On-line Identification and Model Structure Modification of Membrane Fouling in Membrane Bioreactor Systems

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Preface

This thesis which I am proud to present is the result of five months hard work. Students who have some work experience after their bachelor study (BSc) are allowed to do a minor thesis instead of internship for their masters study. Since I had worked a couple of years after my BSc, I chose this minor thesis to replace my internship. I have good mathematical skills and chose a subject in Systems and Control Group (SCO) for both my major and minor thesis. I find the doing of research and discovery of results for practical and daily life problems very rewarding. However, it is not easy and requires commitment and patience.

Finding the correct answer to a research question is never easy and requires the use of knowledge acquired both from past experiences and during the period of the project itself. A lot of new skills are required for the successful completion of any project, in particular that of scientific writing which is absolutely indispensable.

Special thanks to my wife who supported me during my study as much as she could by releasing me from housekeeping duties and spending a lot time with our son Aryan. Without her steadfast support I would have had many more difficulties completing this project.

My special gratitude to my supervisors, Karel Keesman and Paula van den Brink. Karel for his constant support and theoretical insights which greatly aided me and provided me with invaluable assistance for my computer programming and Matlab work. He also advised me to write this report using \TeX, which was not without difficulties, but proved to be an excellent program to write reports, especially mathematical texts. Paula provided me with this research project and the data which were produced at Wetsus in Leeuwarden. She also arranged a presentation opportunity for me at Wetsus to present my research results on 7th January 2010. It was a valuable experience presenting to a large audience at a top research and educational organization.

I would also like to thank all of the students and staff at the department of SCO and Farm Technology, who were always willing to answer and help me on various questions.
Summary

A system can refer to a process or an object. It may also denote a set of interacting or interdependent processes or objects. System identification is a general scientific field that develops and applies algorithms that build dynamical models from measured data and prior knowledge. Given measured data and mathematical equations describing the system, the unknown parameters and states in the equations can be estimated, if some technical conditions are fulfilled. In the parameter and/or state estimation calculations, two main types of errors have to be dealt with. Both measurement and modeling errors have significant influence on the accuracy of the estimates. Depending on the system and the working situation, the parameter estimates might be time-varying and thus not constant. It is therefore very important to choose appropriate estimation methods so as to be sure that the system under study is identified in a reliable way.

In this research project a membrane bioreactor system (MBR) has been studied. In order to allow the estimates of the time-varying parameter, a so-called recursive parameter estimation scheme put into operation. Based on given physical equations from literature, see [13], both parameter and state estimation steps were performed. The recursive parameter estimates suggest a model structure modification of the membrane fouling process under study.

Three experimental data sets were used where the transmembrane pressure (TMP) was measured. The membrane fouling process essentially contains one parameter; the unknown coefficient, $\alpha$. The TMP parameter, $\alpha$, has been estimated by both off-line and on-line estimation methods. The estimates from the two estimation methods were compared and used for model modification purposes. The Kalman filter is used for on-line parameter and state estimation purposes.

Off-line parameter estimation resulted in three different parameter values using three different data sets. Recursive parameter estimation using two sets of data showed similar results, namely the TMP parameter, $\alpha$, is a time-varying parameter. The estimates of $\alpha$ from the recursive algorithm fitted a hyperbolic function in the form of $\alpha \cdot t = c$. The results suggest that the unknown parameter, $\alpha$, should be estimated on-line. The transmembrane pressure model will not fit many experimental data if the parameter $\alpha$ is
estimated off-line.
Contents

Preface ................................................................. iii
Summary ................................................................. v

1 Introduction ......................................................... 1
  1.1 Problem Definition .......................................... 2
  1.2 Objectives .................................................... 2
  1.3 Approach ...................................................... 3
  1.4 Outline of Thesis ............................................ 3

2 Basic Equations on Local Sub-critical Flux ....................... 5

3 Theory .................................................................. 9
  3.1 Kalman filter Estimator ....................................... 9
  3.2 Permeate Local Flux Concept ................................ 11
  3.3 Darcy’s Law ..................................................... 11

4 Parameter Estimation ............................................. 13
  4.1 Off-line Estimation of TMP parameter, $\alpha$ .............. 13
  4.2 Recursive Estimation of TMP parameter, $\alpha$ ............ 14

5 State Estimation ................................................... 17
  5.1 The necessity of state estimation in MBR systems .......... 17
  5.2 System Definition .............................................. 17
  5.3 System properties ............................................. 19
  5.4 Relationship between the two proportionality constants .... 19

6 Results and Discussion .......................................... 21
  6.1 Parameter Estimation .......................................... 21
    6.1.1 Off-line estimation of $\alpha$ .............................. 21
    6.1.2 Recursive estimation of $\alpha$: Data Set I .............. 23
    6.1.3 Recursive estimation of $\alpha$: Data Set III ............ 24
  6.2 Model Structure Modification ................................ 26
  6.3 Interpretation of the time-varying property of $\alpha$ .......... 28
  6.4 State Estimation .............................................. 28
# CONTENTS

6.4.1 Output Equation Definition ........................................ 28  
6.4.2 Results from State Estimation .................................... 30  
6.5 Results for $k_1k_2$ relationship .................................... 32  

7 Conclusions ................................................................. 35  

8 Recommendation .......................................................... 37  
  8.1 An Algebraic Equation for Proportionality Parameters ............ 37  
  8.2 Future Research Outlook ............................................. 37  

Appendix:  
A Symbols and Abbreviations ............................................... 41  
B Derivation of differential equation of TMP ............................ 43  
C Glossary ........................................................................... 45  
D Matlab Routines .............................................................. 47
Chapter 1

Introduction

Issues on clean water have always been of great impact to human beings. The following quote from [15] goes back to the ancient Greek Pindar (ca 522-438 BC):

Water is the best of all things.

The following quote was published by the World Bank Institute in November 1999 [15], showing that water is still a central issue and remains a great importance to mankind.

Water is essential for all dimensions of life. Over the past few decades, use of water has increased, and in many places water availability is falling to crisis levels. [. . .]. Ecosystems are being destroyed, sometimes permanently. Over one billion people lack safe water and three billion lack sanitation, eighty percent of infectious diseases are waterborne, killing millions of children each year.

Currently, membrane bioreactors (MBR) are broadly used for municipal wastewater treatment. The MBR systems replace the conventional activated sludge (CAS) systems, where the sludge is separated from the treated water by secondary clarification, also called settling, [10]. An MBR applies direct membrane filtration of the mixed-liquor in the bioreactor to separate the treated water (permeate) from the sludge. Compared to CAS systems, an MBR has three major advantages: (i) It uses a smaller footprint since there is no clarifying section (area) required; (ii) The permeate obtained from an MBR has higher effluent quality; and (iii) It has a much larger treatment capacity than a CAS system.

Membranes have a large potential in the wastewater treatment industry [11]. However, they are prone to fouling, leading to a conservative operation, i.e. on average a permeate flux of 20 is chosen instead of $80 \text{ Lm}^{-2}\text{h}^{-1}$ for clean water. In addition to this, a large amount of energy and chemicals are used for periodic cleaning of fouled membranes. According to [10], the energy use for aerating the membranes to limit the fouling, contributes to 38% of the total energy required for the MBR.
CHAPTER 1. INTRODUCTION

1.1 Problem Definition

Membranes are prone to fouling. Hence, they are operated at a lower flux than the maximum possible potential, or a large membrane area is applied to compensate for this. Membrane fouling prevention and cleaning requires a high energy consumption and a large amount of chemicals. There are three membrane fouling mechanisms, also called fouling constituents: (i) Pore blocking, (ii) Adsorption / biofouling and (iii) Cake-forming. Membrane bioreactors are operated over a prolonged period and the fouling mechanisms are likely to change over the course of time because of the heterogeneity of the feed suspension. This has certain consequences on the parameters present in the existing models. Most parameters in the existing models seem to show time-varying behavior, that is they behave as a function of time and are not likely to be constant.

In literature, see e.g. [2, 13], the unknown parameter, $\alpha$, have been estimated off-line. However, when confronted with real experimental data, the transmembrane pressure (TMP) model, [13] does not always fit the data, implying the necessity of a different estimation approach.

The unknown parameter, $\alpha$, will be called the **TMP parameter** throughout this thesis.

1.2 Objectives

Given experimental data and the physical model equations from Ognier et al [13], the objectives of this thesis are (i) parameter estimation, (ii) state estimation and (iii) improving the structure of an existing model. The aims above will lead to a better insight into membrane fouling mechanisms. Properly and accurately estimated parameters will lead to improvements in the models, making them more accurate, and thus will help to interpret the fouling mechanisms more precisely. State estimation in an MBR system is necessary to gain insight into the membrane working conditions in time.

Well defined and accurate models are necessary for optimal control of the system in a later stage of the research.

The research questions are:

1. Which estimation method should be used to estimate the parameters present in the MBR model?

2. How can the new parameter information be incorporated into the models?

3. In what way can the estimated parameters be interpreted and related to membrane fouling mechanisms?

4. Which estimation method should be used to estimate the state variables present in the MBR system?
1.3 Approach

Real experimental data ($\Delta P, t$) of a lab-scale MBR in Wetsus, Leeuwarden will be used in combination with an existing model [13]. A recursive estimation method (the Kalman filter) will be used for on-line parameter and state estimation purposes. The recursive parameter estimates will be incorporated into the present models in order to improve and modify the fit between the models and the experimental data. The state estimates can be used for on-line monitoring of the processes. An example of an on-line process monitoring is the concentration of incoming liquor in the MBR system.

1.4 Outline of Thesis

In Chapter 2 of this MSc report, the literature on physical modeling of membrane fouling processes, with a particular focus on the local sub-critical flux model of Ognier et al. [13], is reviewed. Chapter 3 covers some theory on the Kalman filter algorithm as well as topics which are specific to subjects discussed in the subsequent chapters. Chapter 4 focuses on parameter estimation. The purpose is to estimate an unknown parameter with both off-line and on-line estimation methods and compare the results (see Chapter 6). Chapter 5 pays attention to state estimation. First the need for state estimation in an MBR system is explained. In the second section of this chapter the system under study is defined and finally, the section on system properties closes this chapter. Chapter 6 summarizes and discusses the results of the research. This is a relatively long chapter with results, figures and comparisons from subjects issued in Chapter 1 through 5. Chapter 7 includes the conclusions on the recursive estimation method and its influence on accuracy of parameter and state estimation. The research questions are also answered in this chapter. Finally Chapter 8 covers some recommendations about the entire scope of the project, notably suggestions on controlling membrane bioreactor systems. This report is concluded with a literature reference and four appendices.
CHAPTER 1. INTRODUCTION
Chapter 2

Basic Equations on Local Sub-critical Flux

The physical models in this chapter are based on ideas of Ognier et al. [13]. The experimental data were obtained from Wetsus in Leeuwarden.

In principle, permeate flow, $Q$, depends upon the number of open pores, $n_p$, sectional area, $S_p$, of an open pore and permeate flow rate, $J_p$, through an open pore. This means that $Q$ can be expressed as a function of $J_p$ through the pores and the total open pores sectional area, $n_pS_p$, as in the following equation

$$Q = J_p n_p S_p \tag{2.1}$$

where $n_p S_p$ is in m$^2$, $J_p$ is in m$^3$m$^{-2}$s$^{-1}$ and consequently, the permeate flow, $Q$, in m$^3$/s. Generally, $Q$ is a volumetric flow which is realized by a pump. The permeate flow rate, $J$, is the flow through an area. This induces the following relationship between $Q$ and $J$

$$Q = J \cdot A \quad \text{or} \quad J = Q/A \quad \tag{2.2}$$

This is clearly in accordance with the Eqn (2.1), where the equality, $A = n_p S_p$, holds.

At a sub-critical flux, fouling is assumed to be caused by the interaction between different types of soluble particles and the membrane. In what follows, it is assumed that the change in the mass of particles, $m$, interacting at each moment with the membrane material, and susceptible to being retained in the pores, is proportional to the flow of bioreactor matter (sludge) through the membrane,

$$\frac{dm(t)}{dt} = k_1 C_{\text{solute}} Q \quad \tag{2.3}$$

with $k_1$ [-] the proportionality constant, $t$ in seconds and $C_{\text{solute}}$ in g/m$^3$ the soluble particle concentration in the solution.

The change over time in the number of open pores, $n_p$, is taken as directly proportionate to the mass $m$ of solution particles deposited in a pore and/or interacting with the membrane material at time $t$,

$$\frac{dn_p(t)}{dt} = -k_2 m \quad \tag{2.4}$$
with \( k_2 \) in \( g^{-1}s^{-1} \) a proportionality rate and \( m \) the mass of particles in grams (g) in the pores. Equation (2.4) shows that at time instant \( t \), the number of open pores is \( n_p \) and each pore remaining open is taken as keeping a sectional area \( S_p \) and a resistance \( R_p \) to the flow. The sectional area of each pore and the resistance are assumed to be constant. However, the flow resistance through the pores can vary over time, as we will see in the following chapters.

Using Darcy’s law, the transmembrane pressure \( \Delta P \) at time \( t \) can be expressed as a function of the flow conditions in the pores, where

\[
\Delta P = \mu R_p J_p \tag{2.5}
\]

Variation in the number of open pores, \( n_p \), over time induces instantaneous variation of \( J_p \) and \( \Delta P \) such that, under the assumption that \( \mu \) and \( R_p \) are constant

\[
\frac{d(\Delta P)}{dt} = \mu R_p \frac{d(J_p)}{dt} \tag{2.6}
\]

Taking account of Eqns (2.1) - (2.6), for a proof of this see Appendix B, the following differential equation is obtained

\[
\frac{d(\Delta P)}{dt} = \alpha \Delta P^2 t \tag{2.7}
\]

with

\[
\alpha \triangleq \frac{k_1 k_2 S_p C_{solute}}{\mu R_p} \tag{2.8}
\]

The parameter \( \alpha \) in m/kg can be written as the combination of two new parameters \( \beta \) in \( m^{-1}s^{-1} \) and \( \gamma \) in kg \cdot m\(^{-2}\)s\(^{-1}\) as \( \alpha = \beta / \gamma \), leading to the following equations

\[
\beta \triangleq k_1 k_2 S_p C_{solute} \tag{2.9}
\]

and

\[
\gamma \triangleq \mu R_p \tag{2.10}
\]

Under fixed biological conditions (defined sludge age and hydraulic retention time), \( C_{solute} \) can be considered constant and Eqn (2.7) is easily integrated as

\[
\Delta P(t) = \frac{2\Delta P_0}{2 - \alpha \Delta P_0 t^2} \tag{2.11}
\]

where \( \Delta P \) is always a positive value implying that it must hold \( 2 - \alpha \Delta P_0 t^2 > 0 \) and consequently \( t < t^* = \sqrt{\frac{2}{\alpha \Delta P_0}} \).

Moreover, local flux, \( J_p \), in the pores remaining open over time is expressed as follows

\[
J_p(t) = \frac{2J_{p0}}{2 - \beta J_{p0} t^2} \tag{2.12}
\]

Because no experimental means exist to evaluate the actual \( J_p \) values, it is assumed that the membrane properties, e.g. its geometry, correspond to a model offering an initial \( J_p \) value defined such as

\[
J_{p0} = \frac{Q}{A} \tag{2.13}
\]
where $J_{p0}$ is expressed in m$^3$m$^{-2}$s$^{-1}$ = m/s.

This means that the specific open pore flow rate is expressed with regard to the apparent area $A$ of the membrane. This allows to compare the model prediction with experimental results, especially results showing the critical flux conditions expressed in relation to the parameter $A$ itself.
CHAPTER 2. BASIC EQUATIONS ON LOCAL SUB-CRITICAL FLUX
Chapter 3

Theory

In this chapter some background calculations, theory and algorithms used throughout this thesis, are explained. One such an algorithm is the Kalman filter, used for recursive estimation of system parameters and states. The majority of symbols and the general form used in this chapter correspond to the case studies in the following chapters.

3.1 Kalman filter Estimator

The Kalman filter is a recursive estimator. The word *recursive* implies that only the estimated state from the previous time step, \( \hat{x}_{k-1} \), that indicated by the time index \( k \), and the current measurement, \( y_k \), are needed to compute the estimate for the current step, \( \hat{x}_k \).

It is worth emphasizing that this estimator can be used for estimation of system states as well as for system parameters. In contrast to batch estimation techniques, in Kalman filtering, no history of observations and/or estimates are required.

Assuming that the true state value at time \( t_k \) is evolved from the state value at time \( t_{k-1} \), the basic Kalman filter model has the following general form

\[
x_{k|k-1} = A_{k-1}x_{k-1} + B_{k-1}u_{k-1} + w_{k-1}
\]

where \( x \), \( u \) and \( w \) are vectors; \( A \) and \( B \) are matrices. The overall objective is to estimate \( x_k \), i.e. to find an estimate \( \hat{x}_k \) for \( x_k \). The process noise, \( w_k \), has zero mean and covariance \( Q \) i.e. \( w_k \sim N(0, Q_k) \). At time \( t_k \) an observation (or measurement) of the true state \( x_k \) is made according to

\[
y_k = H_kx_k + v_k
\]

where \( y \) and \( v \) are vectors and \( H \) is a matrix. The observation noise, \( v_k \), has zero mean and covariance \( R \), i.e. \( v_k \sim N(0, R_k) \), and is assumed to be uncorrelated with the error in \( x_k \). \( H_k \) is the observation matrix which maps the true state into the observed state, state measurement.

Assume that at time step \( t_k \) there is an old, unbiased estimate \( \hat{x}_{k-1} \) with a covariance \( P_{k-1} \). The aim is to combine \( \hat{x}_{k-1} \) and \( y_k \) linearly (to keep the computation and analysis
simple), to form a new estimate, $\hat{x}_k$. In other words:

$$\hat{x}_k = J_k \hat{x}_{k-1} + K_k y_k$$

(3.3)

with matrices $J_k$ and $K_k$ chosen to make $\hat{x}_k$ a good estimate. If it is required for $\hat{x}_k$ to be unbiased, it means that for any $x$ and any given $H_k$

$$E\hat{x}_k = J_k E\hat{x}_{k-1} + K_k E y_k = J_k x + K_k H_k x = x$$

(3.4)

Hence

$$J_k + K_k H_k = I$$

(3.5)

And so

$$\hat{x}_k = (I - K_k H_k)\hat{x}_{k-1} + K_k y_k = \hat{x}_{k-1} + K_k(y_k - H_k \hat{x}_{k-1})$$

(3.6)

The term $y_k - H_k \hat{x}_{k-1}$ is known as the *innovation* or *measurement residual*. The matrix $K_k$, which is called the optimal Kalman gain matrix, (see e.g. [12] for details) is equal to

$$K_k = P_{k|k-1} H_k^T (H_k P_{k|k-1} H_k^T + R)^{-1}$$

(3.7)

The minimal covariance of $\hat{x}_k$ is given by

$$P_k = (I - K_k H_k) P_{k-1}$$

(3.8)

**Example**: Kalman filter algorithm.

Suppose two old, unbiased estimates, $x_{k-1}^{(1)} = 5$ and $x_{k-1}^{(2)} = -2$, of two states $x^{(1)}$ and $x^{(2)}$ are to be updated using a new, noisy observation

$$y_k = x^{(1)} + x^{(2)} + v_k = 4.5$$

Furthermore, the covariance of the old estimate $\hat{x}_{k-1}$ and the noise variance of the new observation $y_k$, are also given as

$$cov(\hat{x}_{k-1}) = P_{k-1} = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$

and

$$var(v_k) = R = 5$$

**Solution**:

From the observation equation, matrix $H_k$ is obtained: $H_k = [1 \ 1]$.  

Step 1: using Eqn (3.7) the Kalman gain matrix is calculated

$$K = \begin{bmatrix} K_k^{(1)} \\ K_k^{(2)} \end{bmatrix} = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \left( \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + 5 \right)^{-1}$$

This results in

$$K = \begin{bmatrix} 0.4 \\ 0.1 \end{bmatrix}$$
Using the gain matrix value and Eqn (3.6), an estimate for $x_k$ is found

$$\hat{x}_k = \begin{bmatrix} 5 \\ -2 \end{bmatrix} + \begin{bmatrix} 0.4 \\ 0.1 \end{bmatrix} \begin{bmatrix} 4.5 & 1 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ -2 \end{bmatrix} = \begin{bmatrix} 5.6 \\ -1.86 \end{bmatrix}$$

Finally, from relationship (3.8), the minimum covariance of $\hat{x}_k$ is calculated as follows

$$P_k = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 0.4 \\ 0.1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix} = \begin{bmatrix} 2.4 & -0.4 \\ -0.4 & 0.9 \end{bmatrix}$$

### 3.2 Permeate Local Flux Concept

Local flux is denoted by $J_p$. This is an important concept in the field of membrane bioreactors, worthy of explanation in a separate section. The local flux, $J_p$, is in fact the circulation rate in an open pore. Therefore it is implied that if the number of open pores decreases, the sectional area, $n_p S_p$, decreases as well, which in turn induces the flow rate, $J_p$, through the open pores to increase. The balance between these two factors facilitates the assumption $Q = \text{constant}$ in Eqns (2.1) and (2.3).

### 3.3 Darcy’s Law

To explain Darcy’s law, the figure below is drawn with symbols that are used in the equations.

![Figure 3.1: Darcy’s law](image)

In general, Darcy’s law, see [17], reads as:

$$J_p = \frac{-\kappa(P_b - P_a)}{\mu L}$$

(3.9)

with

$L = \text{pipe length} \ [m]$

$A = \text{cross-sectional area} \ [m^2]$

$\kappa = \text{permeability} \ [m^2]$

$Q = \text{total permeate} \ [m^3/s]$

$J_p = \text{local flux} \ [m/s]$
CHAPTER 3. THEORY

\[ P_a \geq P_b \]
\[ P_a - P_b = \text{pressure drop in Pa.} \] The pressure drop takes place over the length \( L \).
\[ \mu = \text{dynamic viscosity in Pa}\cdot\text{s or kg/m}\cdot\text{s} \]

After multiplying both sides of Eqn (3.9) by the area \( A \) it can be written as

\[ Q = J_pA = -\frac{\kappa A \Delta P}{\mu L} \] (3.10)

Calculating \( \Delta P \) from this equation leads to

\[ \Delta P = \frac{\mu J_p L}{\kappa} \] (3.11)

The factor \( L/\kappa \text{[m}^{-1}\text{]} \) is assumed to be the hydraulic resistance and is denoted by \( R_p \), which is called the open pore hydraulic resistance with dimension \([m}^{-1}\text{]}. Darcy’s law for \( \Delta P \) can be simplified to

\[ \Delta P = \mu R_p J_p \] (3.12)

Eqn (3.12) is used as a basic equation to derive the differential equation of the transmembrane pressure:

\[ \frac{d\Delta P}{dt} = \alpha \Delta P^2 t \] (3.13)

In Chapter 2 is Eqn (3.13) in detail discussed and in Appendix B it is derived analytically using physical relationships on membrane properties.

Moreover, if the change in pressure is negative (in the \( x \)-direction) then the flow will be positive (in the \( x \)-direction). Dividing both sides of the Eqn (3.10) by the area and using more general notation leads to

\[ q = \frac{-\kappa}{\mu} \nabla P \] (3.14)

where \( q \) is the filtration velocity or Darcy flux (discharge per unit area) and \( \nabla P \) is the pressure gradient vector.
Chapter 4

Parameter Estimation

Parameter estimation is an important part of the identification theory from which an appropriate model structure can be obtained using experimental data. The accuracy of a model depends mainly upon the accuracy of the parameter estimates within the model. The estimation method and the choice of algorithm are also of substantial importance in reducing estimation errors and subsequently obtaining an accurate model.

In the previous chapters, an algebraic equation for TMP has been derived as follows

$$\Delta P(t) = \frac{2 \Delta P_0}{2 - \alpha \Delta P_0 t^2}$$  \hspace{1cm} (4.1)

The unknown parameter $\alpha$ in this equation is a key parameter which is defined as in Eqn (2.8). In this chapter two methods used to estimate the so-called transmembrane pressure parameter, $\alpha$, are discussed. First, an off-line method is briefly explained. Second, a recursive estimation method is elaborated upon for estimation of this parameter.

4.1 Off-line Estimation of TMP parameter, $\alpha$

In literature, see e.g. [2, 13], the parameter $\alpha$ is estimated off-line. In this thesis, the TMP parameter is also estimated off-line in order to compare the off-line estimation outcomes with the recursive estimation results.

For off-line parameter estimation, a nonlinear least squares method is usually used to estimate the parameter. In Matlab, this estimation method is referred to as \texttt{lsqnonlin}. For a Matlab code of this, refer to Appendix D. Three sets of experimental data are used for the calculation of $\alpha$. The estimation results are presented in Chapter 6.

For a set of measurement data ($t$, $\Delta P$), the unknown parameter $\alpha$ is estimated off-line. Using the TMP model, i.e. Eqn (2.11), each of the estimates of $\alpha$ is calculated by

$$\hat{\alpha} = \frac{2}{t^2} \left[ \frac{1}{\Delta P_0} - \frac{1}{\Delta P} \right]$$  \hspace{1cm} (4.2)

The results are depicted as follows
Figure 4.1: A scatter plot of \( \alpha \) tends to be a function of time.

The values of \( \alpha \) in Figure 4.1 are estimated off-line. The scatter plot gives as a first impression that the unknown parameter, \( \alpha \), would be a time-varying parameter.

4.2 Recursive Estimation of TMP parameter, \( \alpha \)

Figure 4.1 in previous section is a scatter plot of \( \alpha \) in which the TMP model is confronted with a set of experimental data. It shows a different value for estimates of \( \alpha \) on each time \( t_k \). This pattern reminds a different approach for the estimation of \( \alpha \).

A recursive estimation method should be used to estimate this parameter of the model more accurately. For this purpose the well-known Kalman filter is used to estimate the parameter \( \alpha \) present in the model. Note that, recursive estimation means repeatedly updating the estimates based on use of the measurement, \( z \). During each update only one output observation is processed.

In order to define an output equation for the model, the TMP relation, Eqn (2.11), is rewritten. The following expression is obtained for the model output, \( y \)

\[
y = \Delta P - \Delta P_0 = (\frac{1}{2} \Delta P_0 \Delta P t^2) \alpha
\]

In Eqn (4.3) the parameter \( \alpha \) and model output variable, \( y \), are linearly related. Concerning the general form of equations in (3.1) and (3.2), a suitable equation form is found for recursive estimation of \( \alpha \) using the state space model

\[
\begin{align*}
\alpha_{k|k-1} &= \alpha_{k-1} + w_k \\
y_k &= (\frac{1}{2} \Delta P_0 \Delta P t^2) \alpha_k + v_k
\end{align*}
\]
Comparing this result with Eqn (3.1) and (3.2), the following matrices are obtained

\[
\begin{align*}
A &= 1, \quad B = 0, \quad u = 0 \\
H &= \frac{1}{2} \Delta P_0 \Delta P t^2
\end{align*}
\]

Where, $\alpha$ is a scalar parameter to be estimated; the vectors $w$ and $v$ are the system noise and the measurement noise respectively with the assumption that a zero-mean exists, i.e. $E(w) = E(v) = 0$. The uncorrelated Gaussian random processes $\{w_k\}$ and $\{v_k\}$ have covariances $Q_k$ and $R_k$, respectively, at time $t_k$, where $k$ is the time index. For the output variable, as mentioned earlier, it holds that $y_k = \Delta P_k - \Delta P_0$. In all corresponding Kalman filter equations the initial value for $\alpha_0$ and initial value for the covariance matrix $P_0$ has to be specified.
Chapter 5

State Estimation

5.1 The necessity of state estimation in MBR systems

Some readers might ask themselves the question: why is, in addition to parameter estimation, state estimation in an MBR system necessary? The model defined in this chapter can even be solved analytically. It can also be simulated by e.g. using an ODE function from Matlab. Then why state estimation? To answer this question, a concise explanation on the necessity of state estimation in an MBR system is given here.

With both system simulation and state estimation, insight is acquired into the membrane fouling and working conditions. By calculation of state estimates up to date information can be obtained on the mass of solutes in the MBR and the number of open pores on the membrane at time $t_k$. However, two major drawbacks are present when simulating the system: (i) there is a high risk that the resulting estimates significantly deviate from the true state estimates, and (ii) the initial state values are always unknown. A large deviation in initial state values can negatively influence the optimal state trajectory.

State estimation on the other hand, does not have these drawbacks and has even more advantages: Firstly, state initial values can be taken from the experimental measurements, and secondly, by on-line state estimation, the state estimates are related to the measurements from practical experiments. This is a very important step which is not possible with either system simulation or analytical solving of the system equations. Involving practical measurements in the state estimation can have numerous advantages, such as error correction arising from the estimation procedure at each time. Also, the error arising from model output is somewhat corrected by this method. This can also be useful if the system is a control system or if the system must be controlled over time.

5.2 System Definition

A system with two states is defined. The change of mass, $m$, interacting at each time with the membrane material and being susceptible to retention in the pores is proportional to the flow of matter through the membrane. As the first state, the mass, $m(t)$, is defined as
follows
\[ \frac{dm(t)}{dt} = k_1 C_{\text{solute}} Q \tag{5.1} \]

The assumption is that at the beginning of the experiment, at \( t = 0 \), there is no mass interaction with the membrane material, implying \( m(0) = 0 \).

The second state is chosen as the number of open pores, \( n_p \), at each given time. The change in number of open pores is proportionate with the mass, \( m \), and is defined as follows
\[ \frac{dn_p(t)}{dt} = -k_2 m \tag{5.2} \]

At the beginning of the experiment, it is assumed that all pores are open: \( n_p(0) = n_{p0} \gg 0 \).

During the entire experiment the transmembrane pressure, \( \Delta P \), is measured. The system output equation is defined on the basis of the following relationship
\[ y(t) = \Delta P = \mu R_p J_p \tag{5.3} \]

Since \( J_p = Q/(n_p S_p) \), the output equation can be rewritten as
\[ y(t) = \frac{\mu Q R_p}{S_p n_p} \tag{5.4} \]

In the state space form, the system is written as follows
\[
\begin{cases}
\frac{dm}{dt} = k_1 C_{\text{solute}} Q \\
\frac{dn_p}{dt} = -k_2 m \\
y(t) = \frac{\mu Q R_p}{S_p n_p}
\end{cases} \tag{5.5}
\]

with the initial state values, \( m(0) = 0 \) and \( n_p(0) = n_{p0} \gg 0 \). The state space from in Eqn (5.5) has the following general form
\[
\begin{cases}
\frac{dx}{dt} = Ax + Bu \\
y = g(x, u)
\end{cases} \tag{5.6}
\]

From the state space model, Eqn (5.5), the system matrices can be read: \( A = \begin{bmatrix} 0 & 0 \\ -k_2 & 0 \end{bmatrix} \), \( B = [1 \ 0]^T \), \( x = [m \ n_p]^T \) and \( u = k_1 C_{\text{solute}} Q \)

The system is not linear because the output, \( y(t) \), is nonlinearly dependent on the second state variable, \( n_p \). Linearization of the system results in the following equation
\[ \frac{dg}{dx} = \begin{bmatrix} 0 & -\mu R_p Q \\ 0 & S_p n_p \end{bmatrix} \tag{5.7} \]

The matrix, \( C \), of the linearized system thus can be defined as
\[ C = \begin{bmatrix} 0 & -\mu R_p Q \\ 0 & S_p n_p \end{bmatrix} \]
5.3 System properties

In this section important properties of the system, which has been defined in the previous section, are elaborated on. Properties in particular stability and controllability, are discussed.

The eigenvalues of the system matrix defined in previous section are equal to \([0 \ 0]\), which implies that the system is stable though not asymptotically stable. System observability is a necessary property for state estimation purposes. Hence, its observability is analyzed below.

The observability matrix of the system is defined as

\[
O = \begin{bmatrix}
C \\
CA
\end{bmatrix}
\]

\[
\Rightarrow O = \begin{bmatrix}
0 & -\mu R_p Q \\
k_2 \mu R_p Q & \frac{k_2 \mu R_p Q}{2 \eta P n_p^2} & 0
\end{bmatrix}
\]

with matrices \(A\) and \(C\) as given in the previous section. The matrix \(O\), which is composed from the matrices \(A\) and \(C\), is a non-zero, off-diagonal matrix. It can easily be calculated that rank \(O = 2\), which implies that this matrix has a full rank, and hence the system in Eqn (5.5) is observable.

The controllability matrix, \(\mathcal{R}\), is defined being \([B \ AB]\), with \(A\) and \(B\) as in the previous section. The system is controllable if \(\mathcal{R}\) has a full rank.

\[
\mathcal{R} = [B \ AB] = \begin{bmatrix}
1 & 0 \\
0 & -k_2
\end{bmatrix}
\]

(5.8)

The matrix \(\mathcal{R}\) has rank 2, hence the system Eqn (5.5) is a controllable system. Since the system is controllable and observable, the system is deemed to be minimal.

5.4 Relationship between the two proportionality constants

To perform the state estimation procedure as accurately as possible, there is a need to estimate the two proportionality constants, \(k_1\) and \(k_2\). The system defined in Section 5.2, can be solved analytically. From the analytical solution, the product, \(k_1 k_2\), of the two proportionality constants, \(k_1\) and \(k_2\), can be calculated. Analytical solutions of the solutes mass, \(m\), from Eqn (5.1) and the number of open pores, \(n_p\), from Eqn (5.2) result in the following equations, respectively for \(m\) and \(n_p\).

\[m(t) = k_1 C_{\text{solutes}} Q t, \quad m(0) = 0\]  

(5.9)

and for \(n_p\)

\[n_p(t) = -\frac{1}{2} k_1 k_2 C_{\text{solutes}} Q t^2 + n_p(0), \quad n_p(0) = n_p(0) \gg 0\]  

(5.10)
On the sub-critical time interval, \( t = [0, \ t^*] \), where the TMP model is valid, an interval value for the final values of \( [n_p(t)]^* \) can be defined as the following

\[
[n_p(t)]^* \in [0, \ \bar{n}_p]
\]

where \( \bar{n}_p \) is an arbitrarily chosen upper limit for \( [n_p(t)]^* \) at time \( t^* \). It can be assumed that at the end of the experiment not all membrane pores are closed, but e.g. 5% or 10% or \( r \) percent. In this case it holds that \( \bar{n}_p = r \cdot n_p(0)/100 \).

For \( [n_p(t)]^* = 0 \), Eqn (5.10) results in the following formula for the product \( k_1 k_2 \)

\[
k_1 k_2 = \frac{n_p(0)}{2C_{\text{solute}}Q t^2}
\]

and for \( [n_p(t)]^* = \bar{n}_p \), this product is calculated such that

\[
k_1 k_2 = \frac{n_p(0) - \bar{n}_p}{2C_{\text{solute}}Q t^2}
\]

From the latter two equations, an interval value for the product \( k_1 \cdot k_2 \) is obtained

\[
k_1 k_2 \in \left[ \frac{n_p(0) - \bar{n}_p}{2C_{\text{solute}}Q t^2}, \ \frac{n_p(0)}{2C_{\text{solute}}Q t^2} \right]
\]

For more details and results on \( k_1 - k_2 \) relationship, refer to Chapter 6.
Chapter 6

Results and Discussion

6.1 Parameter Estimation

In this section the results of the estimation of unknown parameter $\alpha$ are presented using both off-line and on-line estimation methods. Two different data sets are used for off-line parameter estimation and three for recursive estimation purposes.

Recall the equations $\beta = k_1 k_2 S_p C_{solute}$ and $\gamma = \mu R_p$, i.e. Equations (2.9) and (2.10) from Chapter 2. The parameter $\alpha$ can be written as a combination of $\beta$ and $\gamma$, i.e.

$$\alpha = \frac{\beta}{\gamma}$$

(6.1)

Substituting this parameter combination into the TMP model, Eqn (2.11), results in the following equation

$$\Delta P(t) = \frac{2\Delta P_0}{2 - \frac{\beta}{\gamma} \Delta P_0 t^2}$$

(6.2)

An attempt has been made to estimate the two parameters $\beta$ and $\gamma$ separately instead of $\alpha$ in its entirety. Looking at Eqn (6.2) however, because of the construction $\beta/\gamma$, these parameters are not separately identifiable. Hence, the unknown parameter $\alpha$ is studied as a whole.

6.1.1 Off-line estimation of $\alpha$

The estimation results of the TMP parameter, $\alpha$, together with the standard deviation of the residuals, $\sigma_\epsilon$, are shown in Table 6.1. The parameter estimation results are presented for three TMP data sets, I, II and III.

<table>
<thead>
<tr>
<th>Data set</th>
<th>$\hat{\alpha}$</th>
<th>$\sigma_\epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$4.0931 \times 10^{-4}$</td>
<td>0.5702</td>
</tr>
<tr>
<td>II</td>
<td>$1.4232 \times 10^{-6}$</td>
<td>0.6012</td>
</tr>
<tr>
<td>III</td>
<td>$6.074 \times 10^{-5}$</td>
<td>19.6921</td>
</tr>
</tbody>
</table>
Using the first two estimates of $\alpha$, the TMP model (2.11) is fitted to the experimental data. The results are depicted in Figures 6.1 and 6.2 using Data Set I and Data Set II, respectively.

Figure 6.1: Model fitting results when $\alpha$ is estimated off-line, Data Set I

And

Figure 6.2: Model fitting results when $\alpha$ is estimated off-line, Data Set II

It is clear from the Figures 6.1 and 6.2 that off-line estimation of $\alpha$ does not result in a good fit between the proposed model and the real experimental data. This was also observed by [2], where time-variability of $\alpha$ is suggested. In the following section, the TMP parameter $\alpha$ is estimated on-line using a Kalman filter algorithm. For this purpose the data sets I and III are chosen. It should be noticed that using different data sets result
in similar outcomes.

6.1.2 Recursive estimation of $\alpha$: Data Set I

The estimation results in Figure 6.3 show that the parameter $\alpha$, using Data Set I, is not a constant parameter but a time-varying parameter.

![Figure 6.3: Estimates of $\alpha$ using the Kalman filter](image)

In the upper panel of Figure 6.3, the recursive estimates of parameter $\alpha$ are plotted. These estimates are calculated using the Kalman filter. The upper graph in Figure 6.3 once again plotted in Figure 6.4 together with the hyperbolic fitted values of the estimates of $\alpha$. This figure shows that the obtained estimates fit a hyperbolic function.

![Figure 6.4: Recursive estimates of $\alpha$ (circled) and fitted values of estimates (solid line)](image)
The circled curve shows the recursive estimates of $\alpha$, i.e. $\hat{\alpha}$-values. The solid line is plotted by using the hyperbolic function $\dot{\alpha}t = c$. Alternatively, the fitted curve from Figure 6.4 and the scatter plot of $\alpha$ from Figure 4.1 are plotted in the same figure, as follows.

![Figure 6.5: off-line estimates of $\alpha$ (circled), and the estimates from the Kalman filter fitted](image)

where, the dashed line is the hyperbolic fitting of the recursive estimates of $\alpha$, i.e $\dot{\alpha}t = c$, and the circled line a scatter plot of $\alpha$-estimates, which are estimated off-line from the Eqn (2.11). As Figures 6.4 and 6.5 show, the estimates of $\alpha$ in both using a recursive or off-line parameter estimation method tend to fit a hyperbolic function in the form of $\dot{\alpha}t = c$.

### 6.1.3 Recursive estimation of $\alpha$: Data Set III

The estimation results in Figure 6.6 show that the parameter $\alpha$, using a different set of experimental data exhibits a time-varying pattern.
Considering Figures 6.3 - 6.6, there is strong evidence that the TMP parameter $\alpha$ is a time-varying parameter and not constant. In what follows, an attempt is made to model the recursive estimates of $\alpha$ presented in Figures 6.3 and 6.6. Using a curve fitting algorithm, it was discovered that the estimates of $\alpha$ perfectly fit a hyperbolic relationship in the following form

$$\alpha \cdot t = c$$

(6.3)

where $c$ is a constant, yet to be estimated. The constant $c$ can be estimated from

$$\hat{c} = \frac{1}{N} \sum_{t=1}^{N} \hat{\alpha}_t \cdot t$$

(6.4)

where $\hat{\alpha}_t$ is the recursive estimates obtained from the Kalman filter estimation and $t$ is the time index. Hereto, the Matlab command $\text{mean}(\hat{\alpha} \ast t)$ is used to obtain an estimate for the constant $\hat{c}$. In Figure 6.7, the estimates of $\alpha$ from Figure 6.6 are plotted together with hyperbolic fitted values of that estimates.
Figure 6.7: The estimates from the Kalman filter obey a hyperbolic function

In Figure 6.7, the dashed line shows the estimates resulting from the Kalman filter, i.e. $\hat{\alpha}_t(KF)$, and the solid curve refers to the hyperbolic fitting of the Kalman filter estimates, i.e. $\hat{\alpha} = \hat{c}/t$.

### 6.2 Model Structure Modification

From the Figures 6.3 and 6.6 in the previous section, a hyperbolic relationship for estimates of $\alpha$ were found in the following form

$$\dot{\alpha}(t) = \frac{c}{t} \quad (6.5)$$

This hyperbolic relationship will be used in the TMP equation, (2.11), for model structure modification purposes. Substituting this function into Eqn (2.11) will lead to a new equation, which will be the new modified model for transmembrane pressure, $\Delta P(t)$.

In the previous section it was demonstrated that the model (2.11), proposed by Ognier et al. [13] does not fit the real experimental data obtained from Wetsus, Leeuwarden. This was due to time-varying characteristics of $\alpha$. In this section, therefore, the TMP model from Eqn (2.11) is adapted using the new relationship for $\alpha$, namely

$$\alpha t = c \quad (6.6)$$

A new TMP model is calculated by replacing $\alpha \cdot t$ in Eqn (2.11) by the constant $c$, which is estimated from $\dot{\alpha}(t)t = c$. See Chapter 3 for more details. The estimates for $\dot{\alpha}_t$ were calculated by applying the Kalman filter. A new model for calculating TMP is then obtained as follows
6.2. MODEL STRUCTURE MODIFICATION

\[ \Delta P(t) = \frac{2\Delta P_0}{2 - c\Delta P_0 t} \]  

(6.7)

This model seems to fit the experimental data much better than Eqn (2.11). The improved model structure resulting from the use of Eqn (6.7) is demonstrated graphically in Figure 6.8.

![Figure 6.8: Experimental data fitted by an adopted model, Data Set I](image)

Using a different experimental data set showed similar corresponding results with the newly adopted model, Eqn (6.7). The result is depicted in the following figure.

![Figure 6.9: Experimental data fitted by an adopted model, Data Set II](image)
6.3 Interpretation of the time-varying property of $\alpha$

A very important and interesting question to be answered is: what does it mean that $\alpha$ is a time-varying parameter and not a constant? The answer to this question is related to the parameter $R_p$, the open pores hydraulic resistance. According to our findings, this parameter is not a constant value, as was assumed by Ognier et al. [13], but is rather a time-varying variable. Recall from Chapter 2 the following relationship for the parameter $\alpha$

$$\alpha = \frac{\beta}{\gamma} = \frac{\beta}{\mu R_p}$$  \hspace{1cm} (6.8)

where $\beta \triangleq k_1 k_2 S_p C_{solutes}$

As was shown in Sections 4.2 and 6.1, the parameter $\alpha$ is not a constant, but it fits a hyperbolic relationship as a function of time $t$

$$\alpha = \frac{c}{t}$$  \hspace{1cm} (6.9)

where $c$ is a constant, estimated from Eqn (6.4).

By combing the two relationships, Eqn (6.8) and Eqn (6.9), a time-depended equation for open pores hydraulic resistance, $R_p$, is found as follows

$$R_p = \frac{\beta}{c\mu} t$$  \hspace{1cm} (6.10)

As it is seen, $R_p$ depends linearly on time $t$. Taking the derivative from Eqn (6.10) provides a differential equation that can be seen as a new system equation in the state space formulation and is written as

$$\frac{dR_p}{dt} = \frac{\beta}{c\mu} = \delta$$  \hspace{1cm} (6.11)

By Eqn (6.11) the new state variable, $R_p$, is introduced, which is a linear function of time and could be considered as one of the differential equations of a new system.

It should be noticed that integrating Eqn (6.11) with respect to time variable $t$ results again in Eqn (6.10) with $R_p(0) = 0$. The initial value of $R_p$ is zero since there is no solutes-open pore interaction and consequently no resistance at time instance $t = 0$.

6.4 State Estimation

6.4.1 Output Equation Definition

For state estimation purposes, the Kalman filter is used for estimation of the states $m(t)$ and $n_p(t)$, defined in Eqn (5.5). As it is seen, the system is a non-linear system because of nonlinearity in the output equation, $y$. It is a so-called rational system, implying that the Kalman filter can not be directly applied for state estimation purposes. To apply the
Kalman filter to this system it must be transformed into a linear form, [3, 8].

Recall Darcy’s law for transmembrane pressure, $\Delta P$, from Chapter 2 defined as

$$
\Delta P = \mu R_p J_p
$$

(6.12)

where the local flux rate, $J_p$, is the flow through an open pore. Refer back to Chapter 2 for more details on $J_p$

$$
J_p = \frac{Q}{n_p S_p}
$$

(6.13)

Substituting Eqn (6.13) in Eqn (6.12) the following expression is obtained for $\Delta P$

$$
\Delta P = \mu R_p \frac{Q}{n_p S_p}
$$

(6.14)

Rewriting Eqn (6.14) results in the following equality

$$
n_p S_p \Delta P(t) = \mu R_p Q
$$

(6.15)

Recall that $n_p$ is chosen as one of the two states in the system under study. Based on the system definition in Eqn (5.5), the expression in Eqn (6.15) can also be written as follows

$$
S_p \Delta P x_2 = \mu R_p Q
$$

(6.16)

where the second state variable, $n_p$, is denoted by general state variable $x_2$.

In the previous sections, the TMP parameter, $\alpha$, modified as a time-varying hyperbolic function

$$
\alpha t = c
$$

(6.17)

Combining this model with the expression of $\alpha$ in Eqn (2.8), a time dependent equation is found for the open pore resistance, $R_p$

$$
R_p = \eta t
$$

(6.18)

where $\eta$ is defined as

$$
\eta \triangleq \frac{k_1 k_2 C_{\text{solute}} S_p}{\mu c}
$$

(6.19)

Substituting $R_p$ from Eqn (6.18) into the equality Eqn (6.15), the following expression is obtained

$$
S_p \Delta P n_p = \mu \eta t Q
$$

(6.20)

Finally, from the equality in Eqn (6.20), an output model is defined as follows

$$
y(t) \triangleq \mu \eta t Q = (S_p \Delta P(t)) n_p
$$

(6.21)

The output equation (6.21) is a linear function in the state variables, $n_p$ and $m$. It is therefore used for state estimation objectives. The output-state relating matrix $H$ defined in Eqn (3.2), can be read from Eqn (6.21) as follows

$$
H(t) = [0 \ S_p \Delta P(t)]
$$

(6.22)
where the coefficient of the state $m$ is equal to 0 and that of the second state is equal to $S_p \Delta P(t)$. This is more clear if it is written as

$$
\begin{bmatrix}
0 & S_p \Delta P(t)
\end{bmatrix}
\begin{bmatrix}
m \\
n_p
\end{bmatrix}
$$

with the matrix $H$ as in Eqn (6.23) and state variable vector $x = [m \ n_p]^T$.

### 6.4.2 Results from State Estimation

State estimation is performed for the system defined in Eqn (5.5). For this thesis project two states, $m$, and $n_p$, are chosen and estimated. To plot this figure, the two proportionality constants are specified as: $k_1 = 21$ and $k_2 = 20.1 \times 10^{-5}$.

![Graphs showing state estimates](image)

Figure 6.10: State estimates using Data Set I

The first graph in Figure 6.10 shows a linear relationship between the solutes mass, $m$, and the time variable, $t$. This is also in accordance with the mass differential equation, Eqn (2.3), because the mass rate with respect to time is supposed to be constant. The second graph observes a parabolic equation form with a maximum, and corresponds to the differential equation of the number of open pores as defined in Eqn (2.4). In Table 6.2 the initial and final values from Figure 6.10 are given for possible comparison purposes.

<table>
<thead>
<tr>
<th></th>
<th>$m$ [g]</th>
<th>$n_p$</th>
<th>$v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0</td>
<td>3000</td>
<td>$-7.689 \times 10^{-8}$</td>
</tr>
<tr>
<td>Final</td>
<td>275</td>
<td>103</td>
<td>$-5.209 \times 10^{-9}$</td>
</tr>
</tbody>
</table>
6.4. STATE ESTIMATION

The final values of $m$ and $n_p$ in Table 6.2 require special attention. As was seen in Eqn (5.13), the relationship between the two proportionality parameters, $k_1$ and $k_2$, is $k_1k_2 \in \bar{a}$, where $\bar{a}$ is an interval. It indicates that $k_1$ and $k_2$ are hyperbolically related. This implies that the larger the final value of mass in Figures 6.10 and 6.11, the smaller the final number of open pores, $n_p$, will be. This becomes more clear when it is explained and compared with the final values of, $m$, and, $n_p$, in Table 6.3 below, where Data Set II is used. It is important to note again that the final mass value is influenced by the proportionality of $k_1$, and the final value of $n_p$ is determined by the value of the proportionality constant $k_2$. The results from the state estimation of the second data set are shown in Figure 6.11. To plot the figure, $k_1 = 6$ and $k_2 = 15.2 \times 10^{-5}$ are specified.

The course of the graphs in Figure 6.11 is similar to that in Figure 6.10, with the exception that a different data set is used. The initial and final values read from Figure 6.11 are presented in Table 6.3.

Table 6.3: Initial and final estimates from Data Set II

<table>
<thead>
<tr>
<th></th>
<th>$m$ [g]</th>
<th>$n_p$</th>
<th>$v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0</td>
<td>3000</td>
<td>$-7.914 \times 10^{-8}$</td>
</tr>
<tr>
<td>Final</td>
<td>165</td>
<td>232</td>
<td>$-5.974 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

The final values of solutes mass, $m$, and the number of open pores, $n_p$, can be compared with the value in Table 6.2. In Table 6.3, less final mass value, smaller value for $k_1$, resulted in more open pores at the end of the experiment, thus a larger value for $n_p$. Comparably, in Table 6.2 high mass value, larger value for $k_1$, resulted in less open pores at the end of
the experiment. This is because \( k_1 \) and \( k_2 \) are proportionality constants in the differential equations of \( m \) and \( n_p \), respectively.

6.5 Results for \( k_1k_2 \) relationship

As seen in Eqn (5.13), the two proportionality parameters relate to each other in the following form

\[
k_1k_2 \in \bar{a}
\]  

(6.24)

where \( \bar{a} \) is an interval. In what follows, using the known data from Table 6.4, the relationship between \( k_1 \) and \( k_2 \) is explored. The data in the Table 6.4 corresponds to both practical and experimental situations.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>description</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_p(0) )</td>
<td>total initial number of open pores</td>
<td>3000</td>
</tr>
<tr>
<td>( \bar{n}_p )</td>
<td># of open pores at the end of experiment</td>
<td>5% of ( n_p(0) ) = 150</td>
</tr>
<tr>
<td>( C_{\text{solutes}} )</td>
<td>concentration of solutes in solution</td>
<td>30 g/m(^3)</td>
</tr>
<tr>
<td>( Q )</td>
<td>permeate flow</td>
<td>( 4.167 \times 10^{-6} \text{m}^3/\text{s} )</td>
</tr>
<tr>
<td>( t )</td>
<td>time interval in which experiment is conducted</td>
<td>( s )</td>
</tr>
</tbody>
</table>

The following numerical result is thus calculated for \( k_1 \) and \( k_2 \)

\[
k_1k_2 \in \left[ \frac{2850}{2.5 \times 10^{-4}t^2}, \frac{150}{2.5 \times 10^{-4}t^2} \right]
\]  

(6.25)

where \( t \) is the experimental time interval defined as \( t < t^* = \sqrt{\frac{2}{\Delta \rho \alpha}} \). In Figure 6.12 this relationship is illustrated.
6.5. RESULTS FOR $K_1K_2$ RELATIONSHIP

The relationship between $k_1$ and $k_2$ illustrates a hyperbolic curve. From Eqn (5.13) it is clear that there is a spectrum of suitable curves which can also fit into Figure 6.12, instead of just one curve.

Due to the significantly lower order of magnitude of the $k_2$ values in comparison with those of $k_1$, the $y$-axis in Figure 6.12 is chosen as a logarithmic scale in order to highlight the trend of curve follows.
Chapter 7

Conclusions

The aim of this thesis was to study the physical membrane fouling equations derived by Ognier et al. [13] for parameter and state estimation purposes. The results obtained from parameter estimation were used for modification of a transmembrane pressure model structure.

Three data sets have been taken as starting points for off-line estimation of the TMP parameter, $\alpha$. The outcomes from the estimation results were significantly different from real experimental of three varying data sets. This was also observed by [2] where the following is stated about the parameter $\alpha$

Many components are incorporated into the $\alpha$ parameter, which is assumed to be constant with time. Given that [MBR] operation is over a prolonged period and fouling constituents are likely to change because of the diversity of the feed suspension, this assumption [that $\alpha$ is a constant parameter] may not be valid, such that $\alpha$ should more correctly be expressed as a function of time.

Consequently, the TMP parameter was estimated using a recursive estimation method (the Kalman filter). By applying the Kalman filter estimator, it was found that the parameter $\alpha$ is a time-varying parameter and is not a constant. This is the reason that we suggest an on-line parameter/state estimation method in the MBR systems rather than an off-line estimation algorithm; which provides an answer to Research Question 1.

The recursive estimates, $\hat{\alpha}$, showed a hyperbolic relationship between the estimates and the experimental time, $t$, in the form of $\hat{\alpha} \cdot t = c$. To answer Research Question 2, this hyperbolic relationship can simply be substituted in the TMP algebraic equation, Eqn (2.11). This means that in the denominator of this equation, the factor $\alpha \cdot t$ is replaced by a constant value $c$.

Analyzing the relationship for $\alpha$, i.e. Eqn (2.8), we see what the factor $R_p$ has to do with the so called membrane fouling mechanisms. It should be noted that the other terms
in this equation have been assumed to be constants in this thesis project. This indicates that the time-variability of the parameter $\alpha$, results in the time-variability of the hydraulic open pores resistance, $R_p$. From Eqn (6.10), it is clear that the hydraulic resistance, $R_p$, is a linear function of time as $R_p = \delta \cdot t$, where $\delta$ is a proportionality constant.

It is clear that a complete answer has not been given to the question (Research Question 3): which fouling mechanism is this precisely? There are three types of membrane fouling mechanisms: (i) pore blockage, (ii) adsorption, biofouling and (iii) cake-forming. Due to linearity between $R_p$ and $t$, this mechanism is most likely the cake-forming. More research is needed to find out the characteristics of the three fouling mechanisms and to be sure which mechanism is precisely described by the relationship $R_p = \delta \cdot t$.

Finally, to answer Research Question 4, we must have a good knowledge of membrane bioreactor (MBR) systems and the working situations in which the MBR systems operate. MBR systems have two main working conditions

- Membrane bioreactor systems are operated over a long period
- Heterogeneity of the feed suspension suggests fouling mechanisms (constituents) are likely to change over time.

This gives strong indications that the MBR system states and parameters should be estimated using on-line estimation algorithms, like the Kalman filter, which is used in this thesis to estimate states and parameters present in the models.
Chapter 8

Recommendation

8.1 An Algebraic Equation for Proportionality Parameters

Two differential equations are defined in Chapter 5. The first equation is for interacting solutes mass, \( m \), with membrane material and the second is for the number of open pores, \( n_p \).

Referring to Chapter 5, it is probable that there is a hyperbolic relationship between the two proportionality parameters, \( k_1 \) and \( k_2 \). Using a greater number of real experimental data sets and a suitable parameter estimation technique, a mathematical relationship could be found that relates these two parameters.

8.2 Future Research Outlook

On-line prediction should be performed so as to estimate the fouling outputs. This means that while conducting the experiment, predictions can be done for a limited time interval using the measured data available at that given moment in time. This is useful because of the possibility to estimate error corrections at each \( t_k \).

Recall the system in state space form which is defined in Chapter 5 for state estimation purposes, Eqn (5.5)

\[
\begin{align*}
\frac{dm}{dt} &= k_1 C_{\text{solute}} Q \\
\frac{dn_p}{dt} &= -k_2 m \\
y(t) &= \frac{\mu Q R_0}{S_p n_p}
\end{align*}
\]

where only two states, \( m \) and \( n_p \) are used. The system defined here can be extended to more states and equations. One or more time-varying control variables could be added to the system. The permeate flow rate, \( Q \), can for example be assumed as a control variable. This can lead to the set up of a time-varying control system. Using a time-varying control variable in the system can lead to application of a Model Predictive Control (MPC)
technique to identify the desired system more accurately.

Other possible control variables which may be incorporated in the system are: (i) Sludge inflow ($Q_m$) in m$^3$/s (ii) Airflow rate at the vicinity of the membrane ($q$) in m$^3$/h and (iii) The stirrer speed ($r_s$) in the bioreactor in rpm. For some relevant studies on membrane air sparking concept refer to [1, 2, 9].
Bibliography


# Appendix A

## Symbols and Abbreviations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>total membrane area</td>
</tr>
<tr>
<td>$C_{\text{solute}}$</td>
<td>solutes concentration in solution</td>
</tr>
<tr>
<td>$J$</td>
<td>permeate flux (pure water flux)</td>
</tr>
<tr>
<td>$J_p$</td>
<td>permeate flux through an open pore</td>
</tr>
<tr>
<td>$K$</td>
<td>Kalman gain</td>
</tr>
<tr>
<td>$k_1$</td>
<td>constant in proportionality</td>
</tr>
<tr>
<td>$k_2$</td>
<td>constant in proportionality</td>
</tr>
<tr>
<td>$m$</td>
<td>mass of compounds interacting with membrane material</td>
</tr>
<tr>
<td>$n_p$</td>
<td>number of open pores at time $t$</td>
</tr>
<tr>
<td>$P$</td>
<td>variance-covariance matrix of parameter estimation errors</td>
</tr>
<tr>
<td>$Q$</td>
<td>Permeate flow / volumetric flow rate</td>
</tr>
<tr>
<td>$R$</td>
<td>variance-covariance matrix of output measurement errors</td>
</tr>
<tr>
<td>$R_p$</td>
<td>an open pore hydraulic filtration resistance</td>
</tr>
<tr>
<td>$S_p$</td>
<td>an open pores sectional area</td>
</tr>
<tr>
<td>$t$</td>
<td>time variable</td>
</tr>
<tr>
<td>$t_k$</td>
<td>$k^{\text{th}}$ time instant</td>
</tr>
<tr>
<td>$\text{TMP}$</td>
<td>Transmembrane pressure</td>
</tr>
<tr>
<td>$u$</td>
<td>input variable</td>
</tr>
<tr>
<td>$v$</td>
<td>error covariance (innovations)</td>
</tr>
<tr>
<td>$x$</td>
<td>vector of state variables</td>
</tr>
<tr>
<td>$y$</td>
<td>model output variable</td>
</tr>
<tr>
<td>$z$</td>
<td>measurement data set</td>
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**Greek letters**

<table>
<thead>
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<th>Symbol</th>
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<tbody>
<tr>
<td>$\alpha$</td>
<td>$m/kg$</td>
</tr>
<tr>
<td>$\Delta P$</td>
<td>$\text{Pa}$</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>innovations process errors / residuals</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>$\text{Lm}^{-2}\text{h}^{-1}\text{bar}^{-1}$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>solution (dynamic) viscosity $\text{Pa} \cdot \text{s} = \text{kgm}^{-1}\text{s}^{-1}$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>standard deviation</td>
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**Subscripts**

<table>
<thead>
<tr>
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<th>Description</th>
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<tbody>
<tr>
<td>0</td>
<td>initial value</td>
</tr>
<tr>
<td>$k$</td>
<td>time index</td>
</tr>
<tr>
<td>p</td>
<td>an open pore</td>
</tr>
</tbody>
</table>
Appendix B

Derivation of differential equation of TMP

In this appendix, the differential equation, Eqn (2.7), of transmembrane pressure (TMP) from Chapter 2 is derived. The basic physical equations are in more detail explained in Chapter 2.

The equations for the permeate flux, $Q$, and transmembrane pressure are respectively given as

$$ Q = J_p n_p S_p \quad \text{and} \quad \Delta P = \mu R_p J_p $$

(B.1)

Substituting $J_p$ from the first equation into the second, we obtain

$$ \Delta P = \frac{\mu R_p Q}{S_p n_p} $$

(B.2)

Squaring $\Delta P$ from Eqn (B.2) leads to

$$ \Delta P^2 = \frac{\mu^2 R_p^2}{S_p^2} \cdot \frac{Q^2}{n_p^2} $$

(B.3)

Integrating the solutes mass differential equation from Eqn (2.3) results in

$$ m(t) = k_1 C_{\text{solute}} Q t + m(0) $$

(B.4)

Regarding the physical and practical situation, at the beginning of the experiment, $t = 0$, the solutes mass interacting with the membrane material and the open pores is zero. This means that in Eqn (B.4) the equality $m(0) = 0$ holds.

Substituting the expression for $m(t)$ into the differential equation of number of open pores, $n_p$, from Eqn (2.4), the following differential equation is obtained

$$ \frac{dn_p(t)}{dt} = -k_2 m = -k_1 k_2 C_{\text{solute}} Q t $$

(B.5)
Integrating Eqn (B.5) and assuming that $Q$ is constant, we get

$$n_p(t) = -\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0) \quad (B.6)$$

Substituting Eqn (B.6) into the equation for $\Delta P$, i.e. Eqn (B.2), the following is obtained

$$\Delta P = \frac{\mu R_p}{S_p} \frac{Q}{-\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0)} \quad (B.7)$$

Taking the derivative of $\Delta P$ from Eqn (B.7) with respect to $t$ results in

$$\frac{d\Delta P}{dt} = \frac{\mu R_p}{S_p} \frac{k_1 k_2 C_{\text{solute}} Q t Q}{(-\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0))^2} \quad (B.8)$$

Reorganizing and multiplying the right hand side of the expression in Eqn (B.8) by $(\mu R_p S_p) / (\mu R_p S_p)$, the following is obtained

$$\frac{d\Delta P}{dt} = \frac{\mu R_p}{S_p} \frac{k_1 k_2 C_{\text{solute}} Q^2}{(-\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0))^2} \frac{\mu R_p S_p}{\mu R_p S_p} \quad (B.9)$$

rewriting Eqn (B.9) results in

$$\frac{d\Delta P}{dt} = \frac{\mu^2 R_p^2}{S_p^2} \frac{Q^2}{(-\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0))^2} \frac{k_1 k_2 S_p C_{\text{solute}}}{\mu R_p t} \quad (B.10)$$

where it holds, see Eqn (B.7)

$$\Delta P^2 = \frac{\mu^2 R_p^2}{S_p^2} \frac{Q^2}{(-\frac{1}{2} k_1 k_2 C_{\text{solute}} Q t^2 + n_p(0))^2} \quad (B.11)$$

and by defining

$$\alpha \equiv \frac{k_1 k_2 C_{\text{solute}}}{\mu R_p} \quad (B.12)$$

the following differential equation for transmembrane pressure (TMP) is obtained

$$\frac{d\Delta P}{dt} = \alpha \Delta P^2 t \quad (B.13)$$

\[\square\]
Appendix C

Glossary

Concentration unit
Concentration unit is Molarity; symbol = M = moles solute / liter of solution.
Also mass per volume is used as concentration unit:
mass of solution
liter of solution
identical to kg/m$^3$ which is the unit of density, $\rho$.

Darcy
Henry Philibert Gaspard Darcy (June 10, 1803 - January 3, 1858) was a French engineer
who made several important contributions to hydraulics.

Estimator
In statistics, an estimator is a statistic (a function of the observable sample data) that is
used to estimate an unknown population parameter (which is called the estimand). An
estimate is the result from the function (statistic) using a particular sample of data.

Flux
The word flux comes from Latin: fluxus means "flow", and fluere is "to flow". It has
different meanings in different concepts.

Kalman filter
The Kalman filter is a mathematical estimation method named after Rudolf E. Kalman.
Its purpose is to use measurements that are observed over time that contain noise to
produce better estimates of the true value of the measurements and associated model
(calculated) values by reducing the amount of noise.

Model
A model or mathematical model is a formula that uses mathematical language to de-
scribe a system. Mathematical models are used not only in the natural and engineering
sciences (such as physics, biology, geology, meteorology and engineering) but also in the
social sciences (such as economics, psychology, sociology and political sciences).
Eykhoff [6] defined a mathematical model as 'a representation of the essential aspects of an existing system which presents knowledge of that system in suitable form'. Mathematical models can take many forms, such as dynamical models, statistical models, or differential equations.

**Modeling**
The process of developing a mathematical model is called 'mathematical modeling' (also modeling).

**Off-line estimation**
Off-line estimation is a batch (parameter) estimation method meaning that the estimation procedure occurs after the entire data has been collected over the process. This is opposite to the on-line estimation method in which parameter estimation happens while the data is being collected.

**On-line estimation**
The methods for computing online models are called recursive identification methods. Recursive algorithms are also called recursive parameter estimation, adaptive parameter estimation, and on-line algorithms. An example of recursive estimation is Kalman filter estimator which is used in this thesis.

**Pascal unit**
Pascal (symbol: Pa) is the SI unit for pressure and stress. It is a measure of force per unit area. Pascal defined as one Newton per square meter:

\[ 1 \text{ pascal (Pa)} = 1 \text{ N/m}^2 = 1 \text{ kgm}^{-1}\text{s}^{-2} \]

**System**
System (from Latin systēma) is a set of interacting or independent entities forming an integrating whole. We limit a system by defining its boundary; this means choosing which entities are inside the system and which are outside. We then make simplified models (differential equations) of the system in order to understand and to predict or influence its future behavior. These models may define the structure and/or the behavior of the system.

**TMP parameter**
In this thesis the unknown parameter, \( \alpha \), from the transmembrane pressure equation, \( \Delta P \), is named 'TMP parameter'. This name is chosen since the parameter \( \alpha \) exists in the TMP equation. The naming was necessary because this parameter, as the main unknown parameter, is used frequently throughout the entire text.
Appendix D

Matlab Routines

clear all; clc;

load Data1
t = Data1(8:end,1);  % time in min
dp = Data1(8:end,2);  % mbar
dp0 = dp(1);  % The initial TMP in Pa
N = length(t);
i = 1:N;
alpha = zeros(N,1);
a(i) = 0;
for i=1:N
    a(i) = (2*dp(i)-2*dp0)/(dp(i)*dp0*t(i)*t(i));
end;
alpha(i)=a(i);
semilogx(t,alpha,'LineWidth',2);
axis([13 2000 -0.1e-6 0.5e-5])
xlabel('\textbf{Time [min]}','FontSize',12);
ylabel('\textbf{\alpha}','FontSize',14);

function e = dpfun(alpha0,t,dp)
% Deze functie wordt gebruikt om alfa te schatten van model (8)
dp0 = dp(1);
% the calculated values from the model
Mout = dp0./(1-(alpha0*dp0*t.^2)/2);  % try to fit eq. (8) from the article
e = Mout-dp;
end

clear all; clc;
% Dit roept dpfun aan en schat door lsqnonlin een alfahat voor model (8)
% Model (8) in Ognier et al.
APPENDIX D. MATLAB ROUTINES

load Data1
t = Data1(8:end,1)/60;  % time in hour
dp = Data1(8:end,2)/10;  % kPa
alpha0 = (2*dp(end)-2*dp(1))/(dp(end)*dp(1)*t(end)^2);
display(alpha0);
[alphahat,resnorm,residual,exitflag,output,lambda,jacobian] = lsqnonlin(@dpfun,3e-11,[],[],t,dp);
display(alphahat);
save alfa alphahat
J = full(jacobian);  % the Jacobi matrix (=X(theta))
M = inv(J'*J);
display(M);
f = residual;
N = length(f);
MSE = f'*f/(N-1);
cov = MSE*M;
display(MSE);
display(cov);
--------------------------------
% Deze fit de geschatte alpha in model (8)
load alfa  % In alfa is alphahat bewaard
load Data1
t = Data1(8:end,1)/60;  % time in hour
dp = Data1(8:end,2)/10;  % [mbar/10 = kPa]

dp0 = dp(1);
y = dp0./(1-(dp0*alphahat*t.^2)/2);

plot(t,dp,'LineWidth',1);
hold on;
plot(t,y,'r-.','LineWidth',1.5);
xlabel('\textbf{Time [h]}','FontSize',12);
ylabel('\textbf{\DeltaP [kPa]}','FontSize',14);
legenda=legend('[\textbf{experimental data}]','[\textbf{model output}]');
set(legenda,'FontSize',11,'Location','NorthWest');

function [x,P,v]=kf(y,A,C,G,Q,R,x0,P0)
n = 1;  % number of parameters to be estimated
load Data1
t = Data1(9:end,1);
dp = Data1(9:end,2);
dp0 = dp(1);
N=max(size(dp));
%----------------------------
y = dp-dp0;
A=zeros(n,n,N);
C=zeros(1,n,N);
for k=1:N,
    A(:,:,k)=1;
    C(:,:,k)=dp0*dp(k)*t(k)^2/2;
end;
G = A;
Q = 0.1;
R = ones(N,1);
x0 = 1e-7; % initial parameter value(x0 = alpha0)
P0 = 1e3; % covariance of estimate at time t
%----------------------------
n=max(size(x0));
x=x0;
P=P0;
xk(:,1)=x0; %storage of recursive estimates
Pk(:,1)=P0; %storage of covariance matrices of estimates
for k=1:N
    Ak=A(:,:,k); Ck=C(:,:,k);
    Gk=G(:,:,k); Rk=R(k);
    % Old estimates:
    x = Ak*x; % estimate at (t)
    v(k) = y(k)-Ck*x; % prediction error(=innovation)
    P = Ak*P*Ak' + Gk*Q*Gk'; % covariance of system model
    % New updated estimates:
    K(:,k) = P*Ck'*inv(Ck*P*Ck'+Rk);%optimal Kalman gain matrix for updating
    x = x + K(:,k)*v(k); % updated estimate at t+1
    P = (eye(n)-K(:,k)*Ck)*P;% minimal covariance of updated estimate
    xk(:,k+1) = x;
Pk(:,k+1) = P;
end;
x=xk';
P=Pk';
v=v';
%--plot of estimates alphahats
subplot(2,1,1)
plot(0:N,x,'LineWidth',1.5);
axis([0 N -1e-7 1e-6]);
ylabel('f\alpha','FontSize',14);
subplot(2,1,2)
semilogy(0:N,abs(P),'LineWidth',2);
xlabel('f{Time [min]}','FontSize',12);
ylabel('var(\alpha)','FontSize',14);

% Deze fit de geschatte alpha in model (8)
clear all; clc;

load alfa % In alfa is alphahat bewaard
load Data1

\[ t = \frac{Data1(8:end,1)}{60}; \% time in h \]
\[ dp = \frac{Data1(8:end,2)}{10}; \% [mbar/10=kPa] \]

\[ dp0 = dp(1); \]
\[ chat = mean(alphahat.*t); \]
\[ y = \frac{dp0}{1-(Chat*dp0.*t)/2}; \]

% subplot(2,1,1)
plot(t,dp,'LineWidth',2);
hold on;
% subplot(2,1,2)
plot(t,y,'r:','LineWidth',2);
xlabel('f{Time [h]}','FontSize',12);
ylabel('f{\DeltaP [kPa]}','FontSize',14);
legenda=legend('f{experimental data}','f{model output}');
set(legenda,'FontSize',11,'Location','NorthWest');

function \[ [x,P,v]=kf(y,A,C,G,Q,R,x0,P0) \]

n = 2; \% number of states to be estimated
load Data1
\[ t = 60*Data1(6:end,1); \% t in s \]
\[ dp = 100*Data1(6:end,2); \% dp in Pa \% mbar*100 = Pa \]
\[ N = \text{max(size(dp))}; \]
\[ dt = t(15)-t(14); \% in seconds \]

mu = 1.2e-3; \% in Pa.s
k1 = 21; k2 = 20.1e-5;
Csol = 30; \% in g/m^3, [g/m^3=mg/L]
Sp = 7.854e-15;
c = 0.18e-4; Qf = 4.167e-6; % [Qf=Q] in m^-3/s
gama = k1*k2*Csol*Sp/(mu*c);
% mu*gama*t*Q = Sp*dp*x2;
y = mu*Qf*gama.*t;
A = zeros(n,n,N);
C = zeros(1,n,N);

Q = 0.1*eye(2);
R = ones(N,1);
x0 = [0 3000]'; % 3000 initial parameter value (x0 = [m0 np0])
P0 = 1e3*eye(2); % covariance of estimate at time t

n = max(size(x0));
x = x0;
P = P0;
xk(:,1) = x0; % storage of recursive estimates
Pk(:,:,1) = P0; % storage of covariance matrices of estimates
B = [1 0]';
u = k1*Csol*Qf;

for k = 1:N
    Ak = A(:,:,k);
    Ck = C(:,:,k);
    % Gk=G(:,:,k);
    Ak = eye(2) + [0 0; -k2 0]*dt;
    Ck = [0 Sp*dp(k)];
    Rk = R(k);
    % Old estimates:
    % (1) project state ahead
    x = Ak*x + dt*B*u; % estimate at (t)
    % (2) project error covariance ahead
    P = Ak*P*Ak' + Q; % covariance of system model
    % New updated estimates:
    % (1) compute the Kalman gain
    K(:,k) = P*Ck'*inv(Ck*P*Ck'+Rk); % optimal Kalman gain matrix for updating
    % (2) update measurement estimate with measurement zk
    x = x + K(:,k)*v(k); % updated estimate at t+1
    % (3) update the error covariance
    P = (eye(n)-K(:,k)*Ck)*P; % minimal covariance of updated estimate
APPENDIX D. MATLAB ROUTINES

```matlab
xk(:,k+1) = x;
Pk(:,:,k+1) = P;
end;
x=xk';
P=Pk;
v=v';
save innovations v
subplot(3,1,1)
plot(0:N,x(:,1),'LineWidth',1.5);
ylabel('f{m [g]}','FontSize',14);
subplot(3,1,2)
plot(0:N,x(:,2),'LineWidth',1.5);
ylabel('f{n_{p} [-]}','FontSize',14);
subplot(3,1,3)
plot(1:N,v,'LineWidth',1.5);
axis([0 5000 -0.15e-5 0.000001])
xlabel('f{Time [s]}','FontSize',12);
ylabel('v [Pa m^{2}]','FontSize',14);
legend('prediction error (v)',0);

clear all; clc;
load Data1;
t = 60*Data1(8:end,1); %in seconds

np0 = 3000;
npbar = 150;
Csol = 30; %in g/m^3
Q = 4.167e-6; %Q = in m^3/s
%
k1k2LB = (np0-npbar)./(2*Csol*Q*t.^2);
k1k2UB = (np0)./(2*Csol*Q*t.^2);
k1k2Int = [k1k2LB k1k2UB];

k1 = (1:20/(length(t)-1):21)';
k2 = k1k2LB./k1;
semilogy(k1,k2,'LineWidth',2);
xlabel('k_{1}','FontSize',14);
ylabel('k_{2}','FontSize',14);
```