Indian Institute of Technology, Ropar

Bachelor of Technology in Chemical Engineering

CP302: Capstone Project

Design of Bayesian State Estimator for the Bioreactor system

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Contents

1 Introduction

It is always desired to operate the processes near the desired operating conditions. In order to operate successfully we need to have a control on the behavior of the system. Understanding the behavior of the system requires accurate information of the state of the system. The sensors are used to measure the state of system. We can have fast rate measurements (taken at every sampling instant). But not all the process variables are measured at a fast rate. For example concentration and the molecular weight values. To measure these states, first the sample is collected and then experiments are performed in the lab. This way of measuring the variables takes a lot of time. Even the sensors that are available to measure the state variables are very costly. It becomes difficult to have the measurement data for all the states. Also the disturbances in the process corrupts the measurement data and adds noise to it. With the noisy and unmeasured data, it is hard to operate the process. Getting the estimate of the state variables from the given input and measured output is a challenging task. The idea of soft sensing tries to solve this problem.

2 Literature Survey

To reconstruct the missing measurements and to estimate the unmeasured quality variables, the soft sensors are used. The soft sensors are mainly classified into three categories: Model based, Data based and Hybrid based. The model based approach uses the mass, energy and momentum balance equations. The model based soft sensor includes a bayesian and deterministic approach. In this project, the main goal is to develop the Bayesian state estimator for the bioreactor system. In the Bayesian approach, uncertainties in the model and the measurements are handled efficiently. It gives an optimal estimate of the state with the measure of uncertainty in the estimate. The Kalman filter is one of the state estimation methods that is considered a key factor in the success of the Apollo II moon landing [3]. For linear systems, the Kalman filter can be used to reconstruct the missing or the hidden states. It assumes that the state, state uncertainty and measurement noise follow gaussian distribution. The gaussian distribution provides the ease of the computation. In real life, most of the systems are nonlinear in nature. So the Kalman filter can be extended for the nonlinear systems. To solve the nonlinear equations, sampling and non-sampling techniques are used. Under the non sampling based approach, Extended Kalman filter is used in which a nonlinear system is linearised to the linear system by using Taylor series Expansion. For highly nonlinear or discrete systems, sampling based techniques like the particle filter are used.

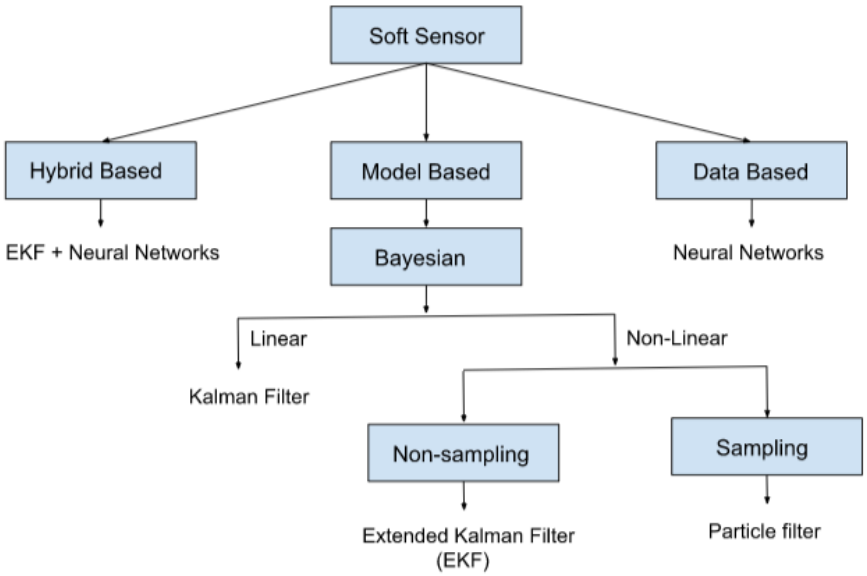

Figure 1: Soft Sensor

2.1 Bayesian State Estimation Problem

The given are the measurement $Y^k = \{y_0, y_1, ...y_k\}$ and input $U^k = \{u_0, u_1, ...u_k\}$. The objective is to estimate $\hat{X}^k = \{\hat{x}_0, \hat{x}_1, ...\hat{x}_k\}$.

The nonlinear continuous time model is given as

$$\frac{dX}{dt} = f(X, U, \theta) \tag{1}$$

It can be converted to a linear continuous time model through Taylor series approximation. Further we can discretize the equation. The discrete time linear pertubation model is given as

$$x_k = \phi x_{k-1} + \Gamma u_{k-1}$$

The linear process model is represented by the below equations.

$$x_k = \phi x_{k-1} + \Gamma u_{k-1} + w_{k-1} \tag{2}$$
$$y_k = Cx_k + v_k \tag{3}$$

Here w_k and v_k represent the uncertainties in state and the measurement. The noise w_k and v_k are white, zero-mean, uncorrelated, and have covariance matrices Q and R respectively[4]. We assumed Q and R to be known. The state x_k, noise w_k and v_k follow gaussian distribution. The objective of the Bayesian state estimation problem is to find the conditional probability density function i.e. $\mathrm{p}(x_k|Y^{k-1})$ from $\mathrm{p}(x_{k-1}|Y^{k-1})$. The process is carried out in two steps : Prediction step and Update step.

Prediction step:

$$p(x_k|Y^{k-1}) = \int p(x_k|x_{k-1})p(x_{k-1}|Y^{k-1})dx_{k-1} \tag{4}$$

This is known as Chapman-Kolmogorov equation. Here the posterior density $\mathrm{p}(x_{k-1}|Y^{k-1})$ at the previous is propagated to the next time step[3].

Update step:

$$p(x_k|Y^k) = \frac{p(y_k|x_k)}{p(y_k|Y^{k-1})}p(x_k|Y^{k-1}) \tag{5}$$

The update step shows the use of Bayes' theorem. The $\mathrm{p}(y_k|x_k)$ is the likelihood term, $\mathrm{p}(x_k|Y^{k-1})$ is the prior density term and $\mathrm{p}(y_k|Y^{k-1})$ represents the evidence term. These terms follow gaussian distribution. Each of these terms can be derived by finding their expectation and covariance. The likelihood function $\mathrm{p}(y_k|x_k)$ can be determined by finding expectation and covariance of measurement model equation (3).

$$E[y_k|x_k] = E[Cx_k + v_k|x_k]$$
$$E[y_k|x_k] = Cx_k$$

where the $\mathrm{E}(v_k)$ is zero as v_k has zero mean.

$$cov[y_k|x_k] = E\{[y_k - E(y_k|x_k)][y_k - E(y_k|x_k)]^T\}$$
$$cov[y_k|x_k] = E\{[y_k - Cx_k][y_k - Cx_k]^T\}$$
$$cov[y_k|x_k] = E\{[v_k][v_k]^T\}$$
$$cov[y_k|x_k] = E\{[v_k - E(v_k)][v_k - E(v_k)]^T\}$$
$$cov[y_k|x_k] = cov(v_k) = R$$

Thus $p(y_k|x_k) \sim N(Cx_k, R)$. Similarly Prior density and Evidence term can be determined.

Likelihood function: $p(y_k|x_k) \sim N(Cx_k, R)$

Prior density: $p(x_k|Y^{k-1}) \sim N(\hat{x}_{k|k-1}, P_{k|k-1})$

Evidence term: $p(y_k|Y^{k-1}) \sim N(C\hat{x}_{k|k-1}, CP_{k|k-1}C^T + R)$

These terms can be represented in the form of gaussian distribution function. Then equation (5) can be converted to an optimization problem to get the estimate x_k that maximizes $p(x_k|Y^k)$. Solving the bayes' theorem, we can obtain the steps of Kalman filter. The below figure shows the steps of Kalman filter algorithm.

Prediction step:
$$\hat{x}_{k|k-1} = \Phi\hat{x}_{k-1|k-1} + \Gamma u_{k-1}$$
$$P_{k|k-1} = \Phi P_{k-1|k-1}\Phi^T + Q$$

Innovation:
$$e_k = y_k - C\hat{x}_{k|k-1}$$

Kalman gain:
$$L_k = CP_{k|k-1}(CP_{k|k-1}C^T + R)^{-1}$$

Update step:
$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k e_k$$
$$P_{k|k} = (I - L_k C)P_{k|k-1}$$

Figure 2: Kalman Filter

The Kalman filter is applied to the linear systems. For nonlinear systems, we have Extended kalman filter(EKF). The main difference between the kalman filter and EKF is the prediction step. Instead of linear model, nonlinear model is taken in account in the prediction step of EKF.The below figure represents the steps of Extended kalman filter.

Prediction step:
$$\hat{x}_{k|k-1} = F[\hat{x}_{k-1|k-1}, u_{k-1}]$$
$$P_{k|k-1} = \Phi_{k-1}P_{k-1|k-1}{\Phi_{k-1}}^T + Q$$
$$\Phi_{k-1} = \left[\frac{\partial F}{\partial x}\right]_{(\hat{x}_{k-1|k-1}, u_{k-1})}$$

Innovation:
$$e_k = y_k - C\hat{x}_{k|k-1}$$

Kalman gain:
$$L_k = CP_{k|k-1}(CP_{k|k-1}C^T + R)^{-1}$$

Update step:
$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k e_k$$
$$P_{k|k} = (I - L_k C)P_{k|k-1}$$

Figure 3: Extended Kalman Filter

3 Methodology

In this project, the focus is on estimating the noise free and unmeasured state for a bioreactor fermenter system. To monitor the quality of contents of the fermenter, state estimation is required. The main motive behind choosing this system is the difficulty that is being faced in measuring the status of these microorganisms in the fermenter. Different specialized sensors like enzyme electrodes (e.g. to measure

glucose, lactate), calorimetric analyzers (e.g., to measure penicillin), and immunosensors (e.g., to measure antigens) are required [2]. These sensors are very costly. The below figure shows a continuous fermenter reactor. The dilution rate D and feed substrate concentration S_f are the manipulated inputs. The biomass concentration X, substrate concentration S and Product concentration P are the process state variables.

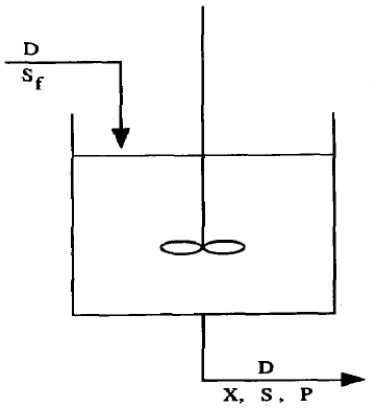

Figure 4: Continuous Fermenter

The dynamic model equations[1] of bioreactor system are given below.

$$\frac{dX}{dt} = -DX + \mu X \tag{6}$$

$$\frac{dS}{dt} = D(S_f - S) - \frac{1}{Y_{X/S}}\mu X \tag{7}$$

$$\frac{dP}{dt} = -DP + (\alpha\mu + \beta)X \tag{8}$$

Where μ is the specific growth rate, $Y_{X/S}$ is the cell mass yield and α and β are the parameters. The specific growth rate model[1] is given as

$$\mu = \frac{\mu_m(1 - \frac{P}{P_m})S}{K_m + S + \frac{S^2}{K_i}} \tag{9}$$

This model contains four model parameters: the maximum specific growth rate μ, the product saturation constant P_m , the substrate saturation constant K_m , and the substrate inhibition constant K_i . We have assumed that the substrate and the biomass concentration measurements are available at every sampling instant. The EKF is implemented to estimate the Product concentration P.

4 Results and Discussion

A step input of 10% from the steady state value is given. The profiles of manipulated input variables: Dilution rate and feed substrate concentration is shown below.

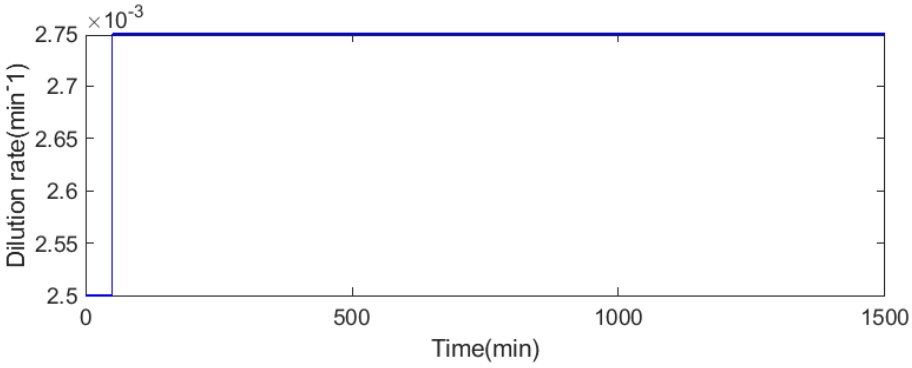

Figure 5: Step change in Dilution Rate

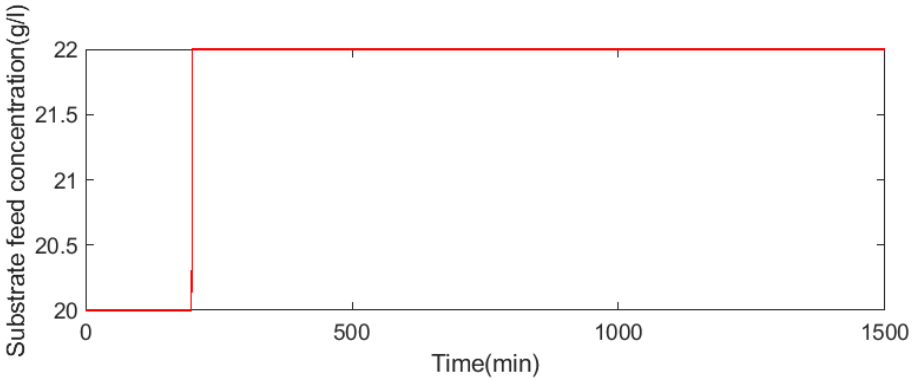

Figure 6: Step change in Substrate Concentration

After providing the step input to the system, the EKF is implemented to estimate the Product concentration and the noise free measurements of Biomass and Substrate concentration. In the below figure, the black line shows the measurement data that is corrupted with the noises. The red line shows the estimated Biomass concentration profile. We can see that EKF is able to filter out the noises in the measurements.

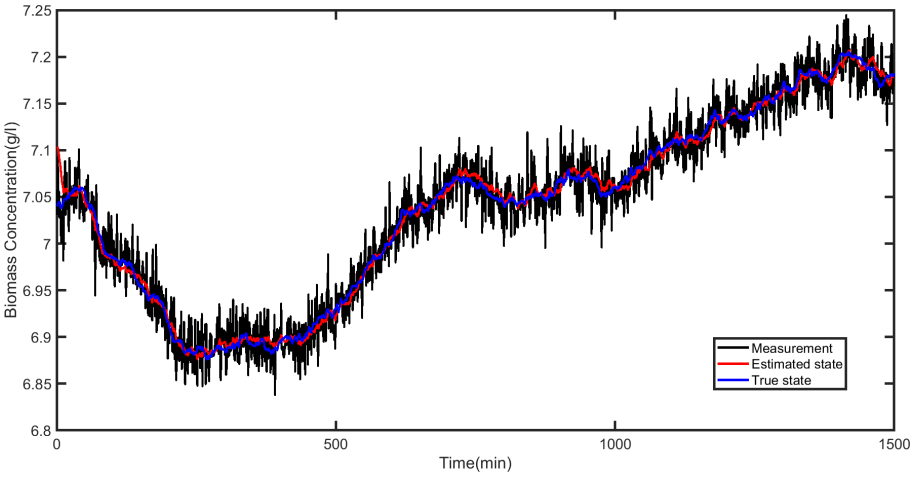

Figure 7: Biomass Concentration Profile

Below figure shows the profile of substrate concentration. Here also black line is showing the measurement

data and red line shows the estimated state.

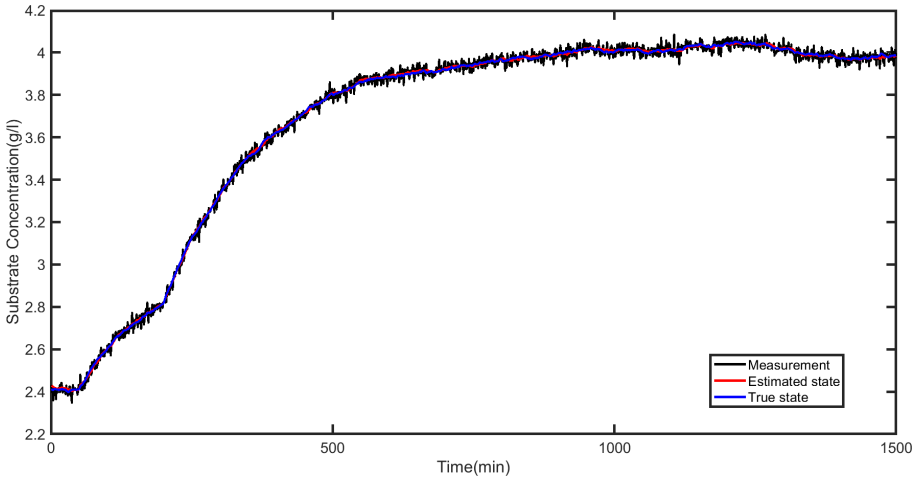

Figure 8: Substrate Concentration Profile

We estimated the product concentration profile by using the input variables (dilution rate, feed substrate concentration) and measured variables (biomass and substrate concentration) information.

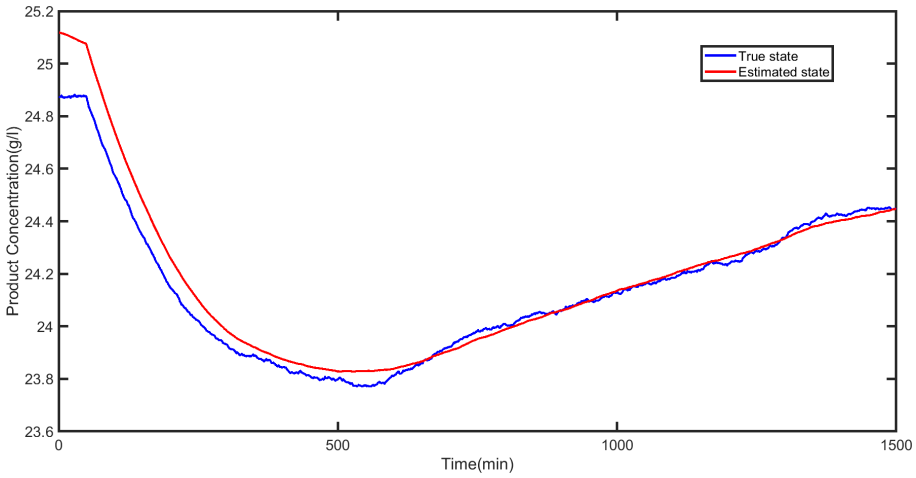

Figure 9: Product Concentration Profile

The error plots for Biomass concentration, Substrate concentration and Product concentration is plotted below.

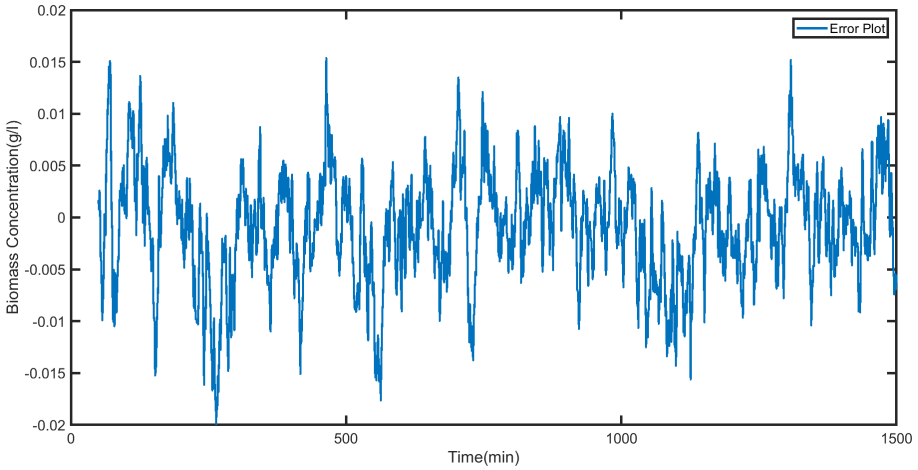

Figure 10: Biomass Concentration Error Plot

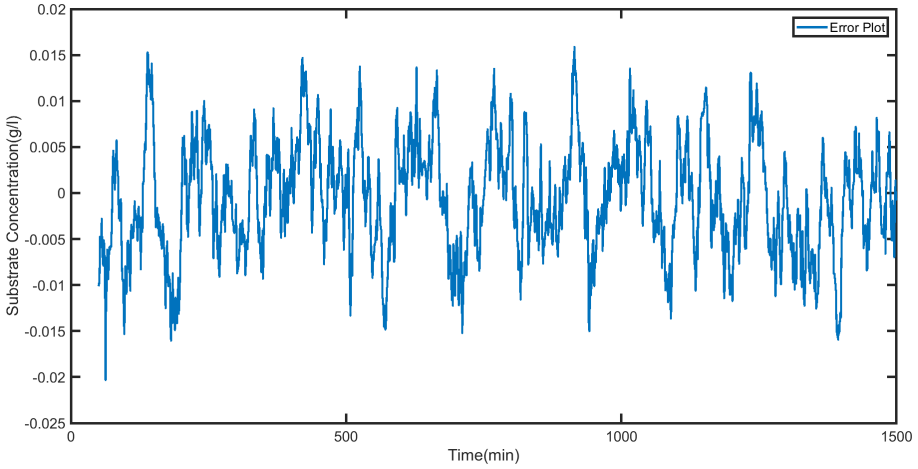

Figure 11: Substrate Concentration Error Plot

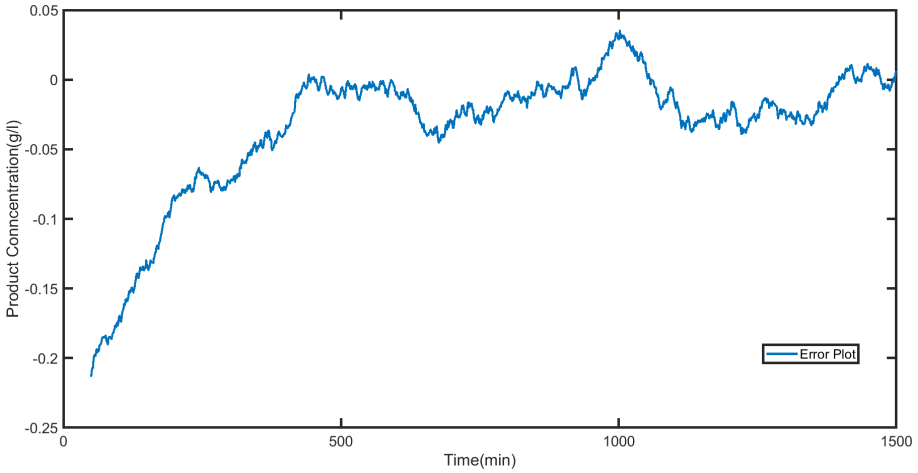

Figure 12: Product Concentration Error Plot

In the Product concentration error plot, we can see that initially the difference between the true and estimated values of Product concentration is large. But over the time the error reduces.

5 Future Scope

In this project, model based techniques like EKF are implemented for estimating the state of the bioreactor system. Here we assumed the process model to be accurate. But in reality process behavior changes over the period of the time. To account for the uncertainties in the model, we can integrate the first principle model with the data driven or ML model. The ML model will take into account the changes happening in the process over the time by discovering the hidden structures in the data. A hybrid based approach (i.e. data + Prior process knowledge) will provide a better understanding of the system. When the number of states increases, the complexity of the process also increases. In future, we can look for the possibilities of applying the state estimation for higher dimension systems like the reactive distillation column. We can further extend our work by developing an integrated advanced process control system.

6 Conclusion

In the Capstone Project,the aim was to design a Bayesian state estimator for the fermenter system. The main reason behind choosing the bioreactor system was due to the challenges associated with it. These systems require specialized and high cost sensor for measuring the status of microorganisms. To resolve this problem, the model based estimator was developed. The extended kalman filter was implemented to estimate the unmeasured state variable, Product concentration. The measured states were also corrupted with the noises. The EKF reduced the noises in the measurements and gave better estimate of the states of the system. In future, the possibilities of integrating the model based estimator with the machine learning models can be explored.

7 References

References

[1] Michael A. Henson and Dale E. Seborg. "Nonlinear control strategies for continuous fermenters". In: *Chemical Engineering Science* 47.4 (1992), pp. 821–835. ISSN: 0009-2509. DOI: https://doi.org/10.1016/0009-2509(92)80270-M. URL: https://www.sciencedirect.com/science/article/pii/000925099280270M.

[2] Gary A. Montague Pankaj Mohan Jarka Glassey. *Process Modeling and Control in Pharmaceutical Operations*.

[3] Sachin C. Patwardhan et al. "Nonlinear Bayesian state estimation: A review of recent developments". In: *Control Engineering Practice* 20.10 (2012). 4th Symposium on Advanced Control of Industrial Processes (ADCONIP), pp. 933–953. ISSN: 0967-0661. DOI: https://doi.org/10.1016/j.conengprac.2012.04.003. URL: https://www.sciencedirect.com/science/article/pii/S0967066112000871.

[4] Dan Simon. *Optimal State Estimation: Kalman, H Infinity, and Nonlinear Approaches*.