} + \sqrt{c} \left( \sqrt{P_{k|k-1}} \right)_i, \\
\hat{x}_{i+1|k-1} &= \hat{x}_{k|k-1} - \sqrt{c} \left( \sqrt{P_{k|k-1}} \right)_i,
\end{align*} \quad (30) \]
for \( i = 1, \ldots, 2n_x \). \( n_x \) is the dimension of the states, \( c = \alpha^2(n_x + \kappa) \), \( \kappa \in [0, 1] \), and we set \( \kappa \) to zero. We compute \( \sqrt{P_{k|k-1}} \) with a cholesky factorization, and \( \left( \sqrt{P_{k|k-1}} \right)_i \) is the \( i \)’th column of \( \sqrt{P_{k|k-1}} \) [43]. We introduce the weights,
\[ \begin{align*}
W_m^{(i)} &= \frac{\lambda}{n_x + \lambda}, \\
W_c^{(i)} &= \frac{\lambda}{n_x + \lambda} + (1 - \alpha^2 + \beta), \\
W_{m'}^{(i)} &= \frac{1}{2(n_x + \lambda)}, \\
W_{c'}^{(i)} &= \frac{1}{2(n_x + \lambda)},
\end{align*} \quad (31) \]
for \( i = 1, \ldots, 2n_x \), where \( \lambda = \alpha^2(n_x + \kappa) - n_x \) [44]. We solve the algebraic equations for each sample,
\[ G(\hat{x}_{k|k-1}, \hat{y}_{k|k-1}, \hat{z}_{k|k-1}) = 0, \quad (32) \]
and evaluate the output:

\[ z_{k|k-1}^m = \sum_{i=0}^{2n_x} W_m^i z_{k|k-1}^m, \]  

(33a)

\[ T_{k|k-1} = \sum_{i=0}^{2n_x} W_c^i \left( z_{k|k-1}^{m,i} - z_{k|k-1}^m \right) \left( z_{k|k-1}^{m,i} - z_{k|k-1}^m \right)' \]  

(33b)

\[ S_{k|k-1} = \sum_{i=0}^{2n_x} W_c^i \left( \hat{x}_{k|k-1}^{i} - \hat{x}_{k|k-1} \right) \left( \hat{x}_{k|k-1}^{i} - \hat{x}_{k|k-1} \right)' \]  

(33c)

The innovation is

\[ e_k = y_k^m - \hat{y}_k^{m|k-1}, \]  

(35)

where \( \hat{y}_k^{m|k-1} = z_{k|k-1}^m \). The Kalman filter gain matrix is

\[ K_{fx,k} = S_{k|k-1}T_{k|k-1}^{-1}. \]  

(36)

The filtered state estimate and the covariance matrix are

\[ \hat{x}_k|k = \hat{x}_k|k-1 + K_{fx,k}e_k, \]  

(37a)

\[ P_{k|k} = P_{k|k-1} - K_{fx,k}T_{k|k-1}K_{fx,k}'. \]  

(37b)

and we solve the algebraic equations for the estimates of the algebraic and adjoint algebraic variables:

\[ G(\hat{x}_k^i, \hat{y}_k^i, \hat{z}_k^i) = 0. \]  

(38)

**B. Time-update**

We introduce \( \tilde{n} = n_x + n_\omega \) and the sets \( N_0 = \{0\}, N_x = \{1, \ldots, 2n_x\} \), and \( N_\omega = \{2n_x + 1, \ldots, 2n_x + 2n_\omega\} \). \( n_x \) is the dimension of the process noise. The process noise in (1) is nonadditive. We therefore compute \( 2\tilde{n} + 1 \) samples of the states:

\[ \hat{x}_{k|i}^{(i)} = \hat{x}_{k|k}, \quad i \in N_0 \cup N_x, \]  

(39a)

\[ \hat{x}_{k|i}^{(i)} = \hat{x}_{k|k} + \sqrt{\hat{c}} \left( \sqrt{P_{k|k}} \right)_i, \quad i = 1, \ldots, n_x, \]  

(39b)

\[ \hat{x}_{k|i}^{(i+n_x)} = \hat{x}_{k|k} - \sqrt{\hat{c}} \left( \sqrt{P_{k|k}} \right)_i, \quad i = 1, \ldots, n_x. \]  

(39c)

\( \hat{c} = \alpha^2 (\tilde{n} + \kappa) \), and we introduce the weights,

\[ \tilde{W}_m^{(0)} = \frac{\hat{\lambda}}{\tilde{n} + \lambda}, \]  

(40a)

\[ \tilde{W}_c^{(0)} = \frac{\hat{\lambda}}{\tilde{n} + \lambda} + (1 - \alpha^2 + \beta), \]  

(40b)

\[ \tilde{W}_m^{(i)} = \frac{1}{2(\tilde{n} + \hat{\lambda})}, \]  

(40c)

\[ \tilde{W}_c^{(i)} = \frac{1}{2(\tilde{n} + \hat{\lambda})}, \]  

(40d)

for \( i = 1, \ldots, 2\tilde{n} \). \( \hat{\lambda} = \alpha^2 (\tilde{n} + \kappa) - \tilde{n} \). We solve the DAEs,

\[ \dot{x}_{k|k}^{(i)}(t_k) = \hat{x}_{k|k}^{(i)}, \]  

(41a)

\[ G(\hat{x}_{k|k}^{(i)}(t), \hat{y}_{k|k}^{(i)}(t), \hat{z}_{k|k}^{(i)}(t)) = 0, \]  

(41b)

\[ d\omega_k^{(i)}(t) = F(\hat{y}_{k|k}^{(i)}(t), u(t))dt, \]  

(41c)

for \( i \in N_0 \cup N_x \) and \( t \in [t_k; t_{k+1}] \). Furthermore, we solve

\[ \delta_k^{(i)}(t_k) = \hat{x}_{k|k}^{(i)}, \]  

(42a)

\[ G(\hat{x}_{k|k}^{(i)}(t), \hat{y}_{k|k}^{(i)}(t), \hat{z}_{k|k}^{(i)}(t)) = 0, \]  

(42b)

\[ d\omega_k^{(i)}(t) = F(\hat{y}_{k|k}^{(i)}(t), u(t))dt + \sigma(\hat{y}_{k|k}^{(i)}(t), u(t))d\omega_k^{(i)}(t), \]  

(42c)

for \( i \in N_\omega \) and \( t \in [t_k; t_{k+1}] \). We sample the increments as

\[ d\omega_k^{(i+2n_\omega)}(t) = \left( \sqrt{\hat{c}} d\tilde{t} \right) e_i, \]  

(43a)

\[ d\omega_k^{(i+2n_\omega)}(t) = - \left( \sqrt{\hat{c}} d\tilde{t} \right) e_i, \]  

(43b)

for \( i = 1, \ldots, n_\omega \). The \( i \)th element of the vector \( e_i \) is one and all other elements are zero. We compute the state estimate and the covariance matrix by

\[ \hat{x}_{k+1|k} = \sum_{i=0}^{2\tilde{n}} \tilde{W}_m^{(i)} \hat{x}_{k+1|k}^{(i)}, \]  

(44a)

\[ P_{k+1|k} = \sum_{i=0}^{2\tilde{n}} \tilde{W}_c^{(i)} \left( \hat{x}_{k+1|k} - \hat{x}_{k+1|k}^{(i)} \right) \left( \hat{x}_{k+1|k} - \hat{x}_{k+1|k}^{(i)} \right)', \]  

(44b)

where \( \hat{x}_{k+1|k}^{(i)} = \hat{x}_{k|k}^{(i)}(t_k+1) \).

**C. Numerical solution of the time-update equations**

We discretize (41) with Euler’s implicit method and (42) with the semi-implicit scheme described in Section III. For each of the \( N_k \) time steps, we solve

\[ D_{k,n+1}^{(i)} \hat{x}_{k,n+1}^{(i)} + G_{k,n+1}^{(i)} \hat{y}_{k,n+1}^{(i)} + \frac{\Delta t_k}{2} \omega_{k,n+1}^{(i)} = 0, \]  

(45)

where \( D_{k,n+1}^{(i)} = D_{k,n+1}^{(i)}(\hat{x}_{k,n+1}^{(i)}, \hat{y}_{k,n+1}^{(i)}, \hat{z}_{k,n+1}^{(i)}, u_k) \) is

\[ D_{k,n+1}^{(i)} = \hat{x}_{k,n+1}^{(i)} - F(\hat{y}_{k,n+1}^{(i)}, u_k)\Delta t_k - \hat{x}_{k,n+1}^{(i)}, \]  

(46)

for \( i \in N_0 \cup N_x \) and

\[ D_{k,n+1}^{(i)} = \hat{x}_{k,n+1}^{(i)} - F(\hat{y}_{k,n+1}^{(i)}, u_k)\Delta t_k - \hat{x}_{k,n+1}^{(i)} - \sigma(\hat{y}_{k,n+1}^{(i)}, u_k)\Delta \omega_{k,n+1}^{(i)} - \hat{x}_{k,n+1}^{(i)}, \]  

(47)

for \( i \in N_\omega \). The increments are

\[ \Delta \omega_{k,n+1}^{(i+2n_\omega)} = \sqrt{\hat{c}} \Delta t_k e_i, \]  

(48a)

\[ \Delta \omega_{k,n+1}^{(i+2n_\omega)} = - \sqrt{\hat{c}} \Delta t_k e_i, \]  

(48b)

for \( i = 1, \ldots, n_\omega \).

**VI. THE PARTICLE FILTER**

We sample \( N_p \) particles, \( \hat{x}_{0|0}^{(i)} \), from the distribution of the initial states, i.e. from \( \mathcal{N}(x_0, P_0) \). Next, we solve the algebraic equations for each of the particles:

\[ G(\hat{x}_{0|0}^{(i)}, \hat{y}_{0|0}^{(i)}, \hat{z}_{0|0}^{(i)}) = 0. \]  

(49)
A. Measurement-update

For each particle, we compute the output,
\[ \hat{z}_{m,i}^{m,k}(i)_{k|k-1} = H(\hat{y}_{i}^{m}(i)_{k|k-1}), \]
and the difference between the output and the measurement:
\[ e_k^m(i) = y_k^m - \hat{z}_{m,i}^{m,k}(i)_{k|k-1}. \]
We compute the relative likelihood that \( y_k^m \) is observed if the particle output, \( \hat{z}_{m,i}^{m,k}(i)_{k|k-1} \), is true:
\[ q^m(i)^{(i)} = \frac{1}{\sqrt{(2\pi)^{n_m}|T_k|}} \exp \left( -\frac{1}{2} \left( \frac{e_k^m(i)}{T_k e_k^m(i)} \right) \right). \]

We use systematic resampling [45], [46]. We sample a single (scalar) uniformly distributed number, \( \tilde{p} \sim U([0,1]) \). Next we compute:
\[ p^i(\tilde{p}) = (\tilde{p} - \tilde{p})/N_p, \quad i = 1, \ldots, N_p. \]
The resampled particles, \( \{\hat{x}_{i}^{m,k}|_{k=1}\}_{i=1}^{N_p} \), contain \( m(i) \) copies of \( \hat{x}_{i}^{m,k-1} \) where \( m(i) \) is the number of indices, \( l \), for which \( p^{l}(\tilde{p}^l) \) is in the interval \( \sum_{j=1}^{l-1} q(j); \sum_{j=1}^{l} q(j) \). We compute the state estimate and the covariance matrix by
\[ \hat{x}_{k|k} = W_m \sum_{i=1}^{N_p} \hat{x}_{i,k|k}^{m}, \quad \tag{55a} \]
\[ P_{k|k} = W_c \sum_{i=1}^{N_p} \left( \hat{x}_{i,k|k}^{m} - \hat{x}_{k|k} \right) \left( \hat{x}_{i,k|k}^{m} - \hat{x}_{k|k} \right)^{T}, \quad \tag{55b} \]
where \( W_m = 1/N_p \) and \( W_c = 1/(N_p - 1) \). Next, we solve the algebraic equations:
\[ G(\hat{x}_{k|k}, \hat{y}_{k|k}, \hat{z}_{k|k}) = 0. \]

B. Time-update

For each particle, we solve the stochastic DAE,
\[ \dot{x}_{k|k}^{m}(i)(t) = \hat{x}_{k|k}^{m}(i)(t), \quad \tag{57a} \]
\[ G(\hat{x}_{k}^{m}(i)(t), \hat{y}_{k}^{m}(i)(t), \hat{z}_{k}^{m}(i)(t)) = 0, \quad \tag{57b} \]
\[ \dot{\hat{x}}_{k}^{m}(i)(t) = F(\hat{y}_{k}^{m}(i)(t), u(t))dt + \sigma(\hat{y}_{k}^{m}(i)(t), u(t))d\omega(t), \quad \tag{57c} \]
for \( t \in [t_k; t_{k+1}] \) as we described in Section III. The one-step ahead predictions for the \( i \)’th particle are \( \hat{x}_{k+1|k}^{m}(i) = \hat{x}_{k|k}^{m}(i), \hat{y}_{k+1|k}^{m}(i) = \hat{y}_{k|k}^{m}(i), \) and \( \hat{z}_{k+1|k}^{m}(i) = \hat{z}_{k|k}^{m}(i) \).

VII. THE ENSEMBLE KALMAN FILTER

We sample \( N_p \) particles, \( \hat{x}_{0|0}^{m}, \hat{y}_{0|0}^{m}, \hat{z}_{0|0}^{m} \), from \( N(x_0, P_0) \), and solve the algebraic equations for each particle:
\[ G(\hat{z}_{0|0}^{m}, \hat{y}_{0|0}^{m}, \hat{z}_{0|0}^{m}) = 0. \]

A. Measurement-update

We compute the output for each particle:
\[ \hat{z}_{k|k}^{m}(i) = H(\hat{y}_{k|k}^{m}(i)). \]
We compute the state and output means, the covariance, and the cross-covariance:
\[ \hat{x}_{k|k-1} = W_m \sum_{i=1}^{N_p} \hat{x}_{i,k|k-1}^{m}, \quad \tag{60a} \]
\[ \hat{z}_{k|k-1} = W_m \sum_{i=1}^{N_p} s_{m,i}^{m,i}, \quad \tag{60b} \]
\[ T_{k|k-1} = W_c \sum_{i=1}^{N_p} (\hat{x}_{i,k|k-1}^{m} - \hat{x}_{k|k-1}^{m}) (\hat{x}_{i,k|k-1}^{m} - \hat{x}_{k|k-1}^{m})^{T} + T_k, \quad \tag{60c} \]
\[ S_{k|k-1} = W_c \sum_{i=1}^{N_p} (\hat{x}_{i,k|k-1}^{m} - \hat{x}_{k|k-1}^{m}) (\hat{z}_{i,k|k-1}^{m} - \hat{z}_{k|k-1}^{m})^{T}. \]
\[ W_m = 1/N_p \) and \( W_c = 1/(N_p - 1) \). We sample measurements for each particle:
\[ \hat{y}_{k|k}^{m}(i) = \hat{z}_{k|k}^{m}(i) + v_{k|k}^{m}(i). \]
Each of the measurement noise samples, \( v_{k|k}^{m}(i) \), is drawn from \( N(0, T_k) \). The innovation for the \( i \)’th particle is
\[ e_{k|k}^{m}(i) = y_{k|k}^{m} - \hat{z}_{k|k}^{m}(i), \]
and the Kalman filter gain matrix is
\[ K_{f,k} = \frac{S_{k|k-1} F_{k|k-1}}{P_{k|k-1}}. \]
For each particle, we update the states:
\[ \hat{x}_{k|k}^{m}(i) = \hat{x}_{k|k-1}^{m} + K_{f,k} e_{k|k}^{m}(i), \]
The state estimate and covariance matrix are
\[ \hat{x}_{k|k} = W_m \sum_{i=1}^{N_p} \hat{x}_{i,k|k}^{m}, \quad \tag{65a} \]
\[ P_{k|k} = W_c \sum_{i=1}^{N_p} \left( \hat{x}_{i,k|k}^{m} - \hat{x}_{k|k} \right) \left( \hat{x}_{i,k|k}^{m} - \hat{x}_{k|k} \right)^{T} \]
and we compute the estimates of the algebraic and adjoint algebraic variables by solving the algebraic equations,
\[ G(\hat{x}_{k|k}, \hat{y}_{k|k}, \hat{z}_{k|k}) = 0. \]

B. Time-update

The time-update in the EnKF is identical to the time-update in the PF. We solve the stochastic DAEs,
\[ \dot{\hat{x}}_{k}^{m}(t) = F(\hat{y}_{k}^{m}(t), u(t))dt + \sigma(\hat{y}_{k}^{m}(t), u(t))d\omega(t), \]
for \( i = 1, \ldots, N_p \) and \( t \in [t_k; t_{k+1}] \) with the approach described in Section III. The one-step ahead predictions are
\[ \hat{x}_{k+1|k}^{m} = \hat{x}_{k|k}^{m}, \hat{y}_{k+1|k}^{m} = \hat{y}_{k|k}^{m}, \) and \( \hat{z}_{k+1|k}^{m} = \hat{z}_{k|k}^{m} \).
VIII. THE DYNAMIC UV FLASH SEPARATION PROCESS

We consider the separation of a mixture of $N_C$ components. The mixture is separated into a vapor phase (v) and a liquid phase (l). The two phases are in thermodynamic equilibrium. The separator is supplied by a feed stream. The vapor and liquid phases exit the separator from two separate streams. Furthermore, the unit is either heated or cooled. We model the process with 1) vapor-liquid equilibrium conditions and 2) mass and energy conservation equations.

We use an open-source thermodynamic software, ThermoLib [47], [48], to evaluate thermodynamic functions based on the Peng-Robinson equation of state.

A. Vapor-liquid equilibrium

The UV flash problem is a mathematical statement of the second law of thermodynamics, i.e. that the entropy of a closed system in equilibrium is maximal. The internal energy, $U$, the volume, $V$, and the total composition (in moles), $n$, are specified in the UV flash. The equilibrium temperature, $T$, pressure, $P$, and vapor-liquid composition (in moles), $n^v$ and $n^l$, are the solution to the optimization problem,

$$\begin{align*}
\max_{T,P,n^v,n^l} & \quad S = S^v(T,P,n^v) + S^l(T,P,n^l), \\
\text{s.t.} & \quad U^v(T,P,n^v) + U^l(T,P,n^l) = U, \\
& \quad V^v(T,P,n^v) + V^l(T,P,n^l) = V, \\
& \quad n^v_i + n^l_i = n_i, \quad i = 1, \ldots, N_C. 
\end{align*}
$$

(68a) (68b) (68c) (68d)

The UV flash is also called the UVn flash or the isoenergetic-isochoric (constant energy - constant volume) flash. The solution to (68) is characterized by the first-order optimality conditions which the algebraic equations (1a) represent. The optimization variables are the algebraic variables, and the Lagrange multipliers associated with (68) are the adjoint algebraic variables. The state variables are $U$ and $n$.

B. Conservation of mass and energy

The internal energy, $U$, and the total mixture composition, $n$, are determined by the conservation equations,

$$\begin{align*}
\dot{U}(t) &= H^v_P(t) + H^l_P(t) - H^v(t) - H^l(t) + Q(t), \\
\dot{n}_i(t) &= f^v_{F,i}(t) + f^l_{F,i}(t) - v_i(t) - l_i(t), \quad i = 1, \ldots, N_C.
\end{align*}
$$

(69a) (69b)

$H^v_P$ and $H^l_P$ are the enthalpies, and $f^v_{F,i}$ and $f^l_{F,i}$ are the molar flow rates of the vapor and liquid phases of the feed stream. Similarly, $H^v$ and $H^l$ are the enthalpies, and $v_i$ and $l_i$ are the flow rates of the vapor stream and the liquid stream. $Q$ refers to heating if it is positive and to cooling if it is negative. The inputs to the system, e.g. the feed stream and the vapor-liquid output streams, can be uncertain. Similarly, there can be uncertainty related to the thermodynamic parameters. That is what we model with the stochastic part of the differential equations (1b) [49].

<table>
<thead>
<tr>
<th>TABLE I</th>
<th>ACCURACY AND COMPUTATION TIMES FOR A UV FLASH PROCESS WITH 6 DIFFERENTIAL EQUATIONS AND 19 ALGEBRAIC EQUATIONS.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EKF</td>
</tr>
<tr>
<td>Avg. NRMSD</td>
<td>0.0216</td>
</tr>
<tr>
<td>Avg. meas. upd. CPU (ms)</td>
<td>1.27</td>
</tr>
<tr>
<td>Avg. time upd. CPU (ms)</td>
<td>8.44</td>
</tr>
</tbody>
</table>

IX. NUMERICAL EXAMPLE

We consider the separation of a hydrocarbon mixture in a 0.2 m$^3$ separator. The mixture contains 60% C$_1$, 8% C$_2$, 5% C$_3$, 25% n-C$_7$, and 2% CO$_2$. We estimate the states over a 72 h period with the EKF, UKF, PF, and EnKF. We use the parameter values $\alpha = 0.1$ and $\beta = 2$ in the UKF. We sample 100 particles in both the PF and the EnKF. We measure temperature and pressure every 30 min. All filters take $N_k = 6$ time steps of 5 min between the measurements. The separator is cooled with $Q = -9$ MJ/h for $f \in [0 \text{ h}; 24 \text{ h}]$ and with $Q = -4$ MJ/h for the remaining 48 h. The flow rates of the feed, the vapor stream, and the liquid stream are 1000 mol/h, 400 mol/h, and 600 mol/h, respectively. The temperature and pressure measurement noises have standard deviations of 10 K and $10^{-1/2} \approx 0.3$ MPa. We consider a constant diffusion coefficient, i.e. $\sigma(y(t), u(t)) = \sigma = \text{diag}([\sigma_U; \sigma_{C_1}; \sigma_{C_2}; \sigma_{C_3}; \sigma_{n-C_7}; \sigma_{CO_2}])$. The diagonal elements are $\sigma_U = 1$ MJ, $\sigma_{C_1} = \sigma_{C_2} = \sigma_{n-C_7} = 1$ mol, and $\sigma_{C_3} = \sigma_{CO_2} = 0.1$ mol. $x_0$ is a steady-state of the process (without process noise), and $F_0 = \sigma^2$. Fig. 1 shows the state estimates of the four filters together with the true states (blue). The estimates of all four filters are close to the true states. The root-mean-square deviation (RMSD) of the $i$'th state variable is

$$\text{RMSD}_i = \left( \frac{1}{N + 1} \sum_{k=0}^{N} (\hat{x}_{i,k} - x_{i,k})^2 \right)^{1/2},$$

(70)

where $N = 144$ is the number of sampling intervals. The state variables have different units and orders of magnitude. We therefore compute the normalized RMSD (NRMSD). It is $\text{NRMSD}_i = \text{RMSD}_i / \hat{x}_i$, where $\hat{x}_i$ is the average of the true states, $x_{i,k}$, over the index $k$. Table I shows the average NRMSD over the state variables for each filter together with the average computation times for a single measurement-update and time-update. The EKF is significantly faster than the other filters while the PF estimates have the lowest average NRMSD. Fig. 2 illustrates that the state estimation algorithms can be used for soft sensing of the vapor-liquid compositions. It shows the PF estimates of the total mole fractions, the vapor-liquid mole fractions, and the vapor fraction of the mixture.

X. CONCLUSIONS

We describe four nonlinear filters for state estimation of UV flash processes, i.e. the EKF, UKF, PF, and EnKF. We model the UV flash processes with stochastic DAEs in a semi-explicit index-1 form. We describe a model of a UV flash separation process and compare the accuracy and
efficiency of the filters with a numerical example. The PF is slightly more accurate than the other filters in terms of the average NRMSE of the estimates. However, all four filters provide estimates that are very close to the true states of the process. The EKF is significantly faster than the other filters. Finally, we demonstrate that the algorithms can be used for soft sensing of vapor-liquid compositions based on temperature and pressure measurements.

REFERENCES


