UNIVERSITY OF CALIFORNIA SAN DIEGO

State Estimation for Reaction-Diffusion Equations with Applications to Lithium-Ion Batteries

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The dissertation of Leobardo Camacho Solorio is approved, and it is acceptable in quality and form for publication on microfilm and electronically:

Chair

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2019
DEDICATION

A mi padre, mi madre, mi hermana y Mateo
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by

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The dissertation introduces advancements in the theory and the applications of state estimation for systems described by partial differential equations (PDEs) with boundary measurements. State estimation is of great importance to engineering applications since typically full-state knowledge is required for control and decision making but only a limited number of states are directly available from measurements. The estimation problems considered in the dissertation are solved via boundary observers, derived from the backstepping method for PDEs, which is a constructive method for boundary control and estimation. The dissertation is confined to PDEs of parabolic type, including: reaction-diffusion equations,
radial reaction-diffusion equations, systems of coupled reaction-diffusion equations, and systems including ODEs coupled with diffusion equations. Some contributions include: a robustness study for boundary observers with respect to uncertainty in parameters and measurement disturbances in the sense of input-to-state stability, the design of observers for coupled diffusion-reaction equations with an uncoupled target system, the design of observers for the expected value of a randomly switching diffusion-reaction PDE, and the design of observers for coupled ODEs with a radial diffusion equations.

The dissertation is motivated by the state estimation problem from electrochemical models of lithium-ion batteries. Lithium-ion technology is widely use in portable electronics, electrified vehicles, aerospace, medical devices, among many other industries. The safe and optimal operation of a battery relies on the battery management system which requires accurate and reliable estimates of internal states of the battery. Electrochemical models are first principle models that provide a detailed description for the time evolution of the battery states. Among electrochemical models, the single particle model (SPM) is a simple electrochemical model suitable for the design of control and estimation algorithms. The dissertation introduces state estimation methodologies from the SPM adapted for lithium-ion batteries with electrodes of multiple active material, electrodes with non-spherical particle geometries, temperature dependent parameters, state dependent parameters and materials with phase transitions. The results in the dissertation are not restricted to battery applications, in fact, the last chapter studies the state estimation problem for a wellbore reservoir model used in managed pressure drilling applications.
Chapter 1

Introduction

The dissertation introduces advancements in the theory and the applications of state estimation for parabolic partial differential equations (PDEs) with boundary measurements. The estimation problem is solved via boundary observers with the usual observer structure, that is, a copy of the system equations with additive output error feedback. The structure of the observer permits the use of output error to correct for errors in the initial conditions and, in the absence of output error, the observer state is constrained to evolve according to the system equations.

In the observer design problem the choice of observer gains is crucial to achieve convergence. Observers gains are weights that determine how output error feedback is introduced in the system equations, both in the interior of the domain and at the boundaries. Convergence of the estimate to the system state is obtained by choosing observer gains such that the zero solution of the estimation error system is asymptotically stable.

The observers in the dissertation are derived via the backstepping method for PDEs. Briefly speaking, in the backstepping method, one seeks an invertible integral transformation that maps the estimation error system to a carefully chosen stable target system; stability of the target system is establish via Lyapunov analysis. For the transformation between
the original system and the target system to be consistent, a unique set of observer gains are found. The main difficulty in the method is finding a solution to the equations satisfied by the kernel in the integral transformation, but once the well-posedness of the kernel equations has been established, analytical and numerical results are simple to obtain and in some cases closed-form observer gains are available.

The dissertation is motivated by the problem state estimation from electrochemical model of lithium-ion batteries. The electrochemical in the Doyle-Fuller-Newman (DFN) serves as a reference model, but observers are design is based on the Single Particle Model (SPM). A lithium-ion battery cell consists of three main regions: negative electrode, separator and positive electrode; all of them characterized by a porous structure. Each electrode includes active materials, conductive fillers, a current collector and a binder. The porous structure of the electrodes provides a large surface area and small distances between lithium ions and active material surfaces for reactions to occur. The separator is placed between the negative and positive electrodes to forbid the flow of electrons between two electrodes while allowing the movement of lithium ions dissolved in the electrolyte. The active materials, intercalated in the lattices of the corresponding electrode, are insertion compounds, i.e. these are host structures in which lithium can be reversibly inserted or extracted. Electrolyte fills all remaining parts of the battery.

The DFN model is derived based on the porous structure all through the lithium-ion battery. In the DFN model, each electrode is viewed as superposition of active materials, inert filler and electrolyte; justified by the porous configuration. Typically intercalation particles are assumed to be spheres with a uniform, averaged radius, and the battery is formulated as a pseudo two-dimensional model. The first dimension represents the path along the spatial direction from the anode, through the separator, to the cathode; and the second dimension is a radial direction used to represent the intercalation and diffusion of lithium ions in the active materials.
In the SPM, the diffusion of lithium ions in each active material is represented by a single diffusion equation, thus, reducing the complexity of the DFN model, to a finite set of linear diffusion equations, an algebraic equation and a nonlinear output equation.

The outline of the dissertation is as follows. In Chapter 2, an observer is derived for the single particle model for electrodes of multiple materials. In Chapter 3, an observers is derived for the single particle model with particles of planar, cylindrical, or spherical geometries. This chapter also includes identifiers for some of the parameters in the model; using a gradient method. Chapter 4, addresses the dependance on temperature of some of the parameters in the single particle model Chapter 5, addresses the dependence on concentration of the parameters of the single particle model. This study is based on the input-top-state stability property of the radial diffusion equation, establishing bounds on the estimation error based on bounds on the parameters variation. In Chapter 6, an observer is derived for the single particle model with phase transition materials. Chapter 7 discussed the boundary estimation problem for system of coupled diffusion reaction equation. Chapter 8 presents an application of the observer constructed in Chapter 7, to estimate the expected value of a randomly switching, diffusion reaction PDEs. In Chapter 9, the estimation problem for coupled diffusion reaction equation is addressed again, this time, using a pair on integral transformations to achieve an uncoupled target system and allowing for a prescribed converge rate Chapter 10 studies the problem of state estimation for a coupled observable LTI system coupled at the boundaries of a radial diffusion equation. This problem is motivated by the state estimation problem in wellbore reservoir models in managed pressure drilling application, but serves also as a solution to the internal temperature estimation problem for lithium ion batteries with ODE sensor dynamics.
Chapter 2

State Estimation for
Multiple-Material Lithium-Ion Batteries

2.1 Abstract

This chapter presents state estimation for a system of diffusion equations coupled in the boundary appearing in reduced electrochemical models of lithium-ion batteries with multiple active materials in single electrodes. The observer is synthesized from a single particle model and is based on the backstepping method for partial differential equations. The observer is suitable for state of charge estimation in battery management systems and is an extension of existing backstepping observers which were derived only for cells with electrodes of single active materials. Observer gains still can be computed analytically in terms of Bessel and modified Bessel functions. This extension is motivated by the trend in cell manufacturing to use multiple active materials to combine power and energy characteristics or reduce degradation.
2.2 Introduction

Accurate battery estimation algorithms are of great importance due to their application in consumer electronics, electrified transportation and energy storage systems for renewable sources. Electrochemical model-based estimation provides visibility into operating regimes that induce degradation enabling a larger domain of operation to increase performance with respect to energy capacity, power capacity and fast charge rates [1]. Electrochemical model-based estimation is challenging for several reasons. First, measurements of lithium concentrations outside specialized laboratory environments is impractical [2]. Second, the concentration dynamics are governed by partial differential algebraic equations (PDAE) [3]. Finally, the only measurable quantities (voltage and current) are related to dynamic states through a nonlinear function. Manufacturers are using multiple active materials in the positive electrode of lithium-ion cells to combine power and energy characteristics or reduce degradation. For example, Li$_y$Mn$_2$O$_4$ is a promising positive-electrode material because of its high potential, high rate capability, abundance and low cost [4, 5]. However, Li$_y$Mn$_2$O$_4$ has problems with the dissolution of Mn and its migration to the negative electrode where it increases the rate of side reactions and reduces cell life [4, 5]. Adding a layered oxide material such as Li$_y$Ni$_{0.80}$Co$_{0.15}$Al$_{0.05}$O$_2$ in the positive electrode can reduce the rate of dissolution and cells with a mixture of these two positive-electrode materials are now being produced commercially [4].

2.2.1 Relevant Literature

Over the past decade, the engineering literature on battery estimation has grown considerably rich with various algorithms, models, and applications. One may categorize this literature by the battery models each algorithm employs. The first category utilizes equivalent circuit models (ECMs). These models use circuit elements to mimic the
phenomenological behavior of batteries [6]. The seminal paper by Plett [7] was one of the first to apply extended Kalman filtering (EKF) to ECMs for simultaneous state and parameter estimation. Over the past decade, a variety of ECM-based algorithms have been developed, including linear parameter varying observers [8], sliding mode observers [9], polynomial chaos [10], unscented Kalman filters [11], and particle filters [12]. The second category of literature considers electrochemical models, which account for the diffusion, intercalation, and electrochemical kinetics. Although these models can accurately predict internal state variables, their mathematical structure renders observer design challenging. Consequently, most approaches develop estimators for reduced-order models. Among the various reduced models the single particle model (SPM) has been widely used for estimation [13, 14, 15, 16] including extensions to account for electrolyte dynamics [17, 18, 19, 20] and for electrodes with multiple active materials [21]

2.2.2 Main Contributions

The main contributions of this paper are the following:

1. A derivation of a single particle model for lithium-ion batteries with multiple active materials in single electrodes.

2. An observer based on the backstepping method for partial differential equations [22] suitable for state of charge estimation. This observer is an extension of backstepping observers for electrodes of a single active material [23, 15, 20].

2.2.3 Outline

The remainder of the paper is organized as follows. First, section 2 derives a single particle model for lithium-ion batteries with multiple active materials in single electrodes. Then, section 3 presents the derivation of an observer suitable for state of charge estimation.
After that, simulation results are provided in section 4. Finally, conclusions are listed in section 5.

2.3 Model Derivation

First, an extension of the Doyle-Fuller-Newman (DFN) model [3, 1] for cells with multiple active materials is described briefly. This extension follows results in [4] and describes the dynamic behavior of a cell with \( n^+ \) active materials in the positive electrode and \( n^- \) active materials in the negative electrode. Modifications to the original DFN model are the following. Diffusion of lithium in solid phase is described independently for each material

\[
\frac{\partial c_{s,i}}{\partial t}(x,r,t) = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_{s,i} r^2 \frac{\partial c_{s,i}}{\partial r}(x,r,t) \right],
\]

(2.1)

\[
\frac{\partial c_{s,i}}{\partial r}(x,0,t) = 0,
\]

(2.2)

\[
D_{s,i} \frac{\partial c_{s,i}}{\partial r}(x,R_{p,i},t) = -j_{n,i}(x,t),
\]

(2.3)

with \( i \in \{1^-,2^-,...,n^-,1^+,...,n^+\} \). A unique molar ion flux \( j_{n,i}(x,t) \) should be computed for each material

\[
j_{n,i}(x,t) = \frac{i_{0,i}(x,t)}{F} \left[ e^{\frac{\alpha_s F}{RT} \eta_i(x,t)} - e^{\frac{-\alpha_c F}{RT} \eta_i(x,t)} \right],
\]

(2.4)

where \( c_{ss,i}(x,t) = c_{s,i}(x,R_{p,i},t) \) and

\[
i_{0,i}(x,t) = k_i [c_{ss,i}(x,t)]^{\alpha_e} \left[ c_e(x,t) (c_{s\max,i} - c_{ss,i}(x,t)) \right]^{\alpha_a},
\]

(2.5)

\[
\eta_i(x,t) = \phi_s(x,t) - \phi_e(x,t) - U_i(c_{ss,i}(x,t)) c - R_{f,i} F j_{n,i}(x,t).
\]

(2.6)
Charge conservation in electrodes becomes

$$\frac{\partial i_e(x,t)}{\partial x} = \sum_k a_{s,k} F j_{n,k}(x,t), \quad (2.7)$$

where the sum is over all materials in each electrode, $a_{s,i} = 3 \epsilon_{s,i}/R_{p,i}$ is the specific interfacial area and $\epsilon_{s,i}$ is the volume fraction of each active material in the corresponding electrode.

Equations for lithium concentration in the electrolyte $c_e(x,t)$, solid electric potential $\phi_s(x,t)$ and electrolyte electric potential $\phi_e(x,t)$ remain unchanged

$$\frac{\partial c_e}{\partial t}(x,t) = \frac{\partial}{\partial x} \left[ D_e \frac{\partial c_e}{\partial x}(x,t) + \frac{1-t_c^0}{\epsilon_e F} i_e(x,t) \right], \quad (2.8)$$

$$\frac{\partial \phi_s}{\partial x}(x,t) = \frac{I(t) - i_e(x,t)}{\sigma}, \quad (2.9)$$

$$\frac{\partial \phi_e}{\partial x}(x,t) = \frac{i_e(x,t)}{\kappa} + \frac{2RT}{F} (1-t_c^0) \times \left( 1 + \frac{d\ln f_{c/a}}{d\ln c_e}(x,t) \right) \frac{\partial \ln c_e}{\partial x}(x,t) \quad (2.10)$$

Notice that solid and electrolyte electric potential have the same value for all materials in the same electrode. Boundary conditions for the electrolyte-phase diffusion PDE (4.8) are given by

$$\frac{\partial c_e}{\partial x}(0^-,t) = \frac{\partial c_e}{\partial x}(0^+,t) = 0, \quad (2.11)$$

$$\frac{\partial c_e}{\partial x}(L^-,t) = \frac{\epsilon_{e,sep} D_e(0^{sep})}{\epsilon_{e,-} D_e(L^-)} \frac{\partial c_e}{\partial x}(0^{sep},t), \quad (2.12)$$

$$\frac{\partial c_e}{\partial x}(L^{sep},t) = \frac{\epsilon_{e,+} D_e(L^+)}{\epsilon_{e,sep} D_e(L^{sep})} \frac{\partial c_e}{\partial x}(L^+,t), \quad (2.13)$$

$$c_e(L^-,t) = c_e(0^{sep},t), \quad (2.14)$$

$$c_e(L^{sep},t) = c_e(L^+,t). \quad (2.15)$$

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Boundary conditions for the solid-phase potential ODE (4.9) are given by

\[ \frac{\partial \phi_s}{\partial x}(L^-, t) = \frac{\partial \phi_s}{\partial x}(L^+, t) = 0. \] (2.16)

Boundary conditions for the electrolyte-phase potential ODE (4.10) are given by

\[ \phi_e(0^-, t) = 0, \] (2.17)
\[ \phi_e(L^-, t) = \phi_e(0^{\text{sep}}, t), \] (2.18)
\[ \phi_e(L^{\text{sep}}, t) = \phi_e(L^+, t). \] (2.19)

Boundary conditions for the ionic current ODE (2.7) are given by

\[ i_e(0^-, t) = i_e(0^+, t) = 0, \] (2.20)

and \( i_e(x, t) = I(t) \) for \( x \in [0^{\text{sep}}, L^{\text{sep}}] \). The input to the model is the applied current density \( I(t) \) (with positive values used for discharging) and the output is the voltage measured across the current collectors,

\[ V(t) = \phi_s(0^+, t) - \phi_s(0^-, t). \] (2.21)

The main assumptions used to derive the SPM model for electrodes with multiple materials are the following

- **[A1]**: Lithium concentration in both electrodes is constant in space, uniformly in time. Mathematically, \( c_{s,i}(x, t) \) and \( j_{n,i}(x, t) \) are constant in the \( x \) direction.

- **[A2]**: The term \( i_{0,i}(x, t) \) can be approximated by its averaged value \( i_{0,i}(t) \), which is independent of \( x \).
Figure 2.1: Schematic of Doyle-Fuller-Newman (DFN) model for electrodes with multiple active materials. This is a two-dimensional model with two phases: solid and electrolyte. States in the solid evolve in $x$ and $r$ dimensions while states in electrolyte evolve only in the $x$ dimension. The cell is divided in three subdomains: negative electrode, separator and positive electrode.
• [A3]: Lithium concentration is constant in space and time, i.e. \( c_e(x,t) = c_e,0 \).

This ultimately renders a model consisting of: (i) a set of \( n^- + n^+ \) spherical diffusion PDEs modeling concentration in each active material, (ii) a set of nonlinear algebraic equations and (iii) a nonlinear output function mapping boundary values of solid concentration and molar fluxes to terminal voltage. The resulting SPM equations are the following. Using assumption [A1] solid diffusion equations are

\[
\frac{\partial c_{s,i}(r,t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( D_{s,i} r^2 \frac{\partial c_{s,i}(r,t)}{\partial r} \right), \tag{2.22}
\]

\[
\frac{\partial c_{s,i}(0,t)}{\partial r} = 0, \tag{2.23}
\]

\[
D_{s,i} \frac{\partial c_{s,i}(R_{p,i},t)}{\partial r} = -j_{n,i}(t), \tag{2.24}
\]

where the solid-phase concentration no longer depends on \( x \). Using assumption [A1] and boundary conditions (2.20) charge conservation becomes

\[
I(t) = \sum_{k=1}^{n^-} a_{s,k} F L^- j_{n,k}(t), \tag{2.25}
\]

\[
I(t) = - \sum_{k=1}^{n^+} a_{s,k} F L^+ j_{n,k}(t). \tag{2.26}
\]

From assumptions [A1], [A2] and [A3] Butler-Volmer equation in (2.4) becomes

\[
j_{n,i}(t) = \frac{i_{0,i}(t)}{F} \left[ e^{\frac{\alpha_c F}{RT} \eta_i(t)} - e^{-\frac{\alpha_c F}{RT} \eta_i(t)} \right], \tag{2.27}
\]

\[
i_{0,i}(t) = k_i \left[ c_{ss,i}(t) \right]^{\alpha_c} \left[ c_{e,0} (c_{s,max,i} - c_{ss,i}(t)) \right]^{\alpha_s}, \tag{2.28}
\]

with \( c_{ss,i}(t) = c_{s,i}(R_{p,i},t) \). Solid electric potential is constant over each electrode and equal for all materials within the same electrode, therefore any index \( i^- \) or \( i^+ \) can be used to compute \( \phi_{s,-}(t) \) or \( \phi_{s,+}(t) \) respectively, i.e.

\[
\phi_{s,-}(t) = \eta_{i^-}(t) + U_{i^-}(c_{ss,i^-(t)}) + R_{f,i^-} F j_{n,i^-}(t), \tag{2.29}
\]
\[
\frac{3\varepsilon_{s,1}}{R_{p,1}} F L^{-} j_{n,1^{-}} (t) = I(t)
\]

\[
\frac{\partial c_{s,1^{-}}}{\partial r} (R_{p,1^{-}}, t) = - \frac{I(t)}{D_{s,1^{-}} a_{s,1^{-}} F L^{-}}
\]

\[
-\phi_{s,-} (c_{s,1^{-}} (t), j_{n,1^{-}} (t)) + \phi_{s,+} (c_{s,1^{+}} (t), j_{n,1^{+}} (t)) = V(t)
\]

Figure 2.2: Schematic of single particle model for one material in the negative electrode and \( n^{+} \) materials in the positive electrode. This a common configuration of commercial lithium-ion batteries where graphite is used for the negative electrode and a mixture of multiple active materials is used in the positive electrode.

(2.30)

Finally, output voltage is computed as

\[
V(t) = \phi_{s,+} (t) - \phi_{s,-} (t).
\]

(2.31)

Proposition 2.3.1. Lithium in the solid phase is conserved [24]. Mathematically, \( \frac{d}{dt} n_{Li,s}(t) = 0 \) where

\[
n_{Li,s}(t) = \sum_{i} \frac{\varepsilon_{s,i} L_{i}}{4 \pi R_{s,i}^{3}} \int_{0}^{R_{p,i}} 4 \pi r^{2} c_{s,i}(r,t) dr
\]

(2.32)

where the sum is computed over all active materials in both electrodes.

The proof is straight-forward and omitted for brevity. In the following observer estimation gains are selected to conserve lithium in solid phase.
2.4 State Observer Design

In this section an observer is developed for a cell with one active material in the negative electrode and two active materials in the positive electrode, see Fig. 2.2. Extension to more active materials in the positive electrode is straightforward. The observer design process is summarized as follows:

1. Linearization of algebraic equations in the positive electrode

2. Normalization and state transformation of solid diffusion equations in the positive electrode

3. Derivation of backstepping PDE observer for the transformed solid diffusion system

4. Inverse state transformation and un-normalization

5. Derivation of an observer in the negative electrode to conserve lithium in solid

2.4.1 Linearization of Algebraic Equations

First, a linear approximation of the dynamic and algebraic states in the positive electrode is being considered

\[
\phi_{s,+}(t) = U_{i,+}(c_{s,i,+}^\text{eq}) + \bar{\phi}_{s,+}(t), \quad (2.33)
\]

\[
c_{\text{ss},1,+}(t) = c_{s,1,+}^\text{eq} + \bar{c}_{\text{ss},1,+}(t), \quad (2.34)
\]

\[
c_{\text{ss},2,+}(t) = c_{s,2,+}^\text{eq} + \bar{c}_{\text{ss},2,+}(t), \quad (2.35)
\]

\[
j_{n,1,+}(t) = \tilde{j}_{n,1,+}(t), \quad (2.36)
\]

\[
j_{n,2,+}(t) = \tilde{j}_{n,2,+}(t), \quad (2.37)
\]

around the equilibrium \((U_{i,+}(c_{s,i,+}^\text{eq}), c_{s,1,+}^\text{eq}, c_{s,2,+}^\text{eq}, 0, 0)\) to find a linear approximation of the algebraic equation in (2.26) and the pair of algebraic equations in (3.77) (one for each
active material)

\[
I(t) = -\frac{3\varepsilon_{s,1}^+}{R_{p,1}^+} F L \tilde{j}_{n,1}^+(t) - \frac{3\varepsilon_{s,2}^+}{R_{p,2}^+} F L \tilde{j}_{n,2}^+(t),
\]

\[
0 = -\tilde{\phi}_{s,+}(t) + \frac{R T \tilde{j}_{n,1}^+(t)}{(\alpha_a + \alpha_c) i_{0,1}^+(t)} + R_{f,1}^+ F \tilde{j}_{n,1}^+(t) + \frac{\partial U_{1+}}{\partial c_{ss,1+}} (c_{s,1+}^{eq}) \tilde{c}_{ss,1+}(t),
\]

\[
0 = -\tilde{\phi}_{s,+}(t) + \frac{R T \tilde{j}_{n,2}^+(t)}{(\alpha_a + \alpha_c) i_{0,2}^+(t)} + R_{f,2}^+ F \tilde{j}_{n,2}^+(t) + \frac{\partial U_{2+}}{\partial c_{ss,2+}} (c_{s,2+}^{eq}) \tilde{c}_{ss,2+}(t),
\]

and then solve for \(\tilde{j}_{n,1}^+(t)\) and \(\tilde{j}_{n,2}^+(t)\) in terms of \(\tilde{c}_{ss,1+}, \tilde{c}_{ss,2+}\) and \(I(t)\)

\[
\tilde{j}_{n,1}^+(t) = -\rho_{11} \tilde{c}_{ss,1+}(t) - \rho_{12} \tilde{c}_{ss,2+}(t) - \rho_1 I(t),
\]

\[
\tilde{j}_{n,2}^+(t) = -\rho_{21} \tilde{c}_{ss,1+}(t) - \rho_{22} \tilde{c}_{ss,2+}(t) - \rho_2 I(t).
\]

### 2.4.2 Normalization and State Transformation

**Assumption 2.4.1.** The radio \(\frac{D_{s,i}}{(R_{p,i})^2}\) has the same value for all materials in each electrode.

Next normalization and state transformation is used to simplify the mathematical structure of the observer in the positive electrode. First scale the radial \(r\) and time \(t\) coordinates as follows

\[
\bar{r} = \frac{r}{R_{p,i}}, \quad \bar{t} = \frac{D_{s,i}}{(R_{p,i})^2} t.
\]

Bars over the space and time coordinates will be dropped to simplify notation. Next state transformation is used to eliminate the first spatial derivative in the spherical diffusion equations (2.22)

\[
c_i(r, t) = r c_{s,i}(r, t).
\]
This normalization and state transformation produces the following PDE

\[
\frac{\partial}{\partial t}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}(r, t) = \frac{\partial^2}{\partial r^2}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}(r, t),
\]

(2.45)

with boundary conditions

\[
\frac{\partial}{\partial r}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}(1, t) - \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}(1, t) = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}(1, t) + \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}I(t).
\]

(2.47)

where

\[
a_{11} = \frac{R_{p,1^+}}{D_{s,1^+}}\rho_{11}, \quad a_{12} = \frac{R_{p,1^+}}{D_{s,1^+}}\rho_{12},
\]

(2.48)

\[
a_{21} = \frac{R_{p,2^+}}{D_{s,2^+}}\rho_{21}, \quad a_{22} = \frac{R_{p,2^+}}{D_{s,2^+}}\rho_{22},
\]

(2.49)

\[
a_1 = \frac{R_{p,1^+}}{D_{s,1^+}}\rho_1, \quad a_2 = \frac{R_{p,2^+}}{D_{s,2^+}}\rho_2.
\]

(2.50)

### 2.4.3 Backstepping Observer for Positive Electrode

The observer in the positive electrode is a copy of the plant (2.45)-(2.47) plus boundary state error injection

\[
\frac{\partial}{\partial t}\begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix}(r, t) = \frac{\partial^2}{\partial r^2}\begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix}(r, t) + \begin{bmatrix} p_{11}(r) & p_{12}(r) \\ p_{21}(r) & p_{22}(r) \end{bmatrix}\begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix}(1, t),
\]

(2.51)
with boundary conditions

\[
\frac{\partial}{\partial r} \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} (1,t) - \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} (1,t) = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} (1,t) + \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} I(t) \tag{2.53}
\]

\[
+ \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} (1,t) \tag{2.54}
\]

where boundary estimation error is defined as \([\hat{c}_1, \hat{c}_2]^T (r, t) = [c_1, c_2]^T (r, t) - [\tilde{c}_1, \tilde{c}_2]^T (r, t)\)
and values of surface concentration \([c_1, c_2]^T (r, t)\) are assumed to be known or are being estimated from measurements. The estimation error system is

\[
\frac{\partial}{\partial t} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (r, t) = \frac{\partial^2}{\partial r^2} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (r, t) - \begin{bmatrix} p_{11} (r) & p_{12} (r) \\ p_{21} (r) & p_{22} (r) \end{bmatrix} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (1,t), \tag{2.55}
\]

with boundary conditions

\[
\frac{\partial}{\partial r} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (1,t) - \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (1,t) = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (1,t) - \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} (1,t) \tag{2.57}
\]

The backstepping approach seeks to find the upper-triangular transformation

\[
\begin{bmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{bmatrix} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} - \int_r^1 \begin{bmatrix} Q_{11}(r,s) & Q_{12}(r,s) \\ Q_{21}(r,s) & Q_{22}(r,s) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} (s,t) ds, \tag{2.58}
\]
that transforms the original error system (2.55)-(2.57) into the target system

\[
\frac{\partial}{\partial t} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(r,t) = \frac{\partial^2}{\partial r^2} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(r,t) + \begin{bmatrix} \lambda_1 & -\lambda_c \\ \lambda_c & \lambda_2 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(r,t),
\]

(2.59)

with boundary conditions

\[
\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(0,t) = 0,
\]

(2.60)

\[
\frac{\partial}{\partial r} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(1,t) = -\frac{1}{2} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}(1,t),
\]

(2.61)

where \( \lambda_1, \lambda_2 < 1/4 \). For the target system (7.28)-(2.61), equilibrium \([w_1^{eq}, w_2^{eq}](r) = [0,0] \) is exponentially stable in the \( L_2 \)-norm and the proof of this statement is as follows. Considering the positive-definite function

\[
V(t) = \frac{1}{2} \int_0^1 w_1^2(r,t) + w_2^2(r,t) dr,
\]

(2.62)

taking the time derivative and using integration by parts

\[
\dot{V}(t) = -\frac{1}{2} w_1^2(1,t) - \int_0^1 w_1^2,dr + \lambda_1 \int_0^1 w_1^2 dr - \frac{1}{2} w_2^2(1,t) - \int_0^1 w_2^2,dr + \lambda_2 \int_0^1 w_2^2 dr,
\]

(2.63)

using the Poincaré inequality

\[
\dot{V}(t) \leq -\left( \frac{1}{4} - \lambda_1 \right) \int_0^1 w_1^2 dr - \left( \frac{1}{4} - \lambda_2 \right) \int_0^1 w_2^2 dr,
\]

(2.64)

\[
\leq -\left( \frac{1}{2} - 2\lambda_{\text{max}} \right) V(t),
\]

(2.65)
with $\lambda_{\text{max}} = \max(\lambda_1, \lambda_2)$. Comparison principle (Lemma 3.4 in [25]) implies $V(t) \leq V(0) e^{-\left(\frac{1}{4} - 2\lambda_{\text{max}}\right)t}$ or in terms of the norm $\|w(t)\| = \|w(0)\| e^{-\left(\frac{1}{4} - \lambda_{\text{max}}\right)t}$. Then for all $\lambda_1, \lambda_2 < \frac{1}{4}$ equilibrium $[w_{1e}^{\text{eq}}, w_{2e}^{\text{eq}}](r) = [0, 0]$ is exponentially stable. Following the procedure in [22] elements of the kernel in (2.58) are solutions of the PDE

\begin{align*}
Q_{11,rr}(r,s) - Q_{11,ss}(r,s) &= \lambda_1 Q_{11}(r,s), \quad (2.66) \\
Q_{12,rr}(r,s) - Q_{12,ss}(r,s) &= -\lambda_c Q_{12}(r,s), \quad (2.67) \\
Q_{21,rr}(r,s) - Q_{21,ss}(r,s) &= \lambda_c Q_{21}(r,s), \quad (2.68) \\
Q_{22,rr}(r,s) - Q_{22,ss}(r,s) &= \lambda_2 Q_{22}(r,s), \quad (2.69)
\end{align*}

with boundary conditions

\begin{align*}
Q_{11}(0,s) &= 0, \quad Q_{11}(r,r) = \frac{\lambda_1}{2} r, \quad (2.70) \\
Q_{12}(0,s) &= 0, \quad Q_{12}(r,r) = -\frac{\lambda_c}{2} r, \quad (2.71) \\
Q_{21}(0,s) &= 0, \quad Q_{21}(r,r) = \frac{\lambda_c}{2} r, \quad (2.72) \\
Q_{22}(0,s) &= 0, \quad Q_{22}(r,r) = \frac{\lambda_2}{2} r, \quad (2.73)
\end{align*}
defined on \( D = \{(r, s) | 0 \leq r \leq s \leq 1\} \). Output injection gains are

\[
p_{11}^+ (r) = -\frac{1}{2} Q_{11}(r, 1) - Q_{11, s}(r, 1),
\]
\[
p_{12}^+ (r) = -\frac{1}{2} Q_{12}(r, 1) - Q_{12, s}(r, 1),
\]
\[
p_{21}^+ (r) = -\frac{1}{2} Q_{21}(r, 1) - Q_{21, s}(r, 1),
\]
\[
p_{22}^+ (r) = -\frac{1}{2} Q_{22}(r, 1) - Q_{22, s}(r, 1),
\]
\[
q_{11}^+ = a_{11} + \frac{3 - \lambda_1}{2}, \quad q_{12}^+ = a_{12} - \frac{\lambda_c}{2},
\]
\[
q_{21}^+ = a_{21} + \frac{\lambda_c}{2}, \quad q_{22}^+ = a_{22} + \frac{3 - \lambda_2}{2},
\]

The Klein-Gordon PDE (2.66)-(2.69) has a closed form solution

\[
Q_{11}(r, s) = \lambda_1 r \frac{I_1(z_1)}{z_1}, \quad Q_{12}(r, s) = -\lambda_c r \frac{J_1(z_c)}{z_c},
\]
\[
Q_{21}(r, s) = \lambda_c r \frac{I_1(z_c)}{z_c}, \quad Q_{22}(r, s) = \lambda_2 r \frac{I_1(z_2)}{z_2},
\]

where \( z_i := z_i(r, s) = \sqrt{\lambda_i (r^2 - s^2)}, \ i \in \{1, c, 2\} \). Substituting (2.80)-(2.81) in (2.74)-(??)

\[
p_{11} (r) = -\frac{\lambda_1 r}{2 z_1} \left[ I_1(z_1) - \frac{2 \lambda_1}{z_1} I_2(z_1) \right],
\]
\[
p_{12} (r) = \frac{\lambda_c r}{2 z_c} \left[ J_1(z_c) - \frac{2 \lambda_c}{z_c} J_2(z_c) \right],
\]
\[
p_{21} (r) = -\frac{\lambda_c r}{2 z_c} \left[ I_1(z_c) - \frac{2 \lambda_c}{z_c} I_2(z_c) \right],
\]
\[
p_{22} (r) = -\frac{\lambda_2 r}{2 z_2} \left[ I_1(z_2) - \frac{2 \lambda_2}{z_2} I_2(z_2) \right],
\]

where \( J_1(\cdot), J_2(\cdot), I_1(\cdot) \) and \( I_2(\cdot) \) are first and second order Bessel functions and first and second order modified Bessel functions, respectively.
2.4.4 Inverse Transformation and Un-normalization

An observer in the original coordinates $\hat{c}_{s,1+}, \hat{c}_{s,2+}$ can be found by inverting transformation (2.44) and un-normalizing the dimensions (2.43). Since the observer for the positive electrode is based on the linear approximation (2.41) and (2.42), convergence results hold only locally. However, the linearization and the computation of observer gains can be done continuously (using measurements of surface concentration or their estimates) and the final result is an observer for the nonlinear PDAE of the positive electrode

$$
\frac{\partial \hat{c}_{s,1+}}{\partial t}(r,t) = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_{s,1+} r^2 \frac{\partial \hat{c}_{s,1+}}{\partial r}(r,t) \right] + \bar{p}_{11}^+(r) \left[ c_{ss,1+}(t) - \hat{c}_{s,1+}(t) \right] \\
+ \bar{p}_{12}^+(r) \left[ c_{ss,2+}(t) - \hat{c}_{s,2+}(t) \right],
$$

(2.86)

with boundary conditions

$$
\hat{c}_{s,1+}(0,t) = 0,
$$

(2.87)

$$
D_{s,1+} \frac{\partial \hat{c}_{s,1+}}{\partial r}(R_{p,1+},t) = -\hat{j}_{n,1+}(t) \\
+ \bar{q}_{11}^+ \left[ c_{ss,1+}(t) - \hat{c}_{s,1+}(t) \right] + \bar{q}_{12}^+ \left[ c_{ss,2+}(t) - \hat{c}_{s,2+}(t) \right],
$$

(2.88)

and

$$
\frac{\partial \hat{c}_{s,2+}}{\partial t}(r,t) = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_{s,2+} r^2 \frac{\partial \hat{c}_{s,2+}}{\partial r}(r,t) \right] + \bar{p}_{21}^+(r) \left[ c_{ss,1+}(t) - \hat{c}_{s,1+}(t) \right] \\
+ \bar{p}_{22}^+(r) \left[ c_{ss,2+}(t) - \hat{c}_{s,2+}(t) \right],
$$

(2.89)
with boundary condition

\[
\tilde{c}_{s,2+}(0,t) = 0, \quad (2.90)
\]

\[
D_{s,2+} \frac{\partial \tilde{c}_{s,2+}}{\partial r} (R_{p,2+}, t) = -\tilde{\eta}_{n,2+}(t)
\]

\[
+ \eta_{21}^{+} \left[ \tilde{c}_{ss,1+}(t) - \tilde{c}_{ss,1+}(t) \right] + \eta_{22}^{+} \left[ \tilde{c}_{ss,2+}(t) - \tilde{c}_{ss,2+}(t) \right], \quad (2.91)
\]

where \( \tilde{\eta}_{n,1+}(t) \) and \( \tilde{\eta}_{n,2+}(t) \) are obtained by solving the nonlinear algebraic equations

\[
I(t) = -a_{s,1+} F L^+ \tilde{\eta}_{n,1+}(t) - a_{s,2+} F L^+ \tilde{\eta}_{n,2+}(t), \quad (2.92)
\]

\[
0 = -\tilde{\phi}_{s,+}(t) + \tilde{\eta}_{1+} + U_{1+}(c_{ss,1+}(t)) + R_{f,1+} F \tilde{\eta}_{n,1+}(t), \quad (2.93)
\]

\[
0 = -\tilde{\phi}_{s,+}(t) + \tilde{\eta}_{2+} + U_{2+}(c_{ss,2+}(t)) + R_{f,2+} F \tilde{\eta}_{n,2+}(t), \quad (2.94)
\]

\[
\tilde{\eta}_{n,1+}(t) = \frac{i_{0,1+}(t)}{F} \left[ e^{\alpha_{c} F \tilde{r}_{1+}} - e^{-\alpha_{c} F \tilde{r}_{1+}} \right], \quad (2.95)
\]

\[
\tilde{\eta}_{n,2+}(t) = \frac{i_{0,2+}(t)}{F} \left[ e^{\alpha_{c} F \tilde{r}_{2+}} - e^{-\alpha_{c} F \tilde{r}_{2+}} \right]. \quad (2.96)
\]

Observer gains are

\[
p_{11}^{+}(r) = \frac{-\lambda_{1} D_{s,1+}}{2 R_{p,1+}^{2}} \left[ I_{1}(z_{1}) - \frac{2 \lambda_{1}}{z_{1}} I_{2}(z_{1}) \right], \quad (2.97)
\]

\[
p_{12}^{+}(r) = \frac{\lambda_{c} D_{s,1+}}{2 R_{p,1+}^2} \left[ J_1(z_{c}) - \frac{2 \lambda_{c}}{z_{c}} J_2(z_{c}) \right], \quad (2.98)
\]

\[
p_{21}^{+}(r) = \frac{-\lambda_{c} D_{s,2+}}{2 R_{p,2+}^2} \left[ I_1(z_{c}) - \frac{2 \lambda_{c}}{z_{c}} I_2(z_{c}) \right], \quad (2.99)
\]

\[
p_{22}^{+}(r) = \frac{-\lambda_{2} D_{s,2+}}{2 R_{p,2+}^2} \left[ I_1(z_{2}) - \frac{2 \lambda_{2}}{z_{2}} I_2(z_{2}) \right], \quad (2.100)
\]
with \( z_j := z_j(r) = \sqrt{\lambda_j \left( \frac{r^2}{R_{p,j}^2} - 1 \right)} \) and

\[
\begin{align*}
\bar{q}_{11}^+ &= \rho_{11} + \frac{D_{s,1+}(3 - \lambda_1)}{2R_{p,1+}}, \\
\bar{q}_{12}^+ &= \rho_{12} - \frac{D_{s,1+}\lambda_c}{2R_{p,1+}}, \\
\bar{q}_{21}^+ &= \rho_{21} + \frac{D_{s,2+}\lambda_c}{2R_{p,2+}}, \\
\bar{q}_{22}^+ &= \rho_{22} + \frac{D_{s,2+}(3 - \lambda_2)}{2R_{p,2+}}.
\end{align*}
\] (2.101)

2.4.5 Observer for Negative Electrode

The observer for the negative electrode consists of a copy of the plant and surface concentration error injection from the positive electrode as follows

\[
\begin{align*}
\frac{\partial \hat{c}_{s,1-}(r,t)}{\partial t} &= \frac{1}{r^2} \frac{\partial}{\partial r} \left[ D_{s,1-} \frac{\partial \hat{c}_{s,1-}(r,t)}{\partial r} \right] + \bar{p}_1(r) \left[ c_{ss,1+}(t) - \hat{c}_{ss,1+}(t) \right] + \bar{p}_2(r) \left[ c_{ss,2+}(t) - \hat{c}_{ss,2+}(t) \right],
\end{align*}
\] (2.105)

with boundary conditions

\[
\begin{align*}
\hat{c}_{s,1-}(0,t) &= 0, \\
D_{s,1-} \frac{\partial \hat{c}_{s,1-}(r_{p,1-},t)}{\partial r} &= - \frac{I(t)}{F_{a-L}} + \bar{q}_1 \left[ c_{ss,1+}(t) - \hat{c}_{ss,1+}(t) \right] + \bar{q}_2 \left[ c_{ss,2+}(t) - \hat{c}_{ss,2+}(t) \right].
\end{align*}
\] (2.107)
Observer gains $\overline{p}_1^-(r), \overline{p}_2^-(r), \overline{q}_1^-$ and $\overline{q}_2^-$ are selected such that $\frac{d}{dt}\overline{n}_{Li,s}(t) = 0$. This property holds true under the following relations between the estimation gains

\begin{align*}
0 &= a_{s,1} + L^+ D_{s,1} \overline{q}_1^+ + a_{s,2} + L^+ D_{s,2} \overline{q}_2^+ + a_{s,1} - L^- D_{s,1} \overline{q}_1^-, \\
0 &= a_{s,1} + L^+ D_{s,1} \overline{q}_1^+ + a_{s,2} + L^+ D_{s,2} \overline{q}_2^+ + a_{s,1} - L^- D_{s,1} \overline{q}_2^-, \\
0 &= \frac{a_{s,1} L^+}{R_{p,1}^+} \int_0^{R_{p,1}^+} r^2 \overline{p}_{11}^+(r) \, dr + \frac{a_{s,2} L^+}{R_{p,2}^+} \int_0^{R_{p,2}^+} r^2 \overline{p}_{21}^+(r) \, dr \\
&\quad + \frac{a_{s,1} L^-}{R_{p,1}^-} \int_0^{R_{p,1}^-} r^2 \overline{p}_{11}^-(r) \, dr, \\
0 &= \frac{a_{s,1} L^+}{R_{p,1}^+} \int_0^{R_{p,1}^+} r^2 \overline{p}_{12}^+(r) \, dr + \frac{a_{s,2} L^+}{R_{p,2}^+} \int_0^{R_{p,2}^+} r^2 \overline{p}_{22}^+(r) \, dr \\
&\quad + \frac{a_{s,1} L^-}{R_{p,1}^-} \int_0^{R_{p,1}^-} r^2 \overline{p}_{12}^-(r) \, dr,
\end{align*}

There are multiple solutions for gains $\overline{p}_1^-(r)$ and $\overline{p}_2^-(r)$ but constant gains can be found easily

\begin{align*}
\overline{p}_1^- &= -\frac{a_{s,1} L^+}{R_{p,1}^+} \int_0^{R_{p,1}^+} r^2 \overline{p}_{11}^+(r) \, dr + \frac{a_{s,2} L^+}{R_{p,2}^+} \int_0^{R_{p,2}^+} r^2 \overline{p}_{21}^+(r) \, dr \\
&\quad + \frac{a_{s,1} L^-}{R_{p,1}^-} \int_0^{R_{p,1}^-} r^2 \overline{p}_{11}^-(r) \, dr, \\
\overline{p}_2^- &= -\frac{a_{s,1} L^+}{R_{p,1}^+} \int_0^{R_{p,1}^+} r^2 \overline{p}_{12}^+(r) \, dr + \frac{a_{s,2} L^+}{R_{p,2}^+} \int_0^{R_{p,2}^+} r^2 \overline{p}_{22}^+(r) \, dr \\
&\quad + \frac{a_{s,1} L^-}{R_{p,1}^-} \int_0^{R_{p,1}^-} r^2 \overline{p}_{12}^-(r) \, dr,
\end{align*}

and

\begin{align*}
\overline{q}_1^- &= -\frac{a_{s,1} L^+ D_{s,1}^+ \overline{q}_1^+ + a_{s,2} L^+ D_{s,2} \overline{q}_2^+}{a_{s,1} L^- D_{s,1}^-}, \\
\overline{q}_2^- &= -\frac{a_{s,1} L^+ D_{s,1}^+ \overline{q}_1^+ + a_{s,2} L^+ D_{s,2} \overline{q}_2^+}{a_{s,1} L^- D_{s,1}^-}.
\end{align*}
The observer is initialized with the correct value of lithium in the solid phase, \( n_{\text{Li,s}} \) in (2.32), assuming it is known beforehand, i.e.

\[
n_{\text{Li,s}} = \sum_i \frac{\epsilon_{s,i} L_i}{3 \pi R_{p,i}^3} \int_0^{R_{p,i}} 4\pi r^2 \hat{c}_{s,i}(r,0) \, dr.
\] (2.120)

### 2.5 Simulation

For the simulation presented in this section, one particle in the negative electrode and two particles in the positive electrode are being considered. Simulation results are shown in Fig. 2.3 with \( \lambda_1 = \lambda_2 = -10 \) and \( \lambda_c = 10^{-8} \). From top to bottom, the first plot shows the current density profile used in this test which is obtained from the urban dynamometer driving schedule (UDDS) and is representative of the battery use in automotive applications. The second plot shows the estimation error in the output voltage and since measurements are being generated from a SPM, convergence is expected. The third plot shows the real and estimated (normalized) surface concentrations in the two particles of the positive electrode. Finally, the fourth plot shows the real and estimated (normalized) surface concentration in the particle of negative electrode. Here, perfect knowledge of surface concentration in particles of the positive electrode is assumed. For battery management applications values of surface concentration in the positive electrode could be estimated from current and voltage measurements [15, ?, 20]. Initial estimates of lithium concentration are chosen with the correct value of \( n_{L,i} \) (i.e. condition in (2.120) is satisfied).
Figure 2.3: Simulation. Perfect measurement of surface concentration is used from a single particle model and current density (input) is obtained from UDDS. Initial estimates of lithium concentration are chosen with the correct value of \( n_{Li} \) (i.e. condition in (2.120) is satisfied). Normalized values of real and estimated surface concentration are plotted i.e. \( \theta_i = c_{ss,i}(t)/c_{max,s,i} \).
2.6 Conclusions

An observer for a system of diffusion equations appearing in a single particle model of lithium-ion batteries with electrodes of multiple active materials has been derived in this paper. The observer is based on the backstepping method for PDEs and is an extension of previous backstepping observers designed only for single active materials. Simulations where presented showing the effectiveness of the estimation scheme. This observer could be used for other settings apart from the multiple material problem, for example in electrodes with a unique active material (i.e. same OCP functions and all parameters with same values) but with two or more distinct particle sizes (i.e. different $R_p$). An important limitation of the observer is that, since it is derived from a reduced electrochemical model, convergence is only expected in the cases when this reduced model is an appropriate approximation of the full electrochemical model (or battery). Future work includes the test of this observer against the full electrochemical model and the extension to simultaneous parameter and state estimation.

Table 2.1: Multiple Material Model. States and Variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_s$</td>
<td>Concentration of lithium ions in particles</td>
</tr>
<tr>
<td>$c_{ss}$</td>
<td>Surface concentration in particles</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Normalized surface concentration</td>
</tr>
<tr>
<td>$j_n$</td>
<td>Molar ion flux</td>
</tr>
<tr>
<td>$i_0$</td>
<td>Exchange current density</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Overpotential</td>
</tr>
<tr>
<td>$c_e$</td>
<td>Concentration of lithium ions in electrolyte</td>
</tr>
<tr>
<td>$\phi_s$</td>
<td>Electric potential in the solid electrodes</td>
</tr>
<tr>
<td>$\phi_e$</td>
<td>Electric potential in the electrolyte</td>
</tr>
<tr>
<td>$i_e$</td>
<td>Ionic current density</td>
</tr>
<tr>
<td>$f_{c/a}$</td>
<td>Activity coefficient in the electrolyte</td>
</tr>
<tr>
<td>$U$</td>
<td>Open circuit potential functions</td>
</tr>
<tr>
<td>$I$</td>
<td>Current density (input)</td>
</tr>
<tr>
<td>$V$</td>
<td>Voltage (output)</td>
</tr>
</tbody>
</table>
Table 2.2: Multiple Material Model. Parameters and Constants

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_s$</td>
<td>Diffusion coefficient in solid particles</td>
</tr>
<tr>
<td>$R_p$</td>
<td>Particle radius</td>
</tr>
<tr>
<td>$n^-, n^+$</td>
<td>Number of active materials in electrodes</td>
</tr>
<tr>
<td>$\alpha_a, \alpha_c$</td>
<td>Transport coefficients</td>
</tr>
<tr>
<td>$R$</td>
<td>Gas constant</td>
</tr>
<tr>
<td>$T$</td>
<td>Constant temperature</td>
</tr>
<tr>
<td>$F$</td>
<td>Faraday constant</td>
</tr>
<tr>
<td>$k$</td>
<td>Effective reaction rate</td>
</tr>
<tr>
<td>$c^{\text{max}}_s$</td>
<td>Maximum concentration</td>
</tr>
<tr>
<td>$R_f$</td>
<td>Film resistance</td>
</tr>
<tr>
<td>$\epsilon_s$</td>
<td>Volume fraction of active material</td>
</tr>
<tr>
<td>$\epsilon_e$</td>
<td>Volume fraction of electrolyte</td>
</tr>
<tr>
<td>$\alpha_s$</td>
<td>Specific interfacial area</td>
</tr>
<tr>
<td>$D_e$</td>
<td>Diffusion coefficient in electrolyte</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Conductivity in solid electrodes</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Conductivity in electrolyte</td>
</tr>
<tr>
<td>$t_c^0$</td>
<td>Transference number</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of region</td>
</tr>
<tr>
<td>$c_{e,0}$</td>
<td>Constant approximation of $c_e$</td>
</tr>
<tr>
<td>$n_{Li}$</td>
<td>Total lithium in solid particles (per unit area)</td>
</tr>
</tbody>
</table>

2.7 Acknowledgments

Chapter 2, in part, is a reprint of the material as it appears in: L. Camacho-Solorio, R. Klein, A. Mirtabatabaei, M. Krstic, and S. Moura, “State Estimation for an Electrochemical Model of Multiple Material Lithium-Ion Batteries”, ASME Dynamic Systems and Control Conference (DSCC), 2016. The dissertation author was the primary investigator and author of this paper.
Chapter 3

State and Parameter Estimation for Lithium-Ion Batteries with Different Particle Geometry

3.1 State Estimation from SPM

3.1.1 Model for Different Particle Geometries

This model consists of: (i) two diffusion PDEs systems modeling the ‘mean’ lithium concentration dynamics in each electrode (negative and positive), (ii) a linear relationship between the input \( I(t) \) of the model and Neumann boundary values (i.e. concentration flux at the surface) in each diffusion system and (iii) a nonlinear output function relating Dirichlet boundary values (i.e. surface concentration) in the diffusion systems to the output \( V(t) \) of the model.

(i) Diffusion equations
Fick’s laws of diffusion modeling lithium concentration are
\[
\frac{\partial c_{s,i}(r,t)}{\partial t} = D_{s,i} \frac{1}{r} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}(r,t)}{\partial r} \right],
\tag{3.1}
\]
for \( r \in (0, R_{p,i}), t > 0 \), with boundary conditions
\[
\frac{\partial c_{s,i}}{\partial r}(0,t) = 0, \tag{3.2}
\]
\[
D_{s,i} \frac{\partial c_{s,i}}{\partial r}(R_{p,i},t) = -j_i(t), \tag{3.3}
\]
and with initial conditions \( c_{s,i}(r,0) = c_{s,i,0}(r) \in L^2(0, R_{p,i}) \) satisfying the boundary conditions. Subscript \( i \in \{-, +\} \) is used to distinguish between each electrode (negative or positive) and the value of the constant \( n \) in (3.1) is chosen according to the geometry particle in each electrode:

**Table 3.1**: Geometry associated with the integer parameter \( m \).

<table>
<thead>
<tr>
<th>( m )</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m = 1 )</td>
<td>Planar</td>
</tr>
<tr>
<td>( m = 2 )</td>
<td>Cylindrical</td>
</tr>
<tr>
<td>( m = 3 )</td>
<td>Spherical</td>
</tr>
</tbody>
</table>

(ii) **Input to molar flux relationships**

The relationships between current density through the lithium ion cell \( I(t) \) (input of the model) and molar fluxes \( j_i(t) \) (Neumann type boundary condition in (3.3)) are simply
\[
I(t) = +a_{s, -} FL^- j_-(t), \tag{3.4}
\]
\[
I(t) = -a_{s, +} FL^+ j_+(t). \tag{3.5}
\]

(iii) **Output function**

Finally, voltage difference between the terminals in the lithium-ion cell \( V(t) \) (output of the model) is computed as the difference between the ‘mean’ potential in the positive and negative electrode
\[
V(t) = \phi_{s, +}(t) - \phi_{s, -}(t). \tag{3.6}
\]
Potentials \( \phi_{s,i}(t) \equiv \phi_{s,i}(c_{ss,i}(t), j_i(t)) \) are functions of molar fluxes \( j_i(t) \) and surface concentration \( c_{ss,i}(t) = c_{s,i}(R_p,t) \) (i.e. the boundary value in the diffusion systems (3.1)-(3.3)) and are computed as

\[
\phi_{s,i}(t) = \eta_i(c_{ss,i}(t), j_i(t)) + U_i(c_{ss,i}(t)) + R_f F j_i(t),
\]

(3.7)

In (6.11) Open Circuit Potentials (OCP) \( U_i(\cdot) \) are known functions defined for the particular active material in each electrode and overpotentials \( \eta_i(\cdot, \cdot) \) are found solving the equation

\[
\begin{aligned}
  j_i(t) &= \frac{i_{0,i}(t)}{F} \left[ e^{\frac{\alpha_c F}{RT} \eta_i(t)} - e^{-\frac{\alpha_c F}{RT} \eta_i(t)} \right], \\
  i_{0,i}(t) &= k_i [c_{ss,i}(t)]^{\alpha_c} [c_{e,0} (c_{s,max,i} - c_{ss,i}(t))]^{\alpha_a}.
\end{aligned}
\]

(3.8)

(3.9)

The model is depicted as a block diagram in Figure 3.2.

### 3.1.2 Observer Design

#### Observer with Surface Concentration Measurements

**Assumption:** In the first step of the observer design we use the assumption that \( c_{ss,i}(t) \) are available from measurements. We will relax this assumption later and use voltage measurements.
\[
U^+ (\cdot) + \eta^+ (\cdot, t) + R_{f,+} + F^+ - 1 \times a_s, + FL^+ + 1 \times a_s, - FL^+ - \eta^- (\cdot, t) + R_{f,-} - F^-
\]

\[
\partial_t c^{+} (r, t) + (r, t) \partial_t c^{+} (r, t) - (r, t) I (t) V (t) + - + + + + Negative Electrode
Positive Electrode
\]

**Figure 3.2:** Single Particle Model. The only dynamic elements in the SPM are the diffusion subsystems modeling lithium concentration in the positive and negative electrodes.
If \( c_{ss,i}(t) \) is known, then the complete states \( c_{s,i}(r,t) \) can be recovered (asymptotically) using Luenberger observers as follows.

The observer is a copy of the diffusion systems in (3.1)-(3.3) along with surface concentration error injection, i.e.

\[
\frac{\partial c_{s,i}(r,t)}{\partial t} = D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}(r,t)}{\partial r} \right] + P_i(r) \left[ c_{ss,i}(t) - \tilde{c}_{ss,i}(t) \right],
\]

(3.10)

for \( r \in (0,R_{p,i}), t > 0 \), with boundary conditions

\[
\partial \tilde{c}_{s,i} \frac{\partial}{\partial r} (0,t) = 0,
\]

(3.11)

\[
D_{s,i} \frac{\partial \tilde{c}_{s,i}}{\partial r} (R_{p,i},t) = -j_i(t) + Q_i \left[ c_{ss,i}(t) - \tilde{c}_{ss,i}(t) \right].
\]

(3.12)

and with initial conditions \( \tilde{c}_{s,i}(r,0) = c_{s,i,0}(r) \in L^2(0,R_{p,i}) \) satisfying the boundary conditions.

The observer design problem is now the problem of finding gains \( P_i(r) \) and \( Q_i \) such that

\[
\tilde{c}_{s,i}(r,t) \rightarrow c_{s,i}(r,t) \text{ as } t \rightarrow \infty.
\]

(3.13)

Statement (3.13) can rewritten in terms of the estimation error \( \tilde{c}_{s,i}(r,t) = c_{s,i}(r,t) - \tilde{c}_{s,i}(r,t) \) as:

\[
\tilde{c}_{s,i}(r,t) \rightarrow 0 \text{ as } t \rightarrow \infty.
\]

Since \( \tilde{c}_{s,i}(r,t) \) is also a function of \( r \), a more precise convergence property can be formulated using a norm, for example

\[
\| \tilde{c}_{s,i} \|_2(t) \rightarrow 0 \text{ as } t \rightarrow \infty,
\]

(3.14)

where \( \| \cdot \|_2 \) is the \( L^2 \)-norm, i.e.

\[
\| \tilde{c}_{s,i} \|_2(t) = \left( \int_0^{R_p} |\tilde{c}_{s,i}(r,t)|^2 dr \right)^{1/2}.
\]

(3.15)

The convergence property in (3.14) holds if the equilibrium solution \( \tilde{c}_{s,i}(r,t) \equiv 0 \) of the estimation error system ( subtracting (3.10)-(3.12) from (3.1)-(3.3) ):

\[
\frac{\partial \tilde{c}_{s,i}(r,t)}{\partial t} = D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \tilde{c}_{s,i}(r,t)}{\partial r} \right] - P_i(r)\tilde{c}_{s,i}(1,t),
\]

(3.16)
\[
\frac{\partial \tilde{c}_{s,i}}{\partial t}(0,t) = 0,
\]
\[
D_{s,i} \frac{\partial \tilde{c}_{s,i}}{\partial r}(R_{p,i},t) = -Q_i \tilde{c}_{s,i}(1,t).
\]

is asymptotically stable in the \(L^2\)-norm. The estimation problem, as stated now, can be solved using the backstepping method for PDEs as follow.

First, normalization of spatial and time coordinates \(r \rightarrow r(1/R_{p,i})\) and \(t \rightarrow t(D_{s,i}/R_{p,i}^2)\) is used in the estimation error system

\[
\frac{\partial \tilde{c}_{s,i}}{\partial t}(r,t) = \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \tilde{c}_{s,i}}{\partial r}(r,t) \right] - \frac{R_{p,i}^2}{D_{s,i}} P_i(r) \tilde{c}_{s,i}(1,t),
\]
\[
\frac{\partial \tilde{c}_{s,i}}{\partial r}(0,t) = 0,
\]
\[
\frac{\partial \tilde{c}_{s,i}}{\partial r}(1,t) = -\frac{R_{p,i}}{D_{s,i}} Q_i \tilde{c}_{s,i}(1,t).
\]

Then, one seeks an invertible transformation of the form

\[
\tilde{c}_{s,i}(r,t) = w(r,t) - \int_0^1 K_i(r,s) w(s,t) ds,
\]

to map the estimation error system into an appropriate target system. For this problem, the target system is chosen as

\[
\frac{\partial w}{\partial t}(r,t) = \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial w}{\partial r}(r,t) \right] + \lambda_i w(r,t),
\]
\[
\frac{\partial w}{\partial r}(0,t) = 0,
\]
\[
\frac{\partial w}{\partial r}(1,t) = 0.
\]

One can prove that if \(\lambda_i < 0\) then the equilibrium solution \(w(r,t) \equiv 0\) is exponentially stable using for example the Lyapunov function

\[
V(t) = \int_0^1 w(r,t)^2 dr.
\]

Since transformation (9.37) is assumed to be invertible, exponential stability in the target system translates back to exponential stability in the estimation error system. It can be
found that kernel $K(r, s)$ in the transformation (9.37) should satisfy the PDE
\[
\frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial}{\partial r} (K(r, s)) \right] - \frac{\partial}{\partial s} \left[ s^{n-1} \frac{\partial}{\partial s} \left( \frac{K(r, s)}{s^{n-1}} \right) \right] = \lambda_i K(r, s), \tag{3.27}
\]
in the triangle domain $(r, s) \in \{(r, s) \in \mathbb{R}^2 | r \in (0, 1), s \in (r, 1)\}$, with boundary conditions
\[
K(r, r) = \frac{\lambda_i}{2} r, \tag{3.28}
\]
\[
K(r, 0) = 0. \tag{3.29}
\]

Further, observer gains should satisfy
\[
\frac{R_{p,i}^2}{D_{s,i}} P_i(r) = (n - 1) K(r, 1) - \frac{\partial K}{\partial s}(r, 1), \tag{3.30}
\]
\[
\frac{R_{p,i}}{D_{s,i}} Q_i = -K(1, 1). \tag{3.31}
\]

One can verify that the (closed form) solution of the kernel PDE is
\[
K(r, s) = \lambda_i s^{n-1} \frac{I_1[z_i(r, s)]}{z_i(r, s)}, \tag{3.32}
\]
with $z_i(r, s) = \sqrt{\lambda_i (r^2 - s^2)}$. From the closed form solution of the transformation kernel, the observer can be found in closed form
\[
P_i(r) = \frac{D_{s,i}}{R_{p,i}} \frac{\lambda^2}{r^{n-2}} \frac{I_2[z(r, 1)]}{z(r, 1)^2}, \tag{3.33}
\]
\[
Q_i = -\frac{D_{s,i}}{R_{p,i}} \frac{\lambda}{2}. \tag{3.34}
\]

Where $I_\alpha[\cdot]$ are modified Bessel functions of the first kind.

Finally, back in the unnormalized coordinates the state observer reads
\[
\frac{\partial \tilde{c}_{s,i}}{\partial t}(r, t) = D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \tilde{c}_{s,i}}{\partial r}(r, t) \right]
+ \frac{D_{s,i}}{R_{p,i}^2} \frac{\lambda^2}{\left( \frac{r}{R_{p,i}} \right)^{n-2}} \frac{I_2[z(r/R_{p,i}, 1)]}{z(r/R_{p,i}, 1)^2} \tilde{c}_{ss,i}(t), \tag{3.35}
\]
\[
\frac{\partial \tilde{c}_{s,i}}{\partial r}(0, t) = 0, \tag{3.36}
\]
\[
D_{s,i} \frac{\partial \tilde{c}_{s,i}}{\partial r}(R_{p,i}, t) = -j_i(t) - \frac{D_{s,i}}{R_{p,i}} \frac{\lambda_i}{2} \tilde{c}_{ss,i}(t). \tag{3.37}
\]
Use of voltage measurements

Since $\tilde{c}_{ss,i}(t)$ is not directly available for use in the observer, an approximation is needed. From the linear expansion of voltage around some estimate of surface concentrations $(\tilde{c}_{ss,+}, \tilde{c}_{ss,-})$ a linear relationship between error in surface concentration estimation and error in voltage estimation can be found

$$\tilde{V}(t) = \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right] \tilde{c}_{ss,+}(t) - \left[ \frac{\partial \phi_-}{\partial c_{ss,-}} \right] \tilde{c}_{ss,-}(t),$$

(3.39)

where $\tilde{V}(t) = V(t) - \hat{V}(t)$ and with voltage estimation being computed using surface concentration estimates: $\hat{V}(t) = \phi_{s,+}(\tilde{c}_{ss,+}(t),j(t)) - \phi_{s,-}(\tilde{c}_{ss,-}(t),j(t))$. From the fact for most electrode materials (and under normal operation conditions)

$$\left[ \frac{\partial \phi_-}{\partial c_{ss,-}} \right] < \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right],$$

(3.40)

a crude approximation of $\tilde{c}_{ss,+}(t)$ can be easily derived

$$\tilde{c}_{ss,+}(t)_{approx} = \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t).$$

(3.41)

We will used this approximation to update the concentration estimate in the positive electrode $\tilde{c}_{s,+}(r,t)$. To update concentration estimate in the negative particle, constant observer gains can be chosen to satisfy the property:

$$\frac{d\tilde{n}_{Li}}{dt}(t) = 0,$$

(3.42)

where

$$\tilde{n}_{Li}(t) = \epsilon_{s,+}L_{c_{ss,+},avg}(t) + \epsilon_{s,-}L_{c_{ss,-},avg}(t),$$

(3.43)

$$\tilde{c}_{s,+},avg(t) = \frac{n}{R_{p,+}} \int_0^{R_{p,+}} \tilde{c}_{s,+}(r,t)r^{(n-1)}dr,$$

(3.44)

$$\tilde{c}_{s,-},avg(t) = \frac{n}{R_{p,-}} \int_0^{R_{p,-}} \tilde{c}_{s,-}(r,t)r^{(n-1)}dr.$$

(3.45)

Such gains are

$$P_+ = \frac{\epsilon_{s,+}L_+}{\epsilon_{s,-}L_-} \frac{n}{R_{p,+}} \int_0^{R_{p,+}} P_+(r/R_{p,+})r^{(n-1)}dr,$$

(3.46)

$$Q_+ = \frac{\epsilon_{s,+}L_+/R_{p,+}}{\epsilon_{s,-}L_-/R_{p,-}} Q_+.$$

(3.47)
Since the observer is now being designed to keep the quantity $\tilde{n}_{Li}$ constant, an assumption would be needed.

**Assumption**

$$\tilde{n}_{Li}(0) = n_{Li}. \quad (3.48)$$

where $n_{Li}$ is the constant (preserved) quantity

$$n_{Li} = \epsilon_{s,+}Lc_{s,+} \text{avg}(t) + \epsilon_{s,-}Lc_{s,-} \text{avg}(t), \quad (3.49)$$

$$c_{s,+} \text{avg}(t) = \frac{n}{R_{p,+}} \int_{0}^{R_{p,+}} c_{s,+}(r,t)r^{(n-1)}dr, \quad (3.50)$$

$$c_{s,-} \text{avg}(t) = \frac{n}{R_{p,-}} \int_{0}^{R_{p,-}} c_{s,-}(r,t)r^{(n-1)}dr. \quad (3.51)$$

Later, by solving the problem of simultaneous state and parameter estimation this assumption would allow some uncertainty.

**Summary of observer using voltage measurements**

The observer for the positive electrode reads

$$\frac{\partial c_{s,+}}{\partial t}(r,t) = D_{s,+} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,+}}{\partial r}(r,t) \right]$$

$$+ P_+(r/R_{p,+}) \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t), \quad (3.52)$$

$$\frac{\partial c_{s,+}}{\partial r}(0,t) = 0, \quad (3.53)$$

$$D_{s,+} \frac{\partial c_{s,+}}{\partial r}(R_{p,+},t) = -j_+(t) + Q_+ \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t), \quad (3.54)$$

$$D_{s,+} \frac{\partial c_{s,+}}{\partial r}(R_{p,+},t) = -j_+(t) + Q_+ \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t), \quad (3.55)$$
and for the negative electrode

\[
\frac{\partial \hat{c}_{s,-}}{\partial t}(r,t) = D_{s,-} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \hat{c}_{s,-}}{\partial r}(r,t) \right] + P_- \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t),
\]

(3.56)

\[
\frac{\partial \hat{c}_{s,-}}{\partial r}(0,t) = 0,
\]

(3.57)

\[
D_{s,-} \frac{\partial \hat{c}_{s,-}}{\partial r}(R_{p,-},t) = -j_-(t) + Q_- \left[ \frac{\partial \phi_+}{\partial c_{ss,+}} \right]^{-1} \tilde{V}(t).
\]

(3.58)

with gains

\[
P_+(r) = \frac{D_{s,i}}{R_{p,+}^2} \frac{\lambda^2}{r^{n-2}} \frac{I_2[z(r,1)]}{z(r,1)^2},
\]

(3.59)

\[
Q_+ = -\frac{D_{s,+}}{R_{p,+}^2} \frac{\lambda}{2},
\]

(3.60)

\[
P_- = -\frac{\epsilon_{s,+} L_+}{\epsilon_{s,-} L_-} \frac{n}{R_{p,+}} \int_{0}^{R_{p,+}} P_+(r/R_{p,+}) r^{(n-1)} dr,
\]

(3.61)

\[
Q_- = -\frac{\epsilon_{s,+} L_+ / R_{p,+}}{\epsilon_{s,-} L_- / R_{p,-}} Q_+.
\]

(3.62)

A block diagram of the observer is shown in Figure 3.3.

3.1.3 Numerical Implementation

A numerical simulation is presented with the observer using current and voltage measurements from a SPM. Figures 3.4 - 3.7 show the results.
3.2 State Estimation from SPM - Multiple Active Material

3.2.1 SPM for Multiple Active Materials

The model consisting of: (i) a set of $m_- + m_+$ spherical diffusion PDEs modeling concentration in each active material, (ii) a set of nonlinear algebraic equations relating current density input and molar flux and surface concentrations and (iii) a nonlinear output function mapping boundary values of solid concentration and molar fluxes to terminal
**Figure 3.4:** Current density and voltage error. [Left] Current density profile from the Urban Dynamometer Driving Schedule (UDDS) which is representative of battery use in automotive applications. [Right] Voltage error (plant minus estimation) decays to zero.

**Figure 3.5:** Normalized surface concentration error. [Left] Error in surface concentration at the negative particle normalized with respect to the maximum concentration $c_{s,\text{max},-}$. [Right] Error in surface concentration at the positive particle normalized with respect to the maximum concentration $c_{s,\text{max},+}$. 
Figure 3.6: Normalized state error. [Left] Error in concentration at the negative particle normalized with respect to the maximum concentration $c_{s,\text{max},-}$. [Right] Error in concentration at the positive particle normalized with respect to the maximum concentration $c_{s,\text{max},+}$.

Figure 3.7: Derivatives of output with respect to surface concentration. [Left] Logarithmic plot of (absolute value) of the partial derivative of the output with respect to the surface concentration in the negative electrode. [Right] Logarithmic plot of (absolute value) of the partial derivative of the output with respect to the surface concentration in the positive particle. Note that the for the positive electrode the derivative is, for most of the simulation time, at least one order of magnitude bigger.
voltage.

(i) Diffusion equations

\[ \frac{\partial c_{s,i}}{\partial t}(r,t) = D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}}{\partial r}(r,t) \right], \quad (3.63) \]

for \( r \in (0, R_{p,i}), t > 0 \), with boundary conditions

\[ \frac{\partial c_{s,i}}{\partial r}(0,t) = 0, \quad (3.64) \]

\[ D_{s,i} \frac{\partial c_{s,i}}{\partial r}(R_{p,i},t) = -j_i(t), \quad (3.65) \]

where \( i \in \{1, 2, ..., m_- \} \cup \{1, 2, ..., m_+ \} \).

(ii) Input to molar flux relationships

Now, the relationship between current and molar flux are not simple proportional relationship. Rather, one need to solve a set of \( 2m_- + 1 \) nonlinear algebraic equations in the negative electrode

\[ 0 = I(t) - \sum_{k=1}^{m_-} a_{s,k} F L_{-j_k}(t), \quad (3.66) \]

\[ 0 = -\phi_{s,-}(t) + \eta_{i,-}(t) + U_{i,-}(c_{ss,i,-}(t)) + R_{t,i,-} F j_i(t), \quad (3.67) \]

\[ 0 = -j_{i,-}(t) + \frac{i_{0,i,-}(t)}{F} \left[ e^{\frac{\alpha_e F c_{ss,i,-}(t)}{RT}} - e^{-\frac{\alpha_e F c_{ss,i,-}(t)}{RT}} \right], \quad (3.68) \]

with

\[ i_{0,i,-}(t) = k_{i,-} \left[ c_{ss,i,-}(t) \right]^{\alpha_e} \left[ c_{e,0} \left( c_{s,\text{max},i,-} - c_{ss,i,-}(t) \right) \right]^{\alpha_a}, \quad (3.69) \]

where \( c_{ss,i,-}(t) = c_{s,i,-}(R_{p,i,-},t) \). To simplify notation we refer to this system as

\[ 0 = G_{-} \left( I(t), j_{-}(t), c_{ss,-}(t) \right). \quad (3.70) \]

with \( j_{-}(t) = [j_{1,-}, j_{2,-}, ..., j_{n,-}]^T(t) \) and \( c_{ss,-}(t) = [c_{ss,1,-}, c_{ss,2,-}, ..., c_{ss,n,-}]^T(t) \).

Similarly, for the positive electrode set of \( 2m_+ + 1 \) nonlinear algebraic equations in

\[ 0 = I(t) + \sum_{k=1}^{m_+} a_{s,k} F L_{+j_k}(t), \quad (3.71) \]

\[ 0 = -\phi_{s,+}(t) + \eta_{i,+}(t) + U_{i,+}(c_{ss,i,+}(t)) + R_{t,i,+} F j_i(t), \quad (3.72) \]

\[ 0 = -j_{i,+}(t) + \frac{i_{0,i,+}(t)}{F} \left[ e^{\frac{\alpha_e F c_{ss,i,+}(t)}{RT}} - e^{-\frac{\alpha_e F c_{ss,i,+}(t)}{RT}} \right], \quad (3.73) \]
with
\[ i_{0,i_+}(t) = k_{i_+} [c_{ss,i_+}(t)]^{\alpha_c} \left[ c_{e,0} \left( c_{s,max,i_+} - c_{ss,i_+}(t) \right) \right]^{\alpha_a}, \tag{3.74} \]
and \( c_{ss,i_+}(t) = c_{s,i_+}(R_{p,i_+}, t) \). Again, we use the notation
\[ 0 = G_+(I(t), j_+(t), c_{ss,+}(t)) . \tag{3.75} \]

Note that in this system of equations we use the assumption of electric potential equilibrium, i.e. potentials of all active materials in the same electrode are equal:
\[ \phi_{s,-}(t) = \eta_{i,-}(t) + U_{i,-}(c_{ss,i-}(t)) + R_{l,i-} F j_{i-}(t), \tag{3.76} \]
\[ \phi_{s,+}(t) = \eta_{i,+}(t) + U_{i,+}(c_{ss,i+}(t)) + R_{l,i+} F j_{i+}(t). \tag{3.77} \]

(iii) **Output function**

Finally, output voltage is computed as the difference between the (common) potentials in the positive and negative electrode
\[ V(t) = \phi_{s,+}(t) - \phi_{s,-}(t). \tag{3.78} \]

Note that by solving the nonlinear systems of algebraic equations \( G_+ \) and \( G_- \) for molar fluxes values, one is simultaneously solving for \( \phi_{s,+} \) and \( \phi_{s,-} \) and no additional computation is needed to obtain the output voltage other than subtracting those values.

**3.2.2 Observer Design**

Observer design for the multiple active material problem follows the same procedure as the one carried out in the single active material case. However, since now the values of molar flux \( j_-(t) \) and \( j_+(t) \) are not known exactly (because \( \hat{c}_{ss,i-}(t) \) and \( \hat{c}_{ss,i+}(t) \) are not known exactly) one need to use estimates \( \hat{j}_-(t) \) and \( \hat{j}_+(t) \)
\[ 0 = G_-(I(t), \hat{j}_-(t), \hat{c}_{ss,i-}(t)) , \tag{3.79} \]
\[ 0 = G_+(I(t), \hat{j}_+(t), \hat{c}_{ss,i+}(t)) . \tag{3.80} \]

**Molar flux correction**

On top of the molar flux estimates \( \hat{j}_-(t) \) and \( \hat{j}_+(t) \) one can add a correction from output
\[ \partial_t c_s + (r, t) I(t) V(t) - U + (\cdot) \eta + (\cdot, t) + R_f + F \partial_t c_s + (r, t) + F = 0 \]

\textbf{Figure 3.8:} Block diagram for SPM for electrodes with multiple active materials
voltage error from a linearization of $G_-(\cdot,\cdot,\cdot)$ and $G_+(\cdot,\cdot,\cdot)$. The linearization (around the estimation) is

$$0 = G_-(I(t), \tilde{j}_-(t), c_{ss,-}(t)) + \frac{\partial G_-}{\partial j_-} (I(t), \tilde{j}_-(t), c_{ss,-}(t)) \tilde{j}_-(t),$$  \hspace{1cm} (3.81)

$$+ \frac{\partial G_-}{\partial c_{ss,-}} (I(t), \tilde{j}_-(t), c_{ss,-}(t)) \tilde{c}_{ss,-}(t),$$  \hspace{1cm} (3.82)

and

$$0 = G_+(I(t), \tilde{j}_+(t), c_{ss,+}(t)) + \frac{\partial G_+}{\partial j_+} (I(t), \tilde{j}_+(t), c_{ss,+}(t)) \tilde{j}_+(t),$$  \hspace{1cm} (3.83)

$$+ \frac{\partial G_+}{\partial c_{ss,+}} (I(t), \tilde{j}_+(t), c_{ss,+}(t)) \tilde{c}_{ss,+}(t).$$

Using (3.79) and (3.80) one can find the relationships

$$\begin{bmatrix} \tilde{j}_1(t) \\ \vdots \\ \tilde{j}_n(t) \end{bmatrix} = \begin{bmatrix} a_{1,-,1}(t), \ldots, a_{1,-,n}(t) \\ \vdots \\ a_{n,-,1}(t), \ldots, a_{n,-,n}(t) \end{bmatrix} \begin{bmatrix} \tilde{c}_{ss,1-}(t) \\ \vdots \\ \tilde{c}_{ss,n-}(t) \end{bmatrix},$$  \hspace{1cm} (3.84)

and

$$\begin{bmatrix} \tilde{j}_1(t) \\ \vdots \\ \tilde{j}_n(t) \end{bmatrix} = \begin{bmatrix} a_{1,+1}(t), \ldots, a_{1,+n}(t) \\ \vdots \\ a_{n,+1}(t), \ldots, a_{n,+n}(t) \end{bmatrix} \begin{bmatrix} \tilde{c}_{ss,1+}(t) \\ \vdots \\ \tilde{c}_{ss,n+}(t) \end{bmatrix}.\hspace{1cm} (3.85)$$

As before $\tilde{c}_{ss,i+}(t)$ are not available, but we use the approximation

$$\begin{bmatrix} \tilde{c}_{ss,1+}(t)_{\text{approx}} \\ \vdots \\ \tilde{c}_{ss,n+}(t)_{\text{approx}} \end{bmatrix} = \begin{bmatrix} \left[ \frac{\partial \phi_+}{\partial c_{ss,1+}} \right]^{-1} \\ \vdots \\ \left[ \frac{\partial \phi_+}{\partial c_{ss,n+}} \right]^{-1} \end{bmatrix} \tilde{V}(t).$$  \hspace{1cm} (3.86)

and build the gains in the negative electrode for conservation of $n_{Li}$ which now depends on all active materials.
Figure 3.9: Normalized surface concentration error — Positive electrode with two active materials [Left] Error in surface concentration at the negative particle normalized with respect to the maximum concentration $c_{s,\text{max},-}$. [Right] Error in surface concentrations at the positive particles normalized with respect to the maximum concentrations $c_{s,\text{max},1+}$ and $c_{s,\text{max},2+}$.

3.2.3 Numerical Test

A numerical simulation is presented for an observer for two active materials in the positive electrode using current and voltage measurements from a SPM. Figure 3.9 shows the results.
3.3 Simultaneous Parameter and State Estimation

Uncertainty in parameters is captured in $\epsilon_i$ and $q_i$, which are multiplicative uncertainties. Here, $\epsilon_i = q_i = 1$ represents the nominal model.

$$
\frac{\partial c_{s,i}}{\partial t}(r,t) = \epsilon_i D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}}{\partial r}(r,t) \right], \quad (3.87)
$$

$$
\frac{\partial c_s}{\partial r}(0,t) = 0, \quad (3.88)
$$

$$
D_{s,i} \frac{\partial c_s}{\partial r}(R_{p,i},t) = -q_i(t), \quad (3.89)
$$

The objective of the this section is to identify and track changes in the parameters. We desire to do this as it is necessary to identify correct parameters for accurate SoC estimation, and additionally to track the inherent information about state-of-health (SoH) contained within the parameter evolution.

3.3.1 Parameterized Observer

The observer is a copy of the diffusion system in the positive electrode with error boundary (surface) error injection

$$
\frac{\partial \tilde{c}_{s,i}}{\partial t}(r,t) = \tilde{\epsilon}(t) D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \tilde{c}_{s,i}}{\partial r}(r,t) \right] + P_i(r) [c_{ss,i}(t) - \tilde{c}_{ss,i}(t)], \quad (3.90)
$$

$$
\frac{\partial \tilde{c}_{s,i}}{\partial r}(0,t) = 0, \quad (3.91)
$$

$$
D_{s,i} \frac{\partial \tilde{c}_{s,i}}{\partial r}(R_{p,i},t) = -\tilde{q}_i(t) + Q_i [c_{ss,i}(t) - \tilde{c}_{ss,i}(t)], \quad (3.92)
$$
Figure 3.10: Block diagram for state observer and online parameter identification from SPM. The ‘Plant’ block represent: a SPM, some other electrochemical model, or a real lithium-ion battery cell.
Figure 3.11: Parameter Identification. [Left] Parameter identification in negative electrode. [Right] Parameter identification in positive electrode. In both cases parameters converge close to the nominal value. In the x-axis 1 cycle refers a 3-hour input of: discharge (UDDS), charge (constant) and rest. This cycle is repeated 100 times.
3.3.2 Parameter Identifiers

We utilize a swapping identifier approach. The parameters update via a gradient (steepest descent) approach

\[
\frac{d}{dt} \tilde{\epsilon}_i(t) = \frac{\gamma_{\epsilon,i}}{m_i(t)} \left( \frac{n}{R_{p,i}^n} \int_0^{R_{p,i}} \psi_i(r,t) \tilde{\epsilon}_i(r,t) r^{(n-1)} dr \right),
\]

(3.93)

\[
\frac{d}{dt} \tilde{q}_i(t) = \frac{\gamma_{q,i}}{m_i(t)} \left( \frac{n}{R_{p,i}^n} \int_0^{R_{p,i}} \eta_i(r,t) \tilde{\epsilon}_i(r,t) r^{(n-1)} dr \right).
\]

(3.94)

Here \(\gamma_{\epsilon,i}\) and \(\gamma_{q,i}\) are tunable gains that regulate the rate of convergence. These gains must be selected carefully. The normalization signal \(m_i(t)\) is needed for boundedness properties of the parameter update, and is computed as

\[
m_i(t) = 1 + \|\psi_i\|^2(t) + \|\eta_i\|^2(t) + \|\mu_i\|^2(t),
\]

(3.95)

where \(\|\cdot\|\) denotes the 2-norm. Each function \(\psi_i, \eta_i\) and \(\mu_i\) is the solution of a particular filter PDE, and as are follows: The PDE for the \(\psi\)-filter, which approximates the effect of the second spatial derivative (in the respective geometrical coordinates) of concentration \(c_{s,i}(t)\) is

\[
\begin{align*}
\frac{\partial \psi_i}{\partial t}(r,t) &= \tilde{\epsilon}_i(t) D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \psi_i}{\partial r}(r,t) \right] \\
&\quad + D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}}{\partial r}(r,t) \right], \\
\frac{\partial \psi_i}{\partial r}(0,t) &= 0, \\
D_{s,i} \frac{\partial \psi_i}{\partial r}(R_{p,i},t) &= -\frac{1}{2} \psi_i(R_{p,i},t).
\end{align*}
\]

(3.96)

(3.97)

(3.98)

(3.99)

The PDE for the \(\eta\)-filter, which approximates the effect of the current density \(I(t)\), is

\[
\begin{align*}
\frac{\partial \eta_i}{\partial t}(r,t) &= \tilde{\epsilon}_i(t) D_{s,i} \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \eta_i}{\partial r}(r,t) \right], \\
\frac{\partial \eta_i}{\partial r}(0,t) &= 0, \\
D_{s,i} \frac{\partial \eta_i}{\partial r}(R_{p,i},t) &= -\frac{1}{2} \eta_i(R_{p,i},t) - j_i(t).
\end{align*}
\]

(3.100)

(3.101)

(3.102)
Finally, the PDE for the $\mu$-filter, which approximates the effect of the concentration state $c_{s,i}(t)$, is

$$\frac{\partial \mu_i}{\partial t}(r,t) = \epsilon_i(t) D_{s,i} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \mu_i}{\partial r}(r,t) \right] - \epsilon_i(t) D_{s,i} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,i}}{\partial r}(r,t) \right],$$

(3.103)

$$\frac{\partial \mu_i}{\partial r}(0,t) = 0,$$

(3.104)

$$D_{s,i} \frac{\partial \mu_i}{\partial r}(R_{p,i},t) = -\frac{1}{2}(\mu_i(R_{p,i},t) - c_{s,i}(t)).$$

(3.105)

With the filter equations defined above, we can formulate a prediction error

$$e_i(r,t) = c_{s,i}(r,t) - \epsilon_i(t) \psi_i(r,t) - q_i(t) \eta_i(r,t) - \mu_i(r,t)$$

(3.106)

which satisfies an exponentially stable error PDE (derived from Equations (3.97)-(3.105))

$$\frac{\partial e_i}{\partial r}(r,t) = \epsilon_i D_{s,i} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial e_i}{\partial r}(r,t) \right],$$

(3.107)

$$\frac{\partial e_i}{\partial r}(0,t) = 0,$$

(3.108)

$$D_{s,i} \frac{\partial e_i}{\partial r}(R_{p,i},t) = -\frac{1}{2} e_i(R_{p,i},t),$$

(3.109)

The prediction error $e_i$ is related to an estimation error $\tilde{e}_i(r,t)$, defined as

$$\tilde{e}_i(r,t) = c_{s,i}(r,t) - \epsilon_i(t) \psi_i(r,t) - q_i(t) \eta_i(r,t) - \mu_i(r,t)$$

(3.110)

This estimation error is the error utilized in the gradient update laws.

### 3.3.3 Numerical Test

A numerical simulation is presented with the observer and identification algorithms using current and voltage measurements from a SPM. Figures 3.11 show the results.
Chapter 4

State Estimation from a
Thermal-Electrochemical Model of
Lithium-Ion Batteries

4.1 Abstract

A thermal-electrochemical model of lithium-ion batteries is presented and a linear observer is derived for State-of-Charge (SoC) estimation by recovering the lithium concentration in the electrodes. This first-principles based model is a coupled system of partial and ordinary differential equations, which is a reduced version of the Doyle-Fuller-Newman model. More precisely, the subsystem of Partial Differential Equations (PDEs) is the Single Particle Model (SPM) while the Ordinary Differential Equation (ODE) is a model for the average temperature in the battery. The observer is designed following the PDE backstepping method. Since some coefficients in the coupled ODE-PDE system are time-varying, this results in the time dependency of some coefficients in the kernel function system of the backstepping transformation and it is non-trivial to show well-posedness of the latter
system. Adding thermal dynamics to the SPM serves a two-fold purpose: improving the accuracy of SoC estimation and keeping track of the average temperature which is a critical variable for safety management in lithium-ion batteries. Effectiveness of the estimation scheme is validated via numerical simulations.

4.2 Introduction

4.2.1 Motivation

Due to its high power and energy storage density, its lack of memory effect and low self discharge, lithium-ion technology is a common choice among the rechargeable battery family [26]. Besides its wide employment in portable electronics, lithium-ion batteries are now being adopted in electrified transportation [27] such as electric vehicles and hybrid electric vehicles. Lithium-ion technology is being considered for grid energy storage as well.

The key indicator for the amount of electrical energy available in batteries is the SoC which, simply put, is the ratio of instantaneous remaining battery charge to its maximum capacity [28]. Thus, in order to predict the available power and energy in the battery during operation, online estimation of the SoC serves as an important factor for regulating both charging and discharging. Besides, it is generally required that the SoC remains within appropriate bounds all the time during the battery operation for safety reasons. Hence, a reliable and accurate estimation of the SoC is required for proper battery management.

4.2.2 Lithium-ion battery models

Accuracy of the SoC estimation depends highly on the quality of the selected model. Thus, one is encouraged to compare the different models available for describing the battery dynamics. Models for lithium-ion batteries can be categorized into two classes. The first class consists of empirical models, in which the most frequently used ones are
Equivalent Circuit Models (ECMs) [29, 30]. ECMs use electric circuit elements such as voltage sources, resistances and RC networks to approximate the dynamics of the battery. Currently, most battery management systems employ ECMs for various tasks: power and energy estimation, cell balancing, thermal management, state-of-health estimation and charge/discharge control. The second class of models are based on first principles [31]. These electrochemical models account for the main underlying physics in the battery, more precisely, they offer an explicit description of the battery dynamics in terms of the main electrochemical parameters and variables. The need for accurate SoC estimation as well as visibility of important electrochemical states and parameters, specially in high power and high energy applications, motivates the study of estimation based on electrochemical models. The widely studied electrochemical Doyle-Fuller-Newman (DFN) model has been shown to accurately describe the main phenomena in lithium-ion batteries [28, 32]. However, the complexity of the model is too high for online SoC estimation [24]. Among the various approximations to the DFN model, the SPM [33, 34] is commonly used to derive online SoC estimation algorithms [15]. In the SPM, diffusion of lithium ions in each electrode is simplified as diffusion in a single spherical particle and electrolyte concentration is assumed to be constant. Still, the SPM has several limitations, for example, being accurate only at low currents [28]. Another limitation is that the SPM is restricted to the cases with small variation in internal temperature, which comes from the fact that SPM ignores the dependence of the battery parameters on temperature. In fact, lithium-ion batteries meet issues such as an increase in internal resistance and decrease of capacity, as functions of battery internal average temperature [34, 35].

4.2.3 Estimation algorithms

Extensive efforts have been devoted to developing SoC estimation algorithms, for example, Extended Kalman Filters (EKFs) for ECMs [30] and for the SPM [13]. Estimation
algorithms have also been derived for reduced electrochemical models with temperature dynamics, e.g., a linear observer derived to satisfy the conservation of lithium ions and a linear observer [24]. These estimation algorithms, together with others based on the unscented Kalman filter or particle filters, rely on some discretization of the diffusion phenomena.

Discretization generally implies a trade-off between high accuracy of the approximation, i.e., a large number of states, and a small number of tuning gains in the observer, i.e. a small number of states. The backstepping approach can be employed to design boundary observers for PDEs in which the discretization is not required. The readers can refer to [36] for a preliminary example of boundary observer design for diffusion PDEs via backstepping. This method has been used for the stabilization of various unstable PDE systems, see the tutorial book [22], in which backstepping boundary controllers and observers are designed for some unstable parabolic, hyperbolic PDEs and other types of PDEs.

4.2.4 Contribution

The main contribution of this paper is the derivation of a linear observer for SoC estimation from a simplified thermal-electrochemical model of lithium-ion batteries, i.e., a coupled ODE-PDE model composed by the SPM and a model for the averaged internal temperature [34, 37]. Adding thermal dynamics to SPM serves a two-fold purpose: improving the accuracy of SoC estimation and keeping track of the average temperature which is a critical variable for safety management in lithium-ion batteries.

The observer is designed following the PDE backstepping method. It is worth noting that backstepping observers have not been introduced to the problem of battery SoC estimation until very recently [15], and by this means the discretization of the diffusion PDEs in the model is avoided. We consider the result presented in this paper as an additional step in the efforts to design estimation and control algorithms for lithium-ion
batteries from electrochemical models without relying on the discretization of the PDEs in these models. The main technical challenges in our design consist of proving the well-posedness of the kernel function system for the backstepping transformation. The fact that some coefficients in the thermal-electrochemical model system are time-varying results in a kernel function system with time-varying coefficients, for which the well-posedness is non-trivial to derive. This paper is a continuation of a previous result for SoC estimation from a thermal-electrochemical model of lithium-ion batteries in [37].

4.2.5 Organization

The rest of this paper is organized as follows. In Section 4.3, a temperature-compensated SPM model is presented; and the corresponding SoC estimation problem is formulated in Section 3. In Section 4.5, a linear observer is developed for estimation of the lithium concentration in the electrodes through boundary state measurements via the backstepping method. The observer error system is proved to be exponentially stable with an arbitrarily designated decay rate, for which the well-posedness is derived by making use of the abstract evolution equation theory. It is worth noting that solving the kernel function system for the backstepping transformation is not trivial because of its dependence on the temperature [38, 39]. Under some more relaxed assumptions and simplifications than those in [37], the existence and regularity of the solution to the system is proved in this section. The SoC estimation accuracy is verified by the numerical simulation results presented in Section 4.6. Finally, some concluding remarks and possible future research topics are given in Section 4.7.
4.3 SPM-T Model

In this section, the working mechanism of lithium-ion batteries is briefly introduced through an overview of the DFN model. Then, the single particle model with temperature dynamics [34, 37], named SPM-T model, is presented for the purpose of SoC estimation, which can be viewed either as a simplification of the DFN model or as temperature-compensated SPM.

4.3.1 Working principles of lithium-ion batteries

A lithium-ion battery cell consists of three main regions: negative electrode, separator and positive electrode; all of them characterized by a porous structure. Each electrode includes active materials, conductive fillers, a current collector and a binder. The porous structure of the electrodes provides a large surface area and small distances between lithium ions and active material surfaces for reactions to occur. The separator is placed between the negative and positive electrodes to forbid the flow of electrons between two electrodes while allowing the movement of lithium ions dissolved in the electrolyte. The active materials, intercalated in the lattices of the corresponding electrode, are insertion compounds, i.e. these are host structures in which lithium can be reversibly inserted or extracted. Electrolyte fills all remaining parts of the battery.

The DFN model is derived based on the porous structure all through the lithium-ion battery [28, 35]. In the DFN model, each electrode is viewed as superposition of active materials, inert filler and electrolyte; justified by the porous configuration. As depicted in Fig. 4.1, all intercalation particles are assumed to be spheres with a uniform, averaged radius, and the battery is formulated as a pseudo two-dimensional model. The first dimension represents the path along the spatial direction $x$ from the anode, through the separator, to the cathode; and the second dimension is a radial direction $r_s$ used to
Figure 4.1: DFN schematic.

represent the intercalation and diffusion of lithium ions in the active materials.

Lithium ions move from the negative electrode to the positive electrode during discharging and in the opposite direction during charging. Lithium concentration in the solid phase, i.e. concentration of lithium ions in the active materials, follows the Fick’s law of diffusion:

\[
\frac{\partial c_s^\pm(t,x,r_s)}{\partial t}(t,x,r_s) = \frac{1}{r_s^2} \frac{\partial}{\partial r_s} \left[ D_s^\pm(T(t)) r_s^2 \frac{\partial c_s^\pm(t,x,r_s)}{\partial r_s} \right], \quad t > 0,
\]

\( x \in \left(0^\pm, L^\pm\right), \quad r_s \in \left(0, R_s^\pm\right), \quad (4.1) \)

\[
\frac{\partial c_s^\pm(t,x,0)}{\partial r_s}(t,x,0) = 0, \quad t > 0, \quad x \in \left(0^\pm, L^\pm\right),
\]

\( (4.2) \)

\[
\frac{\partial c_s^\pm(t,x,R_s^\pm)}{\partial r_s}(t,x,R_s^\pm) = -\frac{1}{D_s^\pm(T(t))} j^\pm(t,x), \quad t > 0, x \in \left(0^\pm, L^\pm\right),
\]

\( (4.4) \)

\[
c_s^\pm(0,x,r_s) = c_{s0}(x,r_s), \quad x \in \left[0^\pm, L^\pm\right], r_s \in \left[0, R_s^\pm\right],
\]

\( (4.5) \)

where the temporal variable is \( t \), the spatial variables are \( x \) and \( r_s \). The states of the PDE model (4.2)–(4.5) are \( c_s^\pm(t,x,r_s) \in \mathbb{R} \); the solid phase lithium concentration. The
Table 4.1: Thermal-Electrochemical Model. Variables

<table>
<thead>
<tr>
<th>Variables</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_s )</td>
<td>Lithium concentration in the solid phase</td>
</tr>
<tr>
<td>( c_{ss} )</td>
<td>Lithium concentration at the surface of the particle</td>
</tr>
<tr>
<td>( c_e )</td>
<td>Constant lithium concentration in the electrolyte</td>
</tr>
<tr>
<td>( \bar{c}_s )</td>
<td>Volume averaged lithium concentration in the solid phase</td>
</tr>
<tr>
<td>( j )</td>
<td>Molar flux of lithium at the surface of the particle</td>
</tr>
<tr>
<td>( \phi_s )</td>
<td>Electric potential in the solid phase</td>
</tr>
<tr>
<td>( \phi_e )</td>
<td>Electric potential in the electrolyte</td>
</tr>
<tr>
<td>( \eta )</td>
<td>Reaction overpotential</td>
</tr>
<tr>
<td>( U )</td>
<td>Open-circuit potential</td>
</tr>
<tr>
<td>( i_0 )</td>
<td>Exchange current density</td>
</tr>
<tr>
<td>( i_e )</td>
<td>Electrolyte current density normalized by cross-sectional area</td>
</tr>
<tr>
<td>( T )</td>
<td>Internal average temperature</td>
</tr>
<tr>
<td>( T_{amb} )</td>
<td>Ambient temperature</td>
</tr>
<tr>
<td>( I )</td>
<td>External current density normalized by cross-sectional area</td>
</tr>
<tr>
<td>( V )</td>
<td>Terminal voltage</td>
</tr>
<tr>
<td>( \bar{q}_s )</td>
<td>Volume averaged flux</td>
</tr>
</tbody>
</table>

Molar fluxes \( j^\pm(t,x) \) are related to the reaction overpotential \( \eta^\pm(t,x) \) by the Butler-Volmer equation

\[
    j^\pm(t,x) = \frac{i_0^\pm(t,x)}{F} \left[ e^{\frac{\alpha_a F}{RT(t)} \eta^\pm(t,x)} - e^{-\frac{\alpha_c F}{RT(t)} \eta^\pm(t,x)} \right]. \tag{4.6}
\]

The reaction overpotentials \( \eta^\pm(t,x) \) are computed from

\[
    \eta^\pm(t,x) = \phi_s^\pm(t,x) - \phi_e^\pm(t,x) - U^\pm(c_{ss}^\pm(t,x), T(t)) - FR_t^\pm(T(t)) j^\pm(t,x). \tag{4.7}
\]

Lithium concentration in the liquid phase \( c_e(t,x) \), i.e. concentration of lithium ions in the electrolyte, satisfies the diffusion equation

\[
    \frac{\partial c_e(t,x)}{\partial t} = \frac{\partial}{\partial x} \left[ D_e \frac{\partial c_e(t,x)}{\partial x} + \frac{1-i_e(t,x)}{\varepsilon_e F} i_e(t,x) \right]. \tag{4.8}
\]
Table 4.2: Thermal-Electrochemical Model. Parameters

<table>
<thead>
<tr>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
</tr>
<tr>
<td>$D_s$</td>
</tr>
<tr>
<td>$D_e$</td>
</tr>
<tr>
<td>$c_{s,\text{max}}$</td>
</tr>
<tr>
<td>$R_s$</td>
</tr>
<tr>
<td>$\alpha_a$</td>
</tr>
<tr>
<td>$\alpha_c$</td>
</tr>
<tr>
<td>$r_{\text{eff}}$</td>
</tr>
<tr>
<td>$R_f$</td>
</tr>
<tr>
<td>$R_c$</td>
</tr>
<tr>
<td>$\epsilon_s$</td>
</tr>
<tr>
<td>$\epsilon_e$</td>
</tr>
<tr>
<td>$a_s$</td>
</tr>
<tr>
<td>$F$</td>
</tr>
<tr>
<td>$R$</td>
</tr>
<tr>
<td>$N_{Li,s}$</td>
</tr>
<tr>
<td>$\sigma$</td>
</tr>
<tr>
<td>$\kappa$</td>
</tr>
<tr>
<td>$\nu_{c,\text{eff}}^0$</td>
</tr>
<tr>
<td>$f_{c/a}$</td>
</tr>
<tr>
<td>$\rho_{\text{avg}}$</td>
</tr>
<tr>
<td>$c_p$</td>
</tr>
<tr>
<td>$h_{\text{cell}}$</td>
</tr>
<tr>
<td>$E$</td>
</tr>
</tbody>
</table>

**Super- and subscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>Positive electrode</td>
</tr>
<tr>
<td>-</td>
<td>Negative electrode</td>
</tr>
<tr>
<td>sep</td>
<td>Separator</td>
</tr>
<tr>
<td>s</td>
<td>Solid phase</td>
</tr>
<tr>
<td>e</td>
<td>Electrolyte</td>
</tr>
</tbody>
</table>
Equations for solid electric potential $\phi_s(t, x)$ and electrolyte electric potential $\phi_e(t, x)$ are

$$ \frac{\partial \phi_s(t, x)}{\partial x} = \frac{i_e(t, x) - I(t)}{\sigma}, \quad (4.9) $$

$$ \frac{\partial \phi_e(t, x)}{\partial x} = - \frac{i_e(t, x)}{\kappa} + \frac{2RT(t)}{F} (1 - t_0) + \left(1 + \frac{\ln f_c}{\ln c_e(t, x)}\right) \frac{\partial \ln c_e(t, x)}{\partial x}, \quad (4.10) $$

where $I(t)$ is the external current density normalized by cross-sectional area. Charge conservation in the electrodes provides a relation between electrolyte current densities $i_e^\pm(x, t)$ and molar fluxes $j_e^\pm(t, x)$:

$$ \frac{\partial i_e^+(t, x)}{\partial x} = -a_s^+ F j_e^+(t, x), \quad (4.11) $$

$$ \frac{\partial i_e^-(t, x)}{\partial x} = a_s^- F j_e^-(t, x), \quad (4.12) $$

with boundary conditions $i_e^-(t, 0^-) = i_e^+(t, L^+) = 0$ and $i_e^-(t, L^-) = i_e^+(t, 0^+) = I(t)$. In the separator, $i_e(t, x) = I(t)$. Output voltage is the difference between the two solid electric potentials computed as

$$ V(t) = \phi_s(t, L^+) - \phi_s(t, 0^-). $$

The readers should refer to [28] for a complete description of the DFN model and for the boundary conditions for equations (4.8)–(4.10). Note that we are using the convention: positive current for discharging and negative current for charging.

### 4.3.2 The SPM-T model

The DFN model accurately describes many aspects of the lithium-ion cells working mechanism; however, the complexity of the model is too high for online SoC estimation. For this reason, we present a simplified model which is the single particle model with temperature dynamics, i.e., the SPM-T model. The SPM-T model [34, 37] is derived by making the following assumptions and simplifications:
- concentration of lithium ions in the electrolyte \( c_e(t, x) \) is uniform in both time and space,
- molar fluxes \( j^\pm(t, x) \) are uniform in the \( x \)-direction,
- concentration of lithium ions in the active materials \( c_s(t, x) \) is uniform in the \( x \)-direction.

Moreover, each electrode is modeled as a single spherical particle in this simplification; representative of all particles in the electrode. Compared with the SPM-T model presented in [34], here we choose not to take into account the electrolyte resistance \( R_{\text{cell}} \), i.e., we set \( R_{\text{cell}} = 0 \) [18]. In the coupled SPM-T model, the SPM subsystem is

\[
\frac{\partial c^\pm_s}{\partial t}(t, r_s) = \frac{1}{r_s^2} \frac{\partial}{\partial r_s} \left[ D^\pm_s(T(t)) r_s^2 \frac{\partial c^\pm_s}{\partial r_s}(t, r_s) \right],
\]

\( t > 0, r_s \in (0, R^\pm_s) \), \hspace{1cm} (4.13)

\[
\frac{\partial c^\pm_s}{\partial r_s}(t, 0) = 0, \hspace{0.5cm} t > 0,
\]

\( \hspace{1cm} (4.14) \)

\[
\frac{\partial c^\pm_s}{\partial r_s}(t, R^\pm_s) = -\frac{1}{D^\pm_s(T(t))} j^\pm(t), \hspace{0.5cm} t > 0,
\]

\( \hspace{1cm} (4.15) \)

\[
c^\pm_s(0, r_s) = c^\pm_s(0, r_s), \hspace{0.5cm} r_s \in [0, R^\pm_s].
\]

\( \hspace{1cm} (4.16) \)

The states of the system (4.77)–(4.16) are \( c^\pm_s(t, r_s) \in \mathbb{R} \), with the temporal variable \( t \) and the spatial variables \( r_s \). The relation between molar fluxes \( j^\pm(t) \) and current \( I(t) \) becomes linear

\[
j^+(t) = -\frac{I(t)}{a^+_s FL^+}, \hspace{0.5cm} j^-(t) = \frac{I(t)}{a^-_s FL^-}.
\]

\( \hspace{1cm} (4.17) \)

By assuming the same value to the anodic and cathodic transfer coefficients, i.e., \( \alpha \triangleq \alpha_a = \alpha_c \),
a simple relation between reaction overpotentials and molar fluxes can be found as

\[ \eta^{\pm}(t) = \frac{RT(t)}{\alpha F} \sinh^{-1} \left( \frac{F}{2i_0^{\pm}(t)} j^{\pm}(t) \right), \]  

(4.18)

where

\[ i_0^{\pm}(t) = r_{\text{eff}}^{\pm}(T(t)) \left[ c_{\text{ss}}^{\pm}(t) \right]^\alpha \left[ c_{\text{e},0} \left( c_{\text{ss}}^{\pm} - c_{\text{ss}}^{\pm}(t) \right) \right]^{\alpha_c}, \]  

(4.19)

with \( c_{\text{ss}}^{\pm}(t) \triangleq c_{\text{s}}^{\pm}(t, R_f^{\pm}) \). The parameter \( c_{\text{e},0} \) in the equation (4.19) denotes the electrolyte concentration at equilibrium. Solid electric potentials are computed from

\[ \phi_{s}^{\pm}(t) = \eta^{\pm}(t) + U^{\pm}(c_{ss}^{\pm}(t), T(t)) + FR_{f}^{\pm}(T(t)) j^{\pm}(t). \]  

(4.20)

Output voltage is now the difference between solid electric potentials in the positive electrode and negative electrode:

\[ V(t) = \phi_{s}^{+}(t) - \phi_{s}^{-}(t) \]

\[ = -\frac{RT(t)}{\alpha F} \left[ \sinh^{-1} \left( \frac{1}{2i_0^{+}(t)} I(t) \right) + \sinh^{-1} \left( \frac{1}{2i_0^{-}(t)} I(t) \right) \right] \]

\[ - \left( \frac{R_{f}^{+}(T(t))}{a^+L^+} + \frac{R_{f}^{-}(T(t))}{a^-L^-} \right) I(t) + U^{+}(c_{ss}^{+}(t), T(t)) - U^{-}(c_{ss}^{+}(t), T(t)). \]  

(4.21)

Parameters \( D_{s}^{\pm}(T(t)), r_{\text{eff}}^{\pm}(T(t)) \) and \( R_{f}^{\pm}(T(t)) \) are functions with an Arrhenius-like dependence [24] on the battery cell internal average temperature \( T(t) \), i.e.,

\[ D_{s}^{\pm}(T(t)) = D_{s}^{\pm}(T(0)) e^{E_{D_{s}^{\pm}}(T(t)-T(0))}, \]  

(4.22)

\[ r_{\text{eff}}^{\pm}(T(t)) = r_{\text{eff}}^{\pm}(T(0)) e^{E_{r_{\text{eff}}^{\pm}}(T(t)-T(0))}, \]  

(4.23)

\[ R_{f}^{\pm}(T(t)) = R_{f}^{\pm}(T(0)) e^{E_{R_{f}^{\pm}}(T(t)-T(0))}. \]  

(4.24)
where $E_{D_k^\pm}$, $E_{r_{\text{eff}}}^\pm$, $E_{R_k^\pm}$, are activation energy coefficients. Internal average temperature satisfies the following ODE [35, Section 12.3.7]

$$\rho_{\text{avg}} c_P \frac{dT}{dt}(t) = h_{\text{cell}} (T_{\text{amb}}(t) - T(t)) - I(t)V(t) + I(t)\left\{U^+(\bar{c}_s^+(t), T(t)) - U^-(\bar{c}_s^-(t), T(t))\right\} - T(t)\left[\frac{\partial U^+}{\partial T}(\bar{c}_s^+(t), T(t)) - \frac{\partial U^-}{\partial T}(\bar{c}_s^-(t), T(t))\right] + R_c I(t)^2, \ t > 0, \ (4.25)$$

$$T(0) = T_{\text{amb}}(0), \ (4.26)$$

where $\bar{c}_s^\pm(t)$ are the average concentrations defined as

$$\bar{c}_s^\pm(t) = \frac{3}{(R_{\text{ss}}^\pm)^3} \int_0^{R_{\text{ss}}^\pm} r_s^2 c_s^\pm(t, r_s) dr_s. \ (4.27)$$

The system states are the solid phase lithium ion concentrations $c_s^\pm(t, r_s) \in \mathbb{R}$ in the PDE (5.77)-(4.16) and the internal average temperature $T(t)$ in the ODE (4.25)-(4.26).

### 4.4 Problem Formulation

#### 4.4.1 Estimation objective

Our objective is to estimate the battery SoC, defined as the normalized averaged lithium concentration in the negative electrode, i.e.,

$$\text{SoC}(t) = \frac{3}{(R_s^-)^3} \int_0^{R_s^-} r_s^2 c_s^-(t, r_s) dr_s = \frac{\bar{c}_s^-(t)}{c_{s,\text{max}}}, \ (4.28)$$

from measurements of the input current $I(t)$ and the output voltage $V(t)$. For this purpose, boundary observers can be constructed to estimate the concentrations of lithium ions in the electrodes $c_s^-(t, r_s)$ by using the boundary values, i.e., the corresponding surface concentrations $c_{ss}^-(t)$. Note however that in (4.21), boundary values $c_{ss}^-(t)$ are not directly
available from measurement of $V(t)$. Instead, they appear in $V(t)$ with a nonlinear fashion, i.e., the nonlinearities within the exchange current densities $i_0^-(t)$ and within the subtraction between the nonlinear Open-Circuit Potential (OCP) functions $U^-(t, c_{ss}^-(t))$. Therefore, in order to overcome the lack of boundary value measurements required by the boundary observers, an inversion of the output function $V(t)$ with respect to the boundary values is needed.

To ease inversion of the output voltage, the lithium concentration dynamics in one of the electrodes will be simplified. Inversion will then be done with respect to the surface concentration of the electrode with unsimplified lithium concentration dynamics. The leading terms in the output voltage are the OCP functions and we are assuming that the OCP functions are invertible with respect to the surface concentration in the corresponding unsimplified electrode. In this paper, we will simplify the lithium concentration dynamics in the negative electrode and invert the output function with respect to the surface concentration in the positive electrode, and a boundary observer will then be derived for estimation of lithium ion concentration in the positive electrode.

**Remark 4.4.1.** The decision of simplifying the negative electrode dynamics instead of the positive one is made based on the sensitivity of OCPs to surface concentrations. For some common lithium ion active materials, $\frac{\partial U^+}{\partial c^+_{ss}}$ is larger than $\frac{\partial U^+}{\partial c^-_{ss}}$ in magnitude, thus making it easier to recover $c^+_{ss}$ from the voltage measurement $V(t)$.

One can easily prove that the total amount of lithium ions in solid phase $N_{Li,s}$ is conserved [24], i.e.,

$$\frac{dN_{Li,s}}{dt} = 0,$$  \hspace{1cm} (4.29)
where

\[ N_{Li,s} = \epsilon^+ L^+ \bar{c}_s^+(t) + \epsilon^- L^- \bar{c}_s^-(t). \]  \hspace{1cm} (4.30)

Since we assume \( N_{Li,s} \) is a known quantity, i.e. a parameter in the model, then we can also compute the battery SoC in the negative electrode from the averaged lithium concentration in the positive electrode, i.e.

\[ \text{SoC}(t) = \frac{N_{Li,s} - \epsilon^+ L^+ \bar{c}_s^+(t)}{\epsilon^- L^- c_{s,\text{max}}^-} . \]  \hspace{1cm} (4.31)

### 4.4.2 Output function inversion

The goal of the output function inversion is to write \( V(t) \) as a function of only of \( c_{ss}^+(t) \) and \( I(t) \).

**Write \( V(t) \) as a function of \( c_{ss}^+(t) \), \( \bar{c}_s^+(t) \) and \( I(t) \)**

The first step is to simplify the internal average temperature dynamics to derive an expression for \( T(t) \) only in terms of time and current, i.e., a time-varying function \( \hat{T}(t) \triangleq \hat{T}(t, I(t), T_{\text{amb}}(t)) \) independent of the concentrations \( c_s^+(t) \), \( c_{ss}^+(t) \). We start by substituting the output voltage equation (4.21) into the original average temperature
equation (4.25),

\[
\rho_{\text{avg}} c_P \frac{dT}{dt} (t) = h_{\text{cell}} (T_{\text{amb}} (t) - T(t)) + I(t) \frac{RT(t)}{\alpha F} \left[ \sinh^{-1} \left( \frac{1}{2 \theta_0^+ (t)} \frac{I(t)}{a^+ L^+} \right) \right. \\
+ \sinh^{-1} \left( \frac{1}{2 \theta_0^- (t)} \frac{I(t)}{a^- L^-} \right) \right] + \left( \frac{R_f^+ (T(t))}{a^+ L^+} + \frac{R_f^- (T(t))}{a^- L^-} - R_c \right) \left( \frac{I(t)}{2} \right)^2 \\
- I(t) \left[ U^+ (c_{ss}^+ (t), T(t)) - U^- (c_{ss}^- (t), T(t)) \right] \\
+ I(t) - \{ U^+ (\bar{c}_s^+ (t), T(t)) - U^- (\bar{c}_s^- (t), T(t)) \} \\
- T(t) \left[ \frac{\partial U^+ (\bar{c}_s^+ (t), T(t))}{\partial T} - \frac{\partial U^- (\bar{c}_s^- (t), T(t))}{\partial T} \right]. 
\]  

(4.32)

We assume that the functions \( U^\pm (\cdot, T(t)) \) and \( i_0^\pm (\cdot) \) are independent of concentrations but possibly time-varying, and we replace their dependence on temperature \( T(t) \) with dependence on the ambient temperature \( T_{\text{amb}} (t) \). For this purpose, denote

\[
\tilde{U}_1^\pm (t) \triangleq U^\pm (c_{ss}^\pm (t), T_{\text{amb}} (t)), \tag{4.33}
\]

\[
\tilde{U}_2^\pm (t) \triangleq U^\pm (\bar{c}_s^\pm (t), T_{\text{amb}} (t)), \tag{4.34}
\]

\[
\tilde{i}_0^\pm (t) \triangleq i_0^\pm (T_{\text{amb}} (t)), \tag{4.35}
\]

where subscript 1 in \( \tilde{U} \) is used to denote the approximation of \( U^\pm (\cdot, T(t)) \) when they are evaluated at the surface concentration and subscript 2 when they are evaluated at the averaged concentration. Similarly, for the temperature dependent parameters \( R_f^\pm (T(t)) \) and \( r_{\text{eff}}^\pm (T(t)) \), we also replace dependence on \( T(t) \) with \( T_{\text{amb}} (t) \), i.e.,

\[
r_{\text{eff}}^\pm (t) \triangleq r_{\text{eff}}^\pm (T_{\text{amb}} (t)), \tag{4.36}
\]

\[
\tilde{R}_f^\pm (t) \triangleq R_f^\pm (T_{\text{amb}} (t)). \tag{4.37}
\]
Thus, we can rewrite the equation (4.32) as

\[
\rho_{\text{avg}} \frac{d\tilde{T}}{dt}(t) = \chi(t)\tilde{T}(t) + \omega(t),
\]

where

\[
\chi(t) = -h_{\text{cell}} + \frac{R}{\alpha F} I(t) \left[ \sinh^{-1} \left( \frac{1}{2i_0^+} \frac{I(t)}{a^+ L^+} \right) + \sinh^{-1} \left( \frac{1}{2i_0^-} \frac{I(t)}{a^- L^-} \right) \right] - I(t) \left[ \frac{\partial \tilde{U}_2^+}{\partial T}(t) - \frac{\partial \tilde{U}_2^-}{\partial T}(t) \right],
\]

\[
\omega(t) = h_{\text{cell}} T_{\text{amb}}(t) + \left( \frac{\tilde{R}^+_t(t)}{a^+ L^+} + \frac{\tilde{R}^-_t(t)}{a^- L^-} - R_c \right) I(t)^2 - I(t) \left[ \tilde{U}_2^+ (t) - \tilde{U}_2^- (t) \right] + I(t) \left[ \tilde{U}_2^+ (t) - \tilde{U}_2^- (t) \right],
\]

then, it holds that

\[
\tilde{T}(t) = \tilde{T}(0) e^{\frac{1}{\rho_{\text{avg}} C_p} \int_0^t \chi(\tau) d\tau} + \frac{1}{\rho_{\text{avg}} C_p} \int_0^t e^{\frac{1}{\rho_{\text{avg}} C_p} \int_0^{\tau} \chi(\sigma) d\sigma} \omega(\tau) d\tau.
\]

Substituting (4.41) into (4.21) yields the following simplified output function:

\[
V(t) = -\frac{R \tilde{T}(t)}{\alpha F} \left[ \sinh^{-1} \left( \frac{1}{2i_0^+} \frac{I(t)}{a^+ L^+} \right) + \sinh^{-1} \left( \frac{1}{2i_0^-} \frac{I(t)}{a^- L^-} \right) \right] - \left( \frac{R^+_t(\tilde{T}(t))}{a^+ L^+} + \frac{R^-_t(\tilde{T}(t))}{a^- L^-} \right) I(t) + U^+(c_{ss}^+(t), \tilde{T}(t)) - U^-(c_{ss}^-(t), \tilde{T}(t)),
\]

\[
\triangleq h_1(t, c_{ss}^+(t), c_{ss}^-(t), I(t)).
\]

**Write \( V(t) \) as a function of \( c_{ss}^+(t) \) and \( I(t) \)**

In order to further simplify the output function, we are to establish relations between \( c_{ss}^+(t) \) and the other concentrations \( c_{ss}^-(t), c_s^+(t), c_s^-(t) \). Consider the following approximate
polynomial solution profiles of the electrode diffusion dynamics [40] 

\[ c_s^\pm(t) = c_{ss}^\pm(t) - \frac{8R_s^\pm}{35}q_s^\pm(t) + \frac{R_s^\pm}{35D_s^\pm(\bar{T}(t))}j^\pm(t), \]  

(4.44)

where the volume averaged fluxes \( \bar{q}_s^\pm(t) \) satisfy

\[ \frac{d}{dt} \bar{q}_s^\pm(t) = -\frac{30D_s^\pm(\bar{T}(t))}{(R_s^\pm)^2} \bar{q}_s^\pm(t) - \frac{45}{2(R_s^\pm)^2}j^\pm(t). \]  

(4.45)

Moreover, from the conservation (4.29) of lithium ions in solid phase \( N_{Li,s} \), we can write the relation

\[ \bar{c}_s^-(t) = \alpha \bar{c}_s^+(t) + \beta, \]  

(4.46)

where \( \alpha = -\frac{e^+L^+}{e^-L^-} \) and \( \beta = \frac{N_{Li,s}}{e^-L^-} \). It then immediately follows from (4.44) and (4.46) that

\[ \bar{c}_s^-(t) = \alpha \left( c_{ss}^+(t) - \frac{8R_s^+}{35}q_s^+(t) + \frac{R_s^+}{35D_s^+(\bar{T}(t))}j^+(t) \right) + \beta, \]  

(4.47)

\[ c_s^\pm(t,r) = \frac{39}{4}c_{ss}^\pm(t) - 3\bar{q}_s^\pm(t)R_s^\pm - \frac{35}{4}c_s^\pm(t) \]

\[ + \left( -35c_{ss}^\pm(t) + 10\bar{q}_s^\pm(t)R_s^\pm + 35c_s^\pm(t) \right) \frac{(r_s^\pm)^2}{(R_s^\pm)^2} \]

\[ + \left( 105c_{ss}^\pm(t) - 7\bar{q}_s^\pm(t)R_s^\pm - 105c_s^\pm(t) \right) \frac{r_s^4}{(R_s^\pm)^4} \]  

(4.43)
and

\[
c_{ss}^{-}(t) = c_{s}^{-}(t) + \frac{8R_{s}^{-}}{35}q_{s}^{-}(t) - \frac{R_{s}^{-}}{35D_{s}^{-}(\hat{T}(t))}j^{-}(t)
\]

\[
= \alpha \left( c_{ss}^{+}(t) - \frac{8R_{s}^{+}}{35}q_{s}^{+}(t) + \frac{R_{s}^{+}}{35D_{s}^{+}(\hat{T}(t))}j^{+}(t) \right) + \beta + \frac{8R_{s}^{-}}{35}q_{s}^{-}(t) - \frac{R_{s}^{-}}{35D_{s}^{-}(\hat{T}(t))}j^{-}(t).
\]

(4.48)

Therefore, from (4.42), (4.44), (4.47) and (4.48), we obtain a further simplified version of the output function:

\[
V(t) = h_{2}(t, c_{ss}^{+}(t), I(t)).
\]

(4.49)

**Inversion of the function \( h_{2} \)**

As long as the function (4.49) is a one-to-one correspondence w.r.t. \( c_{ss}^{+}(t) \), uniformly in \( I(t) \), one could invert it to derive the boundary concentration in the positive electrode as

\[
c_{ss}^{+}(t) = h_{0}(t, V(t), I(t)).
\]

(4.50)

### 4.4.3 Normalization and state transformation

We perform normalization and state transformation to simplify the system and thus also the structure of to-be-designed observer. Let \( r = r_{s}/R_{s}^{+} \) for normalization and proceed the state transformation \( c(t, r) = r sc_{s}^{+}(t, r_{s}) \), then the PDE subsystem (5.77)–(4.16)
is transformed into \(^2\)

\[
\frac{\partial c}{\partial t}(t,r) = \frac{D_s^+ (\bar{T}(t))}{(R_s^+)^2} \frac{\partial^2 c}{\partial r^2}(t,r), \quad t > 0, \quad r \in (0,1), \quad (4.51)
\]

\[
c(t,0) = 0, \quad t > 0, \quad (4.52)
\]

\[
\frac{\partial c}{\partial r}(t,1) - c(t,1) = \frac{R_s^+}{D_s^+ (\bar{T}(t))} \frac{I(t)}{a^+F L^+} \triangleq I_1(t), \quad t > 0, \quad (4.53)
\]

\[
c(0,r) = c_0(r) = R_s^+ r c_a^+(0,R_s^+ r), \quad r \in [0,1]. \quad (4.54)
\]

Our objective now is to design an observer for this normalized and transformed PDE system.

### 4.5 Backstepping State Observer

With the inversion of the output function in Section 4.4.2, the boundary concentration in the positive electrode is then available for observer design. Again, we assume that the internal averaged temperature is a time-varying and concentration-independent function which can be computed from the simplified equation (4.41). Thus, the function \(D_s^+ (\bar{T}(t))\) will be treated as known. Moreover, assume that \(I(t), U^\pm(\cdot, \bar{T}(t))\) and \(V(t)\) are piecewise (real) analytic. In what follows, we only consider the proof piecewisely so that both \(I(t)\) and \(V(t)\) are analytic in each separate time interval. Then, from (4.41) and with the assumption that \(\partial U^\pm/\partial T\) are also analytic in each corresponding time interval, we can prove by induction that the \(n\)-th order derivative of \(\bar{T}(t)\) is differentiable for any nonnegative integer \(n\). Further, we can derive that \(\bar{T}(t)\) is analytic in each time interval.

Without loss of generality, consider \(t \in [0, t_{\text{max}}]\) where \(t_{\text{max}}\) is an appropriate finite time for the regularities to hold.

---

\(^2\)The normalization transformation \(\bar{t} = D_s^+ (\bar{T}(t))/(R_s^+)^2\) employed in [15] is not used in this paper. The reason is that \(T(t)\) is not known a priori in this case, needing to be measured or derived at each time step. Thus, the corresponding inverse transformation can not be trivially obtained.
A Luenberger-type observer for the normalized and transformed PDE system (4.51)–(4.54) can be designed:

\[
\frac{\partial \hat{c}}{\partial t}(t, r) = \frac{D_s^+ (\bar{T}(t))}{(R_s^+)^2} \frac{\partial^2 \hat{c}}{\partial r^2}(t, r) + p_1(t, r)(c(t, 1) - \hat{c}(t, 1)), \; t > 0, \; r \in (0, 1), \quad (4.55)
\]

\[
\hat{c}(t, 0) = 0, \; t > 0, \quad (4.56)
\]

\[
\frac{\partial \hat{c}}{\partial r}(t, 1) - \hat{c}(t, 1) = I_1(t) + p_{10}(t)(c(t, 1) - \hat{c}(t, 1)), \; t > 0, \quad (4.57)
\]

\[
\hat{c}(0, r) = \hat{c}_0(r), \; r \in [0, 1], \quad (4.58)
\]

which is a copy of the plant together with output error injection terms. Here, \( \hat{c}_0(r) \) denotes the initial condition of the observer, and the boundary state error injection gains \( p_1(t, r) \) and \( p_{10}(t) \) are to be determined to guarantee the stability of the estimation error system

\[
\frac{\partial \tilde{c}}{\partial t}(t, r) = \frac{D_s^+ (\bar{T}(t))}{(R_s^+)^2} \frac{\partial^2 \tilde{c}}{\partial r^2}(t, r) - p_1(t, r)\tilde{c}(t, 1), \; t > 0, \; r \in (0, 1), \quad (4.59)
\]

\[
\tilde{c}(t, 0) = 0, \quad (4.60)
\]

\[
\frac{\partial \tilde{c}}{\partial r}(t, 1) - \tilde{c}(t, 1) = -p_{10}(t)\tilde{c}(t, 1), \quad (4.61)
\]

\[
\tilde{c}(0, r) = c_0(r) - \hat{c}_0(r) \triangleq \tilde{c}_0(r), \quad (4.62)
\]

with \( \tilde{c}(t, r) \triangleq c(t, r) - \hat{c}(t, r) \). In order to find the output injection gains, the PDE backstepping method \cite{22} is employed. We would like to find an invertible transformation

\[
\tilde{c}(t, r) = \tilde{w}(t, r) - \int_r^1 p(t, r, \iota)\tilde{w}(t, \iota) d\iota \quad (4.63)
\]
so that $\tilde{w}$ satisfies the following exponentially stable target system:

$$
\frac{\partial \tilde{w}}{\partial t} (t, r) = \frac{D_s^+(\bar{T}(t))}{(R^+_s)^2} \frac{\partial^2 \tilde{w}}{\partial r^2} (t, r) + \lambda \tilde{w}(t, r), \quad (4.64)
$$

$$
\tilde{w}(t, 0) = 0, \quad (4.65)
$$

$$
\frac{\partial \tilde{w}}{\partial r} (t, 1) = -\frac{1}{2} \tilde{w}(t, 1), \quad (4.66)
$$

$$
\tilde{w}(0, r) = \tilde{w}_0(r), \quad (4.67)
$$

where $\tilde{w}_0(r)$ denotes the initial condition to be determined for the target system, and $
\lambda < \min_{t\geq 0}\{D_s^- (\bar{T}(t))\} / (4(R^+_s)^2)$ is a free parameter to be chosen, which determines the convergence rate of the observer state in (4.59)–(4.62) to the system state in (4.51)–(4.54).

The following lemma states the exponential stability of the $\tilde{w}$-system (4.64)–(4.67).

**Lemma 4.5.1.** Let $t \in [0, t_{\text{max}}]$. If

$$
\frac{1}{4(R^+_s)^2} \min_{t\geq 0}\{D_s^+(\bar{T}(t))\}, \quad (4.68)
$$

then for any initial data $\tilde{w}_0(\cdot) \in L^2(0, 1)$, the $\tilde{w}$-system (4.64)–(4.67) admits a (mild) solution $\tilde{w}(t, \cdot) \in L^2(0, 1)$ and is exponentially stable at $\tilde{w} \equiv 0$. Moreover, if the boundary compatibility condition is satisfied, the solution is classical.

**Proof.** Consider the state space $H = L^2(0, 1)$. For every $t \in [0, t_{\text{max}}]$, define a linear operator $A(t) : \text{Dom}(A(t)) \subset H \to H$ as follows:

$$
A(t) \varphi = \frac{D_s^+(\bar{T}(t))}{(R^+_s)^2} \varphi'' + \lambda \varphi, \quad \forall \varphi \in \text{Dom}(A(t)), \quad (4.69)
$$

$$
\text{Dom}(A(t)) = \{ \varphi \in H^2(0, 1); \varphi(0) = 0, \ \varphi'(1) = -\frac{1}{2} \varphi(1) \}. \quad (4.70)
$$
Then, the system (4.64)–(4.67) can be written into the following abstract equation:

\[
\frac{d}{dt} \tilde{w}(t, \cdot) = A(t) \tilde{w}(t, \cdot), \quad 0 \leq t \leq t_{\text{max}},
\]

(4.71)

\[
\tilde{w}(0, \cdot) = \tilde{w}_0(\cdot).
\]

(4.72)

Note that \(\text{Dom}(A(t))\) is dense in \(H\) and independent of \(t\), and it can be proved that \(A(t)\) is for each \(t\) the infinitesimal generator of an exponential stable semigroup. Indeed, all the assumptions (P1)–(P3) in [41, Section 5.6] are satisfied. Thus, from [41, Section 5.6, Theorem 6.1], there exists a unique evolution system corresponding to (4.71)–(4.72) and (4.64)–(4.67) as well. Furthermore, by considering the Lyapunov function \(V(t) = \frac{1}{2} \| \tilde{w}(t, \cdot) \|^2_{L^2(0,1)}\), we get

\[
\dot{V}(t) = \int_0^1 \tilde{w}(t, r) \left[ \frac{D_s^+(\tilde{T}(t))}{(R_s^+)^2} \frac{\partial^2 \tilde{w}}{\partial r^2}(t, r) + \lambda \tilde{w}(t, r) \right] dr
\]

\[
= \frac{D_s^+(\tilde{T}(t))}{(R_s^+)^2} \left[ -\frac{1}{2} \tilde{w}^2(t, 1) - \| \tilde{w}_r(t, \cdot) \|^2_{L^2(0,1)} \right] + \lambda \| \tilde{w}(t, \cdot) \|^2_{L^2(0,1)}
\]

\[
\leq -2 \left( \frac{D_s^+(\tilde{T}(t))}{4(R_s^+)^2} - \lambda \right) V(t),
\]

(4.73)

where (4.64) is used in the first line, (4.65), (4.66) and integration by parts are applied in the second line, and the Poincaré Inequality [?, Lemma 2.1]

\[
\| \tilde{w}(t, \cdot) \|^2_{L^2(0,1)} \leq 4 \| \tilde{w}_r(t, \cdot) \|^2_{L^2(0,1)}
\]

(4.74)

is employed in the last line. As a result, from (4.68), exponential stability of the \(\tilde{w}\)-system (4.64)–(4.67) is proved.

For notation simplicity we will denote the \(L^2(0,1)\)-norm by \(\| \cdot \|\) in the sequel.
Differentiating the transformation (4.63) with respect to \( t \) gives

\[
\tilde{c}_t(t, r) = \frac{D_s^+ (\tilde{T}(t))}{(R_s^+)^2} \left[ \frac{\partial^2 \tilde{w}}{\partial r^2} (t, r) + p(t, r, r) \tilde{w}_r(t, r) + \left( p_t(t, r, 1) + \frac{1}{2} p(t, r, 1) \right) \tilde{w}(t, 1) \right]
+ \left[ \lambda - \frac{D_s^+ (\tilde{T}(t))}{(R_s^+)^2} - p_t(t, r, r) \right] \tilde{w}(t, r)
- \int_r^1 \left[ p_t(t, r, \iota) + \lambda p(t, r, \iota) + \frac{D_s^+ (\tilde{T}(t))}{(R_s^+)^2} p_{\iota \iota}(t, r, \iota) \right] \tilde{w}(t, \iota) d\iota,
\]

where (4.64), (4.66) and integration by parts have been used in the calculation. Differentiating (4.63) with respect to \( r \) gives

\[
\tilde{c}_r(t, r) = \tilde{w}_r(t, r) + p(t, r, r) \tilde{w}(t, r) - \int_r^1 p_r(t, r, \iota) \tilde{w}(t, \iota) d\iota,
\]

\[
\tilde{c}_{rr}(t, r) = \tilde{w}_{rr}(t, r) + p(t, r, r) \tilde{w}_r(t, r) + \left( \frac{d}{dr} p(t, r, r) + p_r(t, r, r) \right) \tilde{w}(t, r)
- \int_r^1 p_{rr}(t, r, \iota) \tilde{w}(t, \iota) d\iota.
\]

From (4.59)–(4.62), (4.63), (4.65)–(4.67) and (4.75)–(4.77), we derive that the kernel function \( p(t, r, \iota) \) needs to satisfy the following PDE system:

\[
p_t(t, r, \iota) = \frac{D_s^+ (\tilde{T}(t))}{(R_s^+)^2} \left[ (p_{rr}(t, r, \iota) - p_{\iota \iota}(t, r, \iota)) \right] - \lambda p(t, r, \iota),
\]

\[
p(t, 0, \iota) = 0,
\]

\[
p(t, r, r) = \frac{(R_s^+)^2}{2D_s^+ (\tilde{T}(t))} \lambda r,
\]

\[
p(0, r, \iota) = p_0(r, \iota),
\]

for which the domain is \( \mathcal{T} = \{(t, r, \iota); 0 \leq t \leq t_{\text{max}}, 0 \leq \iota \leq r \leq 1\} \). Here, \( p_0(r, \iota) \) denotes
the initial condition for the kernel system and satisfies

\[ \int_r^1 p_0(r,\iota) \tilde{w}(t,\iota) \, d\iota = c_0(r) - \hat{c}_0(r) - \tilde{w}_0(r). \]  

(4.82)

Moreover, the observer gains need to be chosen as

\[ p_1(t, r) = -\frac{D_s^+ (\bar{T}(t))}{(R_s^+)^2} \left( p_1(t, r, 1) + \frac{1}{2} p(t, r, 1) \right), \]  

(4.83)

\[ p_{10}(t) = \frac{3}{2} - \frac{(R_+)^2}{2D_s^+ (\bar{T}(t))} \lambda. \]  

(4.84)

In more detail, first, plugging (4.63), (4.75) and (4.77) into (4.59) gives (4.78), (4.83) and the boundary condition

\[ \frac{d}{dr} p(t, r, r) = \frac{(R_s^+)^2}{2D_s^+ (\bar{T}(t))} \lambda. \]  

(4.85)

Second, plugging (4.60) and (4.65) into (4.63) gives (4.79). Third, (4.80) is derived from (4.85) and (4.79). Then, (4.84) is derived from (4.61), (4.63), (4.66), (4.76) and (4.80). Finally, (4.82) is derived by plugging (4.62) and (4.67) into (4.63).

4.5.1 Well-posedness of the kernel function \( p(r, \iota, t) \)

**Lemma 4.5.2.** The initial data \( p_0(\cdot, \cdot) \) is an analytic function in \( \mathbb{T} = \{(r, \iota); 0 \leq \iota \leq r \leq 1\} \), and the system (4.78)–(4.81) admits an analytic solution \( p(t, \cdot, \cdot) \) in \( \mathcal{T} \).

**Proof.** We first transform the system (4.78)–(4.81) into an equivalent integral equation. Let \( \xi = r + \iota, \eta = r - \iota \) and \( q(t, \xi, \eta) = p(t, r, \iota) \), then we have from (4.78)–(4.81)
that \( q \) satisfies the following PDE:

\[
q_t(t, \xi, \eta) = 4 \frac{D^+_s(\bar{T}(t))}{(R^+_s)^2} q_{\xi\eta}(t, \xi, \eta) - \lambda q(t, \xi, \eta),
\]

(4.86)

\[
q(t, \xi, -\xi) = 0,
\]

(4.87)

\[
q(t, \xi, 0) = \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} \lambda \xi,
\]

(4.88)

with the initial condition

\[
q(0, \xi, \eta) = p \left( 0, \frac{\xi + \eta}{2}, \frac{\xi - \eta}{2} \right).
\]

(4.89)

The equation (4.86) can be rewritten as

\[
q_{\xi\eta}(t, \xi, \eta) = \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} (q_t(t, \xi, \eta) + \lambda q(t, \xi, \eta)).
\]

(4.90)

Integrating (4.90) with respect to \( \eta \) from 0 to \( \eta \) and using boundary condition (4.88), we have

\[
q_{\xi}(t, \xi, \eta) = \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} \lambda + \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} \int_0^\eta (q_t(t, \xi, \beta) + \lambda q(t, \xi, \beta)) d\beta.
\]

(4.91)

Integrating (4.91) with respect to \( \xi \) from \( -\eta \) to \( \xi \) gives the following integro-differential equation (IDE):

\[
q(t, \xi, \eta) = \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} \lambda(\xi + \eta) + \frac{(R^+_s)^2}{4D^+_s(\bar{T}(t))} \times \int_{-\eta}^{\xi} \int_0^{(q_t(t, \alpha, \beta) + \lambda q(t, \alpha, \beta)) d\beta d\alpha,
\]

(4.92)

where (4.87) is used.
Second, we apply the method of successive approximation. Let

\[ C = \frac{(R_s^+)^2}{4D_+^+(\hat{T}(0))e^{E_+^+/\hat{T}(0)}}, \quad f(t) = e^{E_+^+/\hat{T}(t)}, \]  

(4.93)

then from (4.22), we look for a solution of (4.92) in the form of

\[ q(t,\xi,\eta) = \sum_{n=0}^{\infty} q^n(t,\xi,\eta), \]  

(4.94)

where

\[ q^0(t,\xi,\eta) = \lambda C(\xi + \eta)f(t), \]  

(4.95)

and

\[ q^{n+1}(t,\xi,\eta) = Cf(t) \int_{-\eta}^{\xi} \int_{0}^{\eta} \left[ q^n_t(t,\alpha,\beta) + \lambda q^n(t,\alpha,\beta) \right] d\beta d\alpha. \]  

(4.96)

Recall that \( \hat{T}(t) \) is analytic, and since it is physically impossible for the temperature to reach zero Kelvin, i.e., \( \hat{T}(t) \neq 0 \), then it is reasonable to assume that \( \frac{1}{\hat{T}(t)} \) is an analytic function in \( t \in [0, t_{\text{max}}] \), and thus there exists a constant \( C_f \) such that for every nonnegative integer \( k \), the following bound holds:

\[ \left| f^{(k)}(t) \right| = \left| \frac{d^k}{dt^k} f(t) \right| \leq C_f^{k+1} k!. \]  

(4.97)

Since the composition of analytic functions is analytic, then \( q^0(t,\xi,\eta) \) is an analytic function in \( t \in [0, t_{\text{max}}] \) and it can be derived from (4.95) and (4.97) that

\[ |\hat{\partial}_t q^0(t,\xi,\eta)| \leq \lambda C C_f^{i+1} i! (\xi + \eta), \quad \forall i \in \mathbb{N}, \]  

(4.98)
with respect to \((\xi, \eta)\), uniformly for \(t \in [0, t_{\text{max}}]\).

In what follows we are to prove by induction that for any integer \(n \geq 0\) the following estimate holds:

\[
|\partial_t^m q^n(t, \xi, \eta)| \leq \lambda C^{n+1} f^{m+n+1}(C_f + \lambda)^n \frac{(m+2n)! \xi^n \eta^n (\xi + \eta)}{2^n n! n!(n+1)!}.  \tag{4.99}
\]

Assume that (4.99) holds for an integer \(n \geq 0\), then, for any integer \(m \geq 0\), we derive from (4.96) that

\[
\left| \partial_t^m q^{n+1}(t, \xi, \eta) \right| = \left| \partial_t^m \left[ C f(t) \int_{-\eta}^{\xi} \int_{0}^{\eta} [q^n(t, \alpha, \beta) + \lambda q^n(t, \alpha, \beta)] d\beta d\alpha \right] \right|
\]

\[
= C \sum_{i=0}^{m} \left( \binom{m}{i} \partial_t^{m-i} f(t) \int_{-\eta}^{\xi} \int_{0}^{\eta} \left[ \partial_t^{i+1} q^n(t, \alpha, \beta) + \lambda \partial_t^{i} q^n(t, \alpha, \beta) \right] d\beta d\alpha \right).  \tag{4.100}
\]

Through further calculation, we obtain the following estimates

\[
\left| \partial_t^m q^{n+1}(t, \xi, \eta) \right| \leq C \sum_{i=0}^{m} \left\{ \binom{m}{i} C_f^{m+n+2} (m-i)! \lambda C^{m+1} \left[ C_f + \frac{\lambda}{i+2n+1} \right] (C_f + \lambda)^n \right. \\
\times \frac{(i+2n+1)!}{2^n n!} \frac{\xi^{n+1} \eta^{n+1} (\xi + \eta)}{(n+1)! (n+2)!} \left. \right\}
\]

\[
\leq \lambda C^{n+2} f^{m+n+2} (C_f + \lambda)^{n+1} \\
\times \sum_{i=0}^{m} \left[ \binom{m}{i} (m-i)! \frac{(i+2n+1)!}{2^n n!} \frac{\xi^{n+1} \eta^{n+1} (\xi + \eta)}{(n+1)! (n+2)!} \right]
\]

\[
= \lambda C^{n+2} f^{m+n+2} (C_f + \lambda)^{n+1} \frac{(m+2(n+1))! \xi^{n+1} \eta^{n+1} (\xi + \eta)}{2^n n! (n+1)! (n+2)!},  \tag{4.101}
\]
where the following equalities have been used:

\[
\int_{-\eta}^{\xi} \int_{0}^{\eta} \frac{\alpha^n \beta^n (\alpha + \beta)}{n!(n+1)!} d\beta d\alpha = \frac{\xi^{n+1} \eta^{n+1} (\xi + \eta)}{(n+1)! (n+2)!}, \tag{4.102}
\]

\[
\sum_{i=0}^{m} \binom{m}{i} (m-i)! (i+j)! = \frac{(m+j+1)!}{j+1}. \tag{4.103}
\]

By induction, (4.99) holds for any integer \( n \geq 0 \).

**Finally, the existence and of** \( q(t, \xi, \eta) \) **and** \( p(t, r, \iota) \) **can be proved.** Fixing \( m = 0 \) in (4.99) gives

\[
|q^n(t, \xi, \eta)| \leq \lambda C^{n+1} C_f^{n+1} (C_f + \lambda)n^{2n} \frac{\xi^n \eta^n (\xi + \eta)}{2^n n! (n+1)!}. \tag{4.104}
\]

Then we can show that the series \( \sum_{n=0}^{\infty} q^n(t, \xi, \eta) \) converges absolutely and uniformly. Indeed, the following bound holds:

\[
|q(t, \xi, \eta)| \leq \sum_{n=0}^{\infty} |q^n(t, \xi, \eta)|
\leq \sum_{n=0}^{\infty} \lambda C^{n+1} C_f^{n+1} (C_f + \lambda)n^{2n} \frac{\xi^n \eta^n (\xi + \eta)}{2^n n! (n+1)!}
= \lambda C C_f (\xi + \eta) \sum_{n=0}^{\infty} \phi_1(\xi, \eta; n), \tag{4.105}
\]

where

\[
\phi_1(\xi, \eta; n) = [CC_f (C_f + \lambda) \xi \eta]^n \frac{(2n)!}{2^n n! n! (n+1)!}. \tag{4.106}
\]
Since
\[
\lim_{n \to \infty} \frac{\phi_1(\xi,\eta;n+1)}{\phi_1(\xi,\eta;n)} = \lim_{n \to \infty} \left[ CC_f(C_f + \lambda) \xi \eta \right] \frac{(2n+1)}{(n+1)(n+2)} = 0,
\]
(4.107)

then from the ratio criterion, the series \( \sum_{n=0}^{\infty} \phi_1(\xi,\eta;n) \) is convergent. Consequently, the existence and of \( q(t,\xi,\eta) \) and \( p(t,r,\iota) \) is established, which are analytic in \( T \). Moreover, the following bound holds for \( p(t,r,\iota) \)
\[
|p(t,r,\iota)| \leq 2\lambda CC_f r \sum_{n=0}^{\infty} \phi_2(r,\iota;n),
\]
(4.109)

where
\[
\phi_2(r,\iota;n) = \phi_1(\xi,\eta;n).
\]
(4.110)

\[ \Box \]

### 4.5.2 Invertibility of the transformation (4.63)

Indeed, the continuity of the kernel \( p(t,r,\iota) \) in (4.63) guarantees the existence of an inverse transformation. We write the inverse transformation as
\[
\tilde{w}(t,r) = \tilde{c}(t,r) + \int_r^1 \rho(t,r,\sigma) \tilde{c}(t,\sigma) d\sigma,
\]
(4.111)

then we could derive from (4.63) and (4.111) that the kernel \( \rho(t,r,\iota) \) needs to satisfy
\[
\rho(t,r,\iota) = p(t,r,\iota) + \int_r^{c} p(t,r,\sigma) \rho(t,\sigma,\iota) d\sigma.
\]
(4.112)
In order to solve the equation (4.112), a similar (successive approximation) procedure as in Subsection 4.5.1 can be followed, see also, [?; Section 4.4]. A similar well-posedness result for its inverse can also be obtained and this derivation is omitted here.

Note also that the initial condition \( \tilde{w}_0(r) \) for the target \( \tilde{w} \)-system (4.64)–(4.67) is determined by \( \hat{c}_0(r) \) and \( \rho_0(r,\iota) = \rho(0,r,\iota) \). Indeed, from (4.62) and (4.111), \( \tilde{w}_0(r) \) can be calculated as

\[
\tilde{w}_0(r) = c_0(r) - \hat{c}_0(r) + \int_r^1 \rho_0(r,\iota)[c_0(\iota) - \hat{c}_0(\iota)]d\iota.
\] (4.113)

### 4.5.3 Exponential convergence of the observer

Some assumptions and simplifications have been made to ease the analysis. For completeness and clarity we summarize these assumptions and simplifications before stating our main result.

**(A1)** To derive an output inversion function, i.e., to recover \( c_{ss}^+(t) \) from the voltage measurement, we have assumed that \( T(t) \) is a time-varying function independent of concentrations. We have used the notation \( \tilde{T}(t) \) and compute its value from equation (4.38). For this assumption to hold, some underlying simplifications and assumptions have been made:

(i). Parameters \( R_f^\pm(T(t)) \) and \( r_{eff}^\pm(T(t)) \) are approximated by \( \tilde{R}_f^\pm(t) \triangleq R_f^\pm(T_{amb}(t)) \) and \( \tilde{r}_{eff}^\pm(t) \triangleq r_{eff}^\pm(T_{amb}(t)) \).

(ii). Functions \( U^\pm(\cdot,T(t)) \) are assumed to be independent of concentrations, and their dependence on \( T(t) \) has been replaced with dependence on \( T_{amb}(t) \). We have used the notation \( \tilde{U}_1^\pm(t) \triangleq U^\pm(c_{ss}^+(t),T_{amb}(t)) \) and \( \tilde{U}_2^\pm(t) \triangleq U^\pm(c_{ss}^+(t),T_{amb}(t)) \).

**(A2)** To derive an output inversion function, diffusion of lithium in the negative electrode has been simplified. This is done by assuming a polynomial solution profile for the
diffusion dynamics in the negative electrode.

(A3) For observer design, we have used $\tilde{T}(t)$ to replace $T(t)$.

(A4) For observer design, functions $I(t)$, $U^\pm(\cdot, T(t))$, $V(t)$ and $\partial U^\pm/\partial T(\cdot, T(t))$ are assumed to be piecewise analytic.

Now, our main result can be presented. Consider an appropriate time interval $[0, t_{\text{max}}]$ for the assumed regularities in (A4) to hold. With the well-posedness of the kernel function in the transformation (4.63) together with the invertibility of the transformation, the following main theorem holds.

**Theorem 4.5.1.** Let $t \in [0, t_{\text{max}}]$. Under the simplifications and assumptions (A1)–(A4), if

$$\lambda < \frac{1}{4(R^+_{s})^{2}} \min_{t \geq 0} \{D^+_s(\tilde{T}(t))\},$$

then for any initial value $\hat{c}(0, \cdot) \in L^2(0,1)$, the observer error $\tilde{c}$-system (4.59)–(4.62) is exponentially stable at $\tilde{c} \equiv 0$ in the $L^2$ norm, which means the designed observer (4.55)–(4.58) is exponentially convergent to the system (4.51)–(4.54).

*Proof.* It follows directly from (4.73) that

$$\|\tilde{w}(t, \cdot)\| \leq \|\tilde{w}(0, \cdot)\| e^{-\left(\frac{D^+_s(\tilde{T}(t))}{4(R^+_{s})^{2}} - \lambda\right)t}.$$  

(4.115)

From the state transformations (4.63) and (4.111), the equivalence of the states $\tilde{c}(t, r)$ and $\tilde{w}(t, r)$ is established, i.e., there exist positive constants $M_1, M_2$ such that

$$M_1\|\tilde{w}(t, \cdot)\| \leq \|\tilde{c}(t, \cdot)\| \leq M_2\|\tilde{w}(t, \cdot)\|.$$  

(4.116)

Then, the proof is completed with (4.115) and (4.116).
Remark 4.5.1. Theorem 4.5.1 is rigidly proved under the assumption that the averaged internal temperature is independent of the lithium ion concentrations in the electrodes; computed from the linear ODE (4.38). Here, we would like to clarify that these assumptions are posed solely for the theoretical derivations. Indeed, in the next section we are to present some simulation results showing that the original unsimplified equation for the averaged internal temperature (4.25) can be used in the implementation of the estimation algorithm, which depends on lithium ion concentrations in the electrodes, and still achieve convergence of the SoC estimate. Since only estimates of lithium ion concentration are available to compute the internal averaged temperature, we are actually computing an open-loop estimate calculated from (4.25) and use the notation $\hat{T}(t)$, i.e.,

$$
\rho_{avg \cdot CP} \frac{d\hat{T}(t)}{dt} = h_{cell} \left(T_{amb}(t) - \hat{T}(t)\right) + I(t) \frac{R\hat{T}(t)}{\alpha F} \left[ \sinh^{-1} \left( \frac{1}{2i_0 \cdot (t) \cdot a^+L^+} \right) \right]
$$

$$
+ \sinh^{-1} \left( \frac{1}{2i_0 \cdot (t) \cdot a^-L^-} \right) + \left( \frac{R^+_e(\hat{T}(t))}{a^+L^+} + \frac{R^-_e(\hat{T}(t))}{a^-L^-} - R_c \right) I(t)^2
$$

$$
- I(t) \left[ U^+(\hat{c}^+_s(t), \hat{T}(t)) - U^-(\hat{c}^-_s(t), \hat{T}(t)) \right]
$$

$$
+ I(t) \left\{ U^+(\hat{c}^+_s(t), \hat{T}(t)) - U^-(\hat{c}^-_s(t), \hat{T}(t)) \right\}
$$

$$
- \hat{T}(t) \left[ \frac{\partial U^+}{\partial T}(\hat{c}^+_s(t), \hat{T}(t)) - \frac{\partial U^-}{\partial T}(\hat{c}^-_s(t), \hat{T}(t)) \right],
$$

(4.117)

where $i_0^\pm(t)$ are computed from (4.19) with concentration values replaced by their estimates.

In the original state variables and unnormalized coordinates, the observer for
lithium-ion concentration in the positive electrode reads

\[
\dot{\hat{c}}_s^+(t, r_s) = \frac{D_s^+(T(t))}{r_s^2} \frac{\partial}{\partial r_s} \left[ r_s^2 \frac{\partial \hat{c}_s^+(t, r_s)}{\partial r_s} \right] + \bar{p}_1(t, r_s)(c_{ss}^+(t) - \hat{c}_{ss}^+(t)), \tag{4.118}
\]

\[
\frac{\partial \hat{c}_s^+(t, 0)}{\partial t} = 0, \tag{4.119}
\]

\[
\frac{\partial \hat{c}_s^+(t, R_s)}{\partial r} = \frac{I(t)}{D_s^+(T(t))a^+F^+L^+} + \bar{p}_{10}(t)(c_{ss}^+(t) - \hat{c}_{ss}^+(t)), \tag{4.120}
\]

with

\[
\bar{p}_1(t, r_s) = \frac{p_1(t, r_s)}{r_s}, \quad \bar{p}_{10}(t) = \frac{p_{10}(t)}{R_s}. \tag{4.121}
\]

The SoC estimation can then be derived from (4.28) and (4.31), with \(c_s^+(t, r_s)\) replaced by their estimated values \(\hat{c}_s^+(t, r_s)\). Additionally, estimates \(\hat{c}_s^-(t, r_s)\) and \(\hat{c}_{ss}^-(t, r_s)\) on the negative electrode can be computed from (4.47)–(4.48), with the estimates \(\hat{c}_{ss}^+(t, r_s)\) and \(\hat{c}_{ss}^+(t, r_s)\) on the positive electrode obtained from (4.118)-(4.121) and the open-loop estimate \(\hat{T}(t)\) from (4.117).

### 4.6 Simulation Results

The ambient temperature is assumed to be constant; \(T_{\text{amb}} = 298 \, [K] = 24.85 \, [^\circ C]\). Simulations are performed with parameters of a LiCoO\(_2\)-LiC\(_6\) cell. Parameters and OCP functions \(U^\pm\) are borrowed from [42] and the references within. Note that the OCP functions depend on the internal average temperature and here a linear approximation is employed:

\[
U^\pm(c_{ss}^\pm(t), T) + U^\pm(c_{ss}^\pm(t), T_{\text{amb}}) + \frac{\partial U^\pm(c_{ss}^\pm(t), T_{\text{amb}})}{\partial T}(T - T_{\text{amb}}). \tag{4.122}
\]
The magnitude of input current is described in terms of the cell C-rate (per unit area), which is computed from

\[
C - \text{rate} = F \frac{\min \{ \epsilon_s^+ L^+, \epsilon_s^+_\text{max}, \epsilon_s^- L^-, \epsilon_s^-\text{max} \}}{3600 \text{[s]}}.
\] (4.123)

### 4.6.1 Simulation tests

Simulation tests are performed to evaluate the effectiveness of the proposed observer with two different current profiles: a square profile (constant charge, discharge and rest) and a current profile obtained from the Urban Dynamometer Driving Schedule (UDDS). For each current profile two cases of measurements are considered: voltage measurements generated from the SPM-T model and voltage measurements generated from the DFN model serving as true data. To generate voltage measurements, lithium concentration in the negative electrode is initialized at 80% of the maximum value and lithium concentration in the positive electrode is initialized at 50% of the maximum value. For the observer, lithium concentration in the negative electrode is initialized at 50% of the maximum value and the one in the positive electrode is initialized at 67% of the maximum value. The tuning parameter \(\lambda\) in the observer is set as \(-1\) for all tests\(^3\)

**Simulation with square current profile**

Figs. 4.2-4.5 correspond to the first set of simulation tests, which use a square current profile shown in Fig. 4.2. The current consists of repeated cycles of: 36 minutes of 1 C-rate constant discharging followed by 54 minutes of resting, i.e., zero input, then 36

\(^3\)Ideally, the convergence rate of the designed observer can be made arbitrarily high by choosing a small enough \(\lambda\), i.e., a large enough \(|\lambda|\). However, since accurate/direct measurement of boundary concentration is not available and approximations required in output inversion unavoidably introduces error in the (calculated) boundary measurement, there exists a design trade-off between high convergence rate of the observer and effective attenuation of the approximation error/measurement noise. In particular, choosing large values for \(|\lambda|\) makes the system more sensitive to measurement noise and results in larger estimation errors.
minutes of 1 C-rate constant charging ending with 54 minutes of zero input. Only the first 250 minutes of the simulation results are shown in the figures. True and estimated SoC are shown in Fig. 4.3 using (a) SPM-T measurements and (b) DFN measurements. The initial errors in SoC estimation are due to intentionally chosen, incorrect initialization of lithium concentrations. Convergence of output voltage coincides with convergence of SoC, and this is shown in Fig. 4.4. The estimate of internal average temperature is shown in Fig. 4.5 using voltage measurements from the (a) SPM-T model and (b) DFN model; compared against the true average temperature of the respective models. Note that, since the internal average temperature is monitored in an open-loop fashion, one needs to correctly initialize its value. This condition is satisfied at thermal equilibrium, i.e., the internal average temperature of the battery coincides with the ambient temperature.

![Figure 4.2: Current profile.](image)

Simulation with UDDS current profile

Figs. 4.6-4.9 correspond to simulation tests using a current input derived from a set of UDDS data and scaled to a current density profile within the range of ±4 C-rate of the battery. This current profile, shown in Fig. 4.6, is representative of current demands
in automotive applications. SoC estimation is shown in Fig. 4.7 with the initial errors coming from incorrect initialization. As seen in Fig. 4.8, convergence of the output voltage coincides with convergence of the SoC as well. Finally, Fig. 4.9 compares the open-loop estimates of internal average temperature with the true internal average temperature from the (a) SPM-T model and (b) DFN model.

Fig. 4.10 shows (a) the difference in output voltage values between SPM-T model and SPM and (b) the difference in temperature values from SPM-T model and DFN model for constant discharge currents. One can see that the difference in output voltage values from SPM-T model and SPM accentuates at high currents rate (a) while temperature values from SPM-T model and DFN model remain relatively close for currents as high as 4 C-rate (b).
Figure 4.3: True and estimated SoC. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.4: True and estimated voltage. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.5: True and estimated internal average temperature. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.6: UDDS Current profile used as input for the numerical test.
Figure 4.7: True and estimated SoC. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.8: True and estimated voltage. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.9: True and estimated interval average temperature. (a). Observer with SPM-T measurements. (b). Observer with DFN measurements.
Figure 4.10: SPM-T model validation. (a) Output voltage error between SPM and DFN, and between SPM-T and DFN. (b) Internal averaged temperature computed from the DFN model and from the SPM-T model.
4.6.2 Numerical implementations

Numerical implementations of the SPM-T and the DFN models follow the equations presented in Subsection 4.3.2 and Subsection 4.3.1, respectively. A finite volume method is used for the spatial discretization of PDEs in the models, and then the Euler-backward method is used for the temporal discretization of the resulting system of ODEs. The observer is implemented using the same discretization procedure. Note that in the numerical implementation of the observer, lithium concentration in the negative electrode is approximated by the polynomial profile presented in [40], as described briefly in Subsection 4.4.2.

For the numerical implementation of the kernel function $p(t, r, ι)$ and the computation of the observer gain, a trapezoidal approximation of the IDE (4.92) is used to obtain an ODE, which is then discretized in time with the Euler-backward method. As mentioned in Section 4.5, time normalization $t' = D^+(T(t))/(R^+_s)^2 t$ by the temperature-dependent function is not preferable; here the normalization is performed by a constant instead, i.e.,

\[ t' = D^+_s(T_{amb})/(R^+_s)^2 t. \]

4.7 Conclusions and Future Work

This paper discusses the problem of SoC estimation for the lithium-ion batteries based on a thermal-electrochemical model. In this regard, an infinite-dimensional Luenberger observer is proposed. For the transformation between the observer error system and the exponentially stable target system, well-posedness of the time-varying PDE backstepping kernel functions are rigorously proved. Then, exponential stability of the observer error system is established, which proves effectiveness of the designed observer. We consider this result as an additional step in the effort to design estimation (and control) algorithms for lithium-ion batteries from electrochemical models, without relying on the discretization.
of the PDEs in these models.

The observer requires only one design/tuning parameter as compared with the possibly large number of tuning parameters required in estimation methods based on finite dimensional battery models, e.g., EKF. Compared with estimation based on the infinite dimensional SPM alone, it takes into account the temperature dependence of model parameters and catches the battery responses better than SPM, especially at high C-rates. Simultaneously, the internal average temperature can be monitored in an open-loop fashion.

Some simplifications are made in this paper, and their relaxation could be considered as a future research direction. Another possible extension is to retain the concentration dynamics in the negative electrode and design one observer for each electrode [20]. One could also consider multiple active materials in the electrodes [21] or add models for degradations (e.g., capacity fade) to the battery model [43]. Observer design for the battery internal, core and surface [44], or even the distributed [45] temperature is a subject worth investigating as well.

4.8 Acknowledgments

Chapter 4, in part, is a reprint of the material as it appears in: S.-X. Tang, L. Camacho-Solorio, Y. Wang and M. Krstic, “State-of-Charge Estimation from a Thermal-Electrochemical Model of Lithium-Ion Batteries”, Automatica, Vol. 83, pp. 206-219, 2017, co-authored with Shuxia Tang, Yebin Wang and Miroslav Krstic. The dissertation author was one of the primary investigators and co-author of this paper.
Chapter 5

Robustness of Boundary Observers for Radial Diffusion Equations to Parameter Uncertainty

5.1 Abstract

Boundary observers for radial diffusion equations can be derived to achieve exponential convergence of the estimation error system provided that coefficients are known; which can be either constant or possibly spatially and time varying. When the coefficients depend on the state, their values are not longer known and this might prevent the estimation error to converge to zero. Here, we address the state estimation problem for a radial diffusion equation in which the diffusion coefficient depends on the spatial average of the state value; using an observer with a constant diffusion coefficient. The error introduced to the observer, in this particular situation, can be quantified from an input-to-state stability (ISS) analysis. This study is motivated mainly by the problem of state estimation from electrochemical models of lithium-ion batteries, namely the Single Particle Model (SPM).
In this application, the variation in the diffusion coefficient as a function of the spatial average of the states is of several orders of magnitude. We consider this result an additional effort in the broader goal of designing estimation algorithms from electrochemical models of lithium-ion batteries without relying in the discretization of the PDEs in these models.

5.2 Introduction

5.2.1 Motivation

Lithium-ion technology is a common choice among the rechargeable battery family due to several attractive characteristics: high power and energy storage density, lack of memory effect and low self-discharge [26]. It has a wide employment in portable electronics and an increasing interest for electrified transportation [27] and grid energy storage.

The safe and optimal use of lithium-ion batteries relies on accurate estimation of electrochemical states and parameters [28]. The availability of detailed electrochemical models [35] is driving a recent effort to design of model-based estimation algorithms; however, the complexity of these models also pose various challenges. One aspect of the models that adds complexity is the dependence of some parameters on the states. The rate at which lithium ions diffuse through the porous electrodes in the battery is one of such parameters. For example, in [46], it was noted that the diffusion coefficient of an NMC electrode varies almost three orders of magnitude as a function of the state of charge.

5.2.2 Contribution

We derive an observer for a radial diffusion equation in $n$-dimensional balls with boundary measurements. When coefficients are constant and known, the observer provides exponentially convergence with an arbitrary convergence rate. On the other hand, if the diffusion coefficient is a function of the state, in particular of the spatial average of the
state, an error arises in the estimation due to the fact the value of the diffusion coefficient is not longer known. The main contribution of this paper is the derivation of bounds in the estimation error that arises in this particular situation. The derivation of these bounds follow recent results on the input-to-state stability of one-dimensional parabolic equations [47, 48]. The main technical challenge is to verify the results in [47, 48] are also valid for radial diffusion equations in $n$-dimensional balls.

The observer design follows the PDE backstepping method. This method has been used for the stabilization of various unstable PDE systems [22]. In [22], backstepping boundary controllers and observers are designed for some unstable parabolic, hyperbolic PDEs and other types of PDEs. Boundary stabilization and estimation of diffusion-reaction equations in $n$-dimensional balls was introduced in [49, 50]; the extension to spatially varying coefficients was derived for the case $n = 2$ in [51] and for the case $n = 3$ in [52]. Boundary observers have been derived previously for simplified electrochemical models of lithium ion batteries, namely, the Single Particle Model (SPM): state and parameter estimation was studied in [23] and [15], state estimation for cells with multiple active materials in [21], an observer for the SPM with electrolyte dynamics was derived in [20] and one for the SPM with averaged thermal dynamics in [53]. In all of these cases, the diffusion coefficients appearing in the SPM model were assumed to be known and independent of states.

We consider the result presented in this paper as an additional step in the broader effort to design estimation and control algorithms for lithium-ion batteries from electrochemical models without relying on the discretization of the PDEs in these models.

### 5.2.3 Organization

The rest of this paper is organized as follows. The problem statement is presented in Section 10.3. The main result appears in Section 5.4. The single particle model is briefly
described in Section 5.5 and the corresponding observer is derived in 5.6. Final remarks appear in Section 10.6. The proof that conditions and assumptions in [47, 48] are satisfied for radial diffusion equations are included in the Appendix.

5.3 Problem Statement

5.3.1 Diffusion with Average-Value-Dependent Coefficients

Consider the radial diffusion equation

\[ u_t(x,t) = \frac{\epsilon(\pi(t))}{x^{n-1}} \left[x^{n-1}u_x(x,t)\right]_x, \quad (5.1) \]

for \( x \in (0,1), t > 0, n \in \mathbb{N} \), with boundary conditions

\[ u_x(0,t) = 0, \quad (5.2) \]
\[ \epsilon(\pi(t))u_x(1,t) = f(t), \quad (5.3) \]

and initial condition \( u_0(x) \in C^2([0,1]) \) and some \( f(t) \in C^2((0,\infty)) \) given. The diffusion coefficient \( \epsilon : [u_{\text{min}},u_{\text{max}}] \to (0,\infty) \) in (5.1) is an affine function of the spatial average value \( \pi(t) \), defined as

\[ \pi(t) = n \int_0^1 u(x,t)x^{n-1}dx. \quad (5.4) \]

Equation (5.1) with boundary conditions (5.2)-(5.3) describe the radial diffusion of the quantity \( u \) in a \( n \)-dimensional sphere. The boundary value \( y(t) = u(1,t) \) is known and the goal is to find an estimate of \( u(x,t) \) from the boundary measurements \( f(t) \) and \( y(t) \).
5.3.2 Observer Design

The proposed observer is copy of the plant (5.1)-(5.3) with linear output error injection, that is

\[
\hat{u}_t(x,t) = \frac{\epsilon(\bar{u}_\star)}{x^{n-1}} \left[ x^{n-1} \hat{u}_x(x,t) \right] + P(x)\tilde{u}(1,t),
\]  

(5.5)

for \( x \in (0,1), t > 0 \) with boundary conditions

\[
\hat{u}_x(0,t) = 0,
\]

(5.6)

\[
\epsilon(\bar{u}_\star)\hat{u}_x(1,t) = f(t) + Q\tilde{u}(1,t),
\]

(5.7)

initial conditions are \( \hat{u}_0(x) \in C^2([0,1]) \) and a fix value \( \bar{u}_\star \in [u_{\min}, u_{\max}] \) used to compute a constant diffusion coefficient. In (5.5) and (5.7), \( P(x) \) and \( Q \) are in-domain and boundary observer gains, respectively. Since \( \epsilon \) is affine, the difference between the diffusion coefficient in the plant and the diffusion coefficient in the observer is proportional to the error between \( \bar{u}(t) \) and \( \bar{u}_\star \), that is, for some \( \epsilon_1 \in \mathbb{R} \) and \( \delta \bar{u}(t) = \bar{u}(t) - \bar{u}_\star \), it follows that

\[
\epsilon(\bar{u}(t)) - \epsilon(\bar{u}_\star) = \epsilon_1 \delta \bar{u}(t).
\]

(5.8)

The estimation error is defined as \( \tilde{u}(x,t) := \hat{u}(x,t) - u(x,t) \), and the estimation error system is obtained by subtracting (5.5)-(5.7) from (5.1)-(5.3), that is

\[
\tilde{u}_t(r,t) = \frac{\epsilon(\bar{u}_\star)}{x^{n-1}} \left[ x^{n-1} \tilde{u}_x(r,t) \right] - P(x)\tilde{u}(1,t) + \delta \bar{u}(t) \frac{\epsilon_1}{x^{n-1}} \left[ x^{n-1} u_x(r,t) \right],
\]

(5.9)
for $x \in (0,1)$, $t > 0$, with boundary conditions

$$\tilde{u}_x(0,t) = 0,$$

(5.10)

$$\epsilon(x) \tilde{u}_x(1,t) = -\epsilon_1 \delta(x) u_x(1,t) - Q \tilde{u}(1,t),$$

(5.11)

and initial conditions $\tilde{u}_0(x) = u_0(x) - \tilde{u}_0(x), \tilde{u}_0(x) \in C^2([0,1])$. The estimation problem is now the problem of choosing gains $P(x)$ and $Q$ to guarantee some stability properties of the estimation error system. More precisely, we will choose $P(x)$ and $Q$ such that $\|\tilde{u}(x,t)\|_2$ is bounded by a term that is asymptotically proportional to $\epsilon_1$. Thus, when $\epsilon_1 = 0$, this choice of $P(x)$ and $Q$, will imply that $\|\tilde{u}(x,t)\|_2 \to 0$ as $t \to \infty$.

### 5.4 Stability of the Estimation Error System

Before showing the stability properties of the estimation error system in (9.10)-(10.17), a set of constants need to be defined.

**Definition 5.4.1.** The positive scalars $A_2$ and $A_3$ quantify the effect of a discrepancy in the value of the diffusion coefficient on the value of the estimation error. These two quantities are computed from the plant and observer parameters as follows

$$A_2 = T^{-1}B_2,$$

(5.12)

$$A_3 = T^{-1}(B_1D_1 + B_2D_2),$$

(5.13)
with

\begin{align*}
B_1 &= \beta \sqrt{\left(1 + \gamma \right) \int_0^1 \left[ I_v \left( \sqrt{\frac{\lambda}{\epsilon(u_s)}} \right) \right]^2 x \, dx,} \\
B_2 &= \sqrt{(1 + \gamma^{-1}) \sum_{m=1}^{\infty} \frac{1}{\sigma_m^2} \, dx},
\end{align*}

(5.14)

(5.15)

for some \( \lambda > 0 \) and \( \gamma > 0 \). The function \( I_v(\cdot) \) in (5.14) is the modified Bessel function of first kind. The term \( \beta \), in (5.14), is

\[ \beta = \frac{\sqrt{1 + b^2}}{\left| b I_v \left( \sqrt{\frac{\lambda}{\epsilon(u_s)}} \right) - \sqrt{\frac{\lambda}{\epsilon(u_s)}} I_{v+1} \left( \sqrt{\frac{\lambda}{\epsilon(u_s)}} \right) \right|}, \]

(5.16)

for some \( b > 0 \), chosen for (5.16) to be finite. For each \( m \in \mathbb{N} \),

\[ \sigma_m = \epsilon(u_s) \mu_m^2 + \lambda, \]

(5.17)

where \( \mu_m \) are the positive roots of

\[ \mu J_v'(\mu) + [b - v] J_v(\mu) = 0, \]

(5.18)

in ascending order, and \( J_v(\cdot) \) is the Bessel function of first kind with \( v = n/2 - 1 \). The positive scalars \( T^{-1} \) and \( T \) are defined as

\[ T = 1 + \|K(x,s)\|_2, \]

(5.19)

\[ T^{-1} = 1 + \|L(x,s)\|_2. \]

(5.20)

Functions \( K(x,s) \) and \( L(x,s) \) take values on \( \mathbb{R} \) and are defined on the unit square \( S := \)
\{(x,s) : 0 \leq x,s \leq 1\} as follows

\[
K(x,s) = -s \frac{\lambda}{\varepsilon(\overline{\mu}_*)} \frac{I_1[\zeta(x,s)]}{\zeta(x,s)},
\]

(5.21)

\[
L(x,s) = -s \frac{\lambda}{\varepsilon(\overline{\mu}_*)} \frac{J_1[\zeta(x,s)]}{\zeta(x,s)},
\]

(5.22)

with

\[
\zeta(x,s) = \sqrt{\frac{\lambda}{\varepsilon(\overline{\mu}_*)} (s^2 - x^2)}.
\]

(5.23)

Constants \(D_1\) and \(D_2\) are

\[
D_1 = \frac{1}{\varepsilon(\overline{\mu}_*)^2},
\]

(5.24)

\[
D_2 = \frac{1}{\varepsilon(\overline{\mu}_*)} \overline{T^{-1}} \max_{x \in [0,1]} K(x,1).
\]

(5.25)

Finally, a third positive scalar \(A_1\) is defined as

\[
A_1 = \overline{T^{-1}} \cdot \overline{T}.
\]

(5.26)

Now, with \(A_1\), \(A_2\), and \(A_3\) defined, the main result regarding the stability of the estimation error system can be stated.

**Theorem 5.4.1.** Consider the estimation error system in (9.10)-(10.17) with initial conditions \(\overline{u}_0(x) \in C^2([0,1])\), for \(n \leq 4\), and observer gains chosen as

\[
P(x) = \frac{\lambda}{z(x)} \left[ \frac{\lambda}{\varepsilon(\overline{\mu}_*)} \frac{I_2(z(x))}{z(x)} + (2 + b - n)I_1(z(x)) \right],
\]

(5.27)

\[
Q = b + \frac{\lambda}{2 \varepsilon(\overline{\mu}_*)},
\]

(5.28)
for some $\lambda, b > 0$, and $z(x)$ defined as

$$z(x) = \sqrt{\frac{\lambda}{\epsilon(u_\star)}} (1 - x^2). \tag{5.29}$$

Then, it follows that

$$\|\tilde{u}(\cdot, t)\|_2 < A_1 \sqrt{\frac{\exp[-\sigma_1 t]}{2 - \exp[-\sigma_1 t]}} \|\tilde{u}_0(\cdot)\|_2 + A_3 |\epsilon_1| |\tilde{\pi}(t)| \max_{\tau \in [0,t]} |f(\tau)|$$

$$+ A_2 |\epsilon_1| |\tilde{\pi}(t)| \max_{\tau \in [0,t]} |g(\tau)| \tag{5.30}$$

with $\sigma_1, A_1, A_2$ and $A_3$ computed following Definition 5.4.1, and

$$g(t) = \max_{x \in [0,1]} |h(x, t)|, \tag{5.31}$$

$$h(x, t) = \frac{1}{x^{n-1}} \left[ x^{n-1} u_x(x, t) \right]_x, \tag{5.32}$$

provided that $f(t) \in C^2(\mathbb{R}_+)$ and $h(x, t) \in C^4(\mathbb{R}_+ \times [0,1])$.

Proof. The proof of Theorem 6.4.1 is a results of the next two lemmas. First, in Lemma 5.4.1, we derive an invertible transformation $T$ that maps the estimation error system (9.10)-(10.17) to an auxiliary system; the target system. Then, in Lemma 5.4.2, we derive an ISS result for the target system. The ISS result for the target system and the invertibility of the transformation $T$ imply the ISS property (5.30) for the estimation error system. \qed

Remark 5.4.1. The regularity condition $h(x, t) \in C^4(\mathbb{R}_+ \times [0,1])$ is a condition on the solutions of the nonlinear PDE (5.1)-(5.3). Whenever the system (5.1)-(5.3) satisfies this condition, or the additional requirements, is beyond the scope of this paper.

Lemma 5.4.1. There exists a bounded and invertible transformation $T : \mathcal{L}^2([0,1]^2) \rightarrow \mathcal{L}^2([0,1])$.
\( \mathcal{L}^2([0,1]^2) \) of the form

\[
T[v] = v(x,t) - \int_x^1 K(x,s)v(s,t)dx,
\]

with inverse

\[
T^{-1}[v] = v(x,t) + \int_x^1 L(x,s)v(s,t)dx,
\]

and \( K(x,s), L(x,s) \) defined in (5.21) and (9.76), which maps the error system (9.10)-(10.17) to the target system

\[
w_t(x,t) = \epsilon(u^\star) - \lambda w(x,t) + \epsilon_1 \delta \bar{\pi}(t) T^{-1} \left[ \frac{1}{x^{n-1}} [x^{n-1} \frac{\partial}{\partial x} w(x,t)]_x \right] - \epsilon_1 \delta \bar{\pi}(t) T^{-1} [K(x,1)] u_x(1,t),
\]

for \( x \in (0,1), t > 0, \) with boundary conditions

\[
w_x(0,t) = 0,
\]

\[
w_x(1,t) = -bw(1,t) - \frac{\epsilon_1 \delta \bar{\pi}(t)}{\epsilon(\bar{\pi}_*)} u_x(1,t),
\]

and initial conditions \( w_0(x) = T^{-1}[\bar{u}_0(\cdot)]. \)

**Proof.** Lemma 5.4.1 is actually an special case of the results in [49, 50] and the proof follows the same steps. \( \square \)

**Lemma 5.4.2.** Consider \( w(x,t) \) satisfying equation (7.28) with boundary conditions (7.29)-(10.27) and initial conditions \( w_0(x) \in C^2([0,1]). \) Then, \( w(x,t) \) satisfies the following
inequality

\[ \| w(\cdot, t) \|_2 \leq \left[ \frac{\exp[-\sigma_1 t]}{2 - \exp[-\sigma_1 t]} \right] \| w_0(\cdot) \|_2 \]

\[ + |\epsilon_1| \| \delta \bar{u}(t) (B_1 D_1 + B_2 D_2) \| \max_{\tau \in [0, t]} |f(\tau)| \]

\[ + |\epsilon_1| \| \delta \bar{u}(t) B_2 \| \max_{\tau \in [0, t]} |g(\tau)|, \]

(5.38)

for \( t > 0 \), with \( g(t) \) defined in (5.31) and \( \sigma_1, B_1, B_2, D_1, D_2 \) from Definition 5.4.1.

Proof. This lemma is a particular, but singular, case of the ISS results in [47, 48]. This singularity originates from the radial diffusion operator and force us to certify that the ISS results are still valid. There are two items that we need verify. First, we need to check that the singular Sturm–Liouville problem

\[ \epsilon (\pi_x) \frac{d}{dx} \left[ x^{n-1} \frac{d\phi_m(x)}{dx} \right] - \lambda x^{n-1} \phi_m(x) = -\sigma_m x^{n-1} \phi_m(x), \]

(5.39)

for \( x \in (0, 1) \) with boundary conditions

\[ \phi_m'(0) = 0, \]

(5.40)

\[ \phi_m'(1) + b \phi_m(1) = 0, \]

(5.41)

has all the same properties as a regular Sturm–Liouville problem; this is in fact true and the proof is in Lemma 5.4.3. Then, we need to verify the convergence of the series

\[ \sum_{m=1}^{\infty} \frac{1}{\sigma_m} \max_{x \in [0,1]} |\phi_m(x)|, \]

(5.42)

where \( \{\sigma_m, \phi_m(x)\} \) are the eigenvalues and eigenfunctions of (5.43) - (5.45). We show in
Lemma 5.4.4 that the series (5.42) is in fact convergent for $n \leq 4$. 

**Lemma 5.4.3.** The singular Sturm-Liouville problem

$$
e(x) \frac{d}{dx} \left[ x^{n-1} \frac{d\phi_m}{dx}(x) \right] - \lambda x^{n-1} \phi_m(x) = -\sigma_m x^{n-1} \phi_m(x), \quad (5.43)$$

for $x \in (0,1)$ with boundary conditions

$$
\phi'_m(0) = 0, \quad (5.44)
$$

$$
\phi'(1) + b\phi(1) = 0, \quad (5.45)
$$

preserves the same elementary properties as regular Sturm-Liouville problems, namely:

1. eigenvalues $\sigma_m \in \mathbb{R}$ form an infinite, increasing sequence $\sigma_1 < \sigma_2 < \cdots < \sigma_m < \cdots$, with $\sigma_m \to \infty$ as $m \to \infty$,

2. to each eigenvalue $\sigma_m$ corresponds exactly one real valued eigenfunction $\phi_m(x) \in C^2([0,1])$, satisfying (5.43) and boundary conditions (5.44), (5.50). Furthermore, eigenfunctions $\phi_m(x)$ form an orthonormal basis of $L^2((0,1); x^{n-1}dx)$.

**Proof.** The solution to equation (5.43) is of the form

$$
\phi(x) = c_1 \phi_1(x) + c_2 \phi_2(x). \quad (5.46)
$$

Here, functions $\phi_1(x)$ and $\phi_2(x)$ are two independent solutions of (5.43) and a closed-form expression is available

$$
\phi_1(x) = x^{-v} J_v(\mu x), \quad (5.47)
$$

$$
\phi_2(x) = x^{-v} Y_v(\mu x), \quad (5.48)
$$

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where $J_v$ and $Y_v$ are the Bessel functions of first and second kind of order $v$ and

$$
\mu = \left( \frac{\sigma - \lambda}{\epsilon} \right)^{1/2}, \quad v = \frac{n}{2} - 1.
$$

(5.49)

Boundary condition (5.44) is to be replaced with a condition on the regularity of solutions; specifically, we require $\phi(x)$ to be square integrable, i.e.

$$
\int_0^1 \phi(x)^2 \, dx < \infty.
$$

(5.50)

The regularity condition implies that $c_2 = 0$. Boundary condition (5.45) provides a characteristic equation, that is, an equation that defines the eigenvalues of the system

$$
\mu J'_v(\mu) + [b - v] J_v(\mu) = 0, \text{ if } b > 0,
$$

(5.51)

$$
\mu J_{v+1}(\mu) = 0, \text{ if } b = 0.
$$

(5.52)

Note that the left hand side of equation (5.51) is the Dini function [? , p.580], that is, $D_{b,v}(\mu) := \mu J'_v(\mu) + [b - v] J_v(\mu)$. Let $\mu_{b,v,m}$ denote the $m$-th positive zero of $D_{b,v}$, then $\mu_{b,v,m}$ satisfies (5.51) and defines the value of the $m$-th eigenvalue for the singular Sturm-Liouville problem for $b > 0$, that is

$$
\sigma_m = \epsilon (\tau^*) \mu_{b,v,m}^2 + \lambda.
$$

(5.53)

The corresponding $m$-th eigenfunction is

$$
\phi_m(x) = c_{1,m} x^{-v} J_v \left( \mu_{b,v,m} x \right),
$$

(5.54)
and \( c_{1,m} \) is chosen to normalize (5.59), that is

\[
c_{1,m} = \frac{\sqrt{2}}{J_v(\mu_{b,v,m})}.
\] (5.55)

Note that \( c_{1,m} \) is well defined in (5.55), since zeros of the Dini function cannot be zeros of Bessel functions because the (non zero) zeros of \( J_v, J_{v+1} \) never coincide. The \( m \)-th positive zero \( \mu_{v+1,m} \) of \( J_{v+1} \), and zero itself, are solutions of (5.52). Thus for \( b = 0 \) and \( n \leq 2 \) the eigenvalues of the problem are

\[
\sigma_m = \lambda, \text{ for } m = 1
\] (5.56)

\[
\sigma_m = \epsilon \mu_{v+1,m-1}^2 + \lambda, \text{ for } m > 1,
\] (5.57)

and, for \( n > 2 \) the eigenvalues of the problem are

\[
\sigma_m = \epsilon \mu_{v+1,m}^2 + \lambda,
\] (5.58)

The corresponding eigenfunctions are

\[
\phi_m(x) = c_{1,m}x^{-v}J_v(\mu_{v+1,m}x),
\] (5.59)

and \( c_{1,m} \) is chosen to normalize (5.59), that is

\[
c_{1,m} = \frac{\sqrt{2}}{J_v(\mu_{v+1,m})}.
\] (5.60)

The statements in the lemma follow directly from properties of the Bessel functions:

1. For \( b > 0 \) and \( v > -1 \), the positive zeros of \( D_{b,v} \) are real and form an infinite increasing sequence [54, p.580, p.597].\(^1\) Similarly, for \( v > -1 \), the positive zeros of \( J_v \) are real

\(^1\)Although these properties hold for \( v \geq -1 \), the exposition in [54] assumes \( v \geq -1/2 \), yet for our problem
and form an infinite and increasing sequence [54, p. 479]. Thus, from (5.49) and (5.51), (5.52) it follows that the eigenvalues of the singular Sturm-Liouville problem are real, positive and form an infinite and increasing sequence.

2. Let \( \{ \mu_{b,v,m} \} \) and \( \{ \mu_{v+1,m} \} \) be the zeros of \( D_{b,v} \) and \( J_{v+1} \), respectively. The fact that \( \{ c_1 x^{-v} J_v[\mu_{b,v,m} x] \} \) and \( \{ c_1 x^{-v} J_v[\mu_{v+1,m} x] \} \) are orthonormal basis of \( \mathcal{L}^2((0,1); x^{n-1} dx) \) is known [54, Chapter 18], [55, Theorem 3].

\[ \square \]

**Lemma 5.4.4.** Let \( \{ \sigma_m \} \) and \( \{ \phi_m(x) \} \) be the eigenvalues and eigenfunctions of the singular Sturm-Liouville problem in Lemma 5.4.3. Then, it holds that

\[ \sigma_1 > 0, \]

and, in the case \( n \leq 4 \)

\[ \sum_{m=1}^{\infty} \frac{1}{\sigma_m} \max_{x \in [0,1]} |\phi_m(x)| < \infty. \]  

**Proof.** For any \( v > -1/2 \), the \( m \)-th positive zero \( \mu_{\alpha,m} \) of the Bessel function \( J_\alpha \) is lower bounded [56] as follows

\[ \mu_{\alpha,m} > m \pi - \frac{\pi - 1}{2} + \alpha. \]  

Let \( \mu_{b,\alpha,m} \) be the \( m \)-th positive zero of the Dini function \( D_{b,\alpha} \). From the Dixon’s theorem on interlacing zeros of Dini functions [? p.480] it follows that

\[ \mu_{b,\alpha,m} > \mu_{b',\alpha,m-1}. \]  

If we let \( b' = 0 \), zeros \( \mu_{b',\alpha,m-1} \) are actually the positive zeros of \( J_{\alpha+1} \), and zero itself,
therefore

\[ \mu_{b,\alpha,1} > 0, \quad (5.65) \]
\[ \mu_{b,\alpha,m} > \mu_{\alpha+1,m-1}, \text{ for } m > 1 \quad (5.66) \]

In the case \( b = 0 \), equation (5.63) implies

\[ \sigma_m > \lambda, \text{ for } m \in \{1, 2\}, \quad (5.67) \]
\[ \sigma_m > \epsilon (m-2)^2 \pi^2 + \lambda, \text{ for } m > 2. \quad (5.68) \]

In the case \( b > 0 \),

\[ \sigma_m > \lambda, \text{ for } m \in \{1, 2, 3\}, \quad (5.69) \]
\[ \sigma_m > \epsilon (m-3)^2 \pi^2 + \lambda, \text{ for } m > 3. \quad (5.70) \]

Clearly the first inequality in the lemma holds.

We use a known bounds on Bessel functions

\[
\max_{x \in [0,1]} |\phi_m(x)| \leq \frac{\sqrt{2}}{J_v(\mu_{b,v,m})} \mu_{b,v,m}^v
\quad (5.71)
\]

For any \( m > 0 \) we have \( J_v(\mu_{b,v,m}) \neq 0 \), and thus all terms in the series are bounded. This allows us to neglect the first \( M \) terms of the series, for any \( M > 0 \), and concern only about the convergence of the tail. From this observation and from (5.68) and (5.70) it follows that convergence of

\[
\sum_{m=M}^{\infty} \frac{1}{J_v(\mu_{b,v,m+3})} \frac{\mu_{b,v,m+3}^v}{m^2}, \quad (5.72)
\]
implies convergence of the original series (5.62). Let

\[ a_m = \frac{1}{\mu_{b,v,m+3}^v J_v \left( \mu_{b,v,m+3} \right)}, \]

(5.73)

\[ b_m = \frac{\mu_{b,v,m+3}^v}{m^2}, \]

(5.74)

It can be verified that

\[ \inf_{m>0} \left| \mu_{b,v,m+3}^v J_v \left( \mu_{b,v,m+3} \right) \right| > 0, \]

(5.75)

thus, the sequence \( \{ |a_m| \} \) is bounded. From the asymptotic location of zeros of Bessel functions, there is \( M > 0 \) such that for \( m > M \) we have

\[ |b_m| < \frac{(m+3) + (v+1)/2}{m^2} \pi^{v+1/2}. \]

(5.76)

Using a one-sided comparison test, the convergence of the series is guarantee to converge if \( v + 1/2 < 2 \); this is the case if \( n \leq 4 \). Boundedness of \( \{ |a_m| \} \) and convergence of \( \{ |b_m| \} \) implies that the original series converges for \( n \leq 4 \).

Now that the proof of the main result is complete, we can proceed with a brief description on how this results is applied to state estimation for lithium-ion batteries from the SPM.

5.5 The Single Particle Model

A simple electrochemical model accounting for some of the main dynamic phenomena in lithium-ion batteries is the SPM [33]. The model includes a pair of diffusion equations describing the diffusion of lithium ions in the intercalation sites of active materials in the
The diffusion coefficients $D_{s,\pm}$ are functions of the average concentration of lithium ions $\overline{c}_{s,\pm}(t)$. The terms $j_{\pm}(t)$ are molar fluxes of lithium ions, i.e., the rate of lithium entering or exiting the intercalation sites. The parameters $R_{p,\pm}$ are the average, or representative, radii of the particles. We view (5.77) - (5.79) as a dynamic system with states $c_{s,\pm}(r,t)$, input $j_{n,\pm}(t)$ and output $c_{ss,\pm}(t) = c_{s,\pm}(R_{p,\pm},t)$. Molar fluxes are computed as a proportion of the current $I(t)$ (per unit area) applied to the lithium-ion cell

$$j_{-}(t) = \frac{nR_{p,-}}{\epsilon_{s,-}FL_{-}}I(t), \quad j_{+}(t) = -\frac{nR_{p,+}}{\epsilon_{s,+}FL_{+}}I(t).$$

(5.80)

Where $\epsilon_{s,\pm}$ are the volume fractions of active material in the electrode, $L_{\pm}$ are the lengths of the electrodes and $F$ is the Faraday constant. Overpotentials $\eta_{\pm}(t)$ are computed by solving a set of nonlinear algebraic equations (in terms of $j_{\pm}$ and $c_{ss,\pm}(t)$)

$$j_{\pm}(t) = \frac{i_{0,\pm}(t)}{F} \left[ e^{\frac{\alpha_{c}F}{RT} \eta_{\pm}(t)} - e^{-\frac{\alpha_{c}F}{RT} \eta_{\pm}(t)} \right],$$

$$i_{0,\pm}(t) = k_{\pm} \left[ c_{ss,\pm}(t) \right]^{\alpha_{c}} \left[ c_{e} (c_{s,\text{max,}\pm} - c_{ss,\pm}(t)) \right]^{\alpha_{a}},$$

(5.81)

(5.82)

where $k_{\pm}$ are (effective) reaction rates, $c_{e}$ is the concentration of lithium-ions in the electrolyte (assumed to be constant), $T$ is the mean temperature in the cell, and $R$ is the...
gas constant. Electric potentials in the electrodes are computed from

\[ \phi_{s,\pm}(t) = \eta\pm(t) + U_i^{-}(c_{ss,\pm}(t)) + R_{f,\pm}F j\pm(t), \quad (5.83) \]

where \( U_{\pm} \) are open-circuit potentials. Finally, the measured voltage in the cell is the difference between the positive and negative electric potential,

\[ V(t) = \phi_{s,+}(t) - \phi_{s,-}(t). \quad (5.84) \]

Concentrations \( c_s(r,t) \) are positive and bounded by \( c_{s,\text{max,}\pm} \), where the possible values of \( c_{s,\text{max,}\pm} \) depend on the specific active material. The current applied to the cell is bounded to keep the concentration within these bounds. For an experimental determination of the dependence of diffusion on the mean concentration of lithium-ions in the electrodes, for a particular material, one can see the results in [46]. An observer, based on the SPM, can be derived to estimate the concentration of lithium ions in the electrode; and thus, estimating the state of charge.

5.6 Observer for the Single Particle Model

We assume \( c_{ss,\pm}(t) \) can be recover perfectly from measurements of current and voltage. Thus, the problem of estimating \( c_{s,\pm}(r,t) \) from known values of \( j_n(t) \) and \( c_{ss,\pm}(t) \) can be solved using the analysis in the previous sections. We consider an observer in the form

\[ \frac{\partial \hat{c}_{s,\pm}(r,t)}{\partial t} = \frac{D_s \left( c_{s,\pm,\star} \right)}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial \hat{c}_{s,\pm}(r,t)}{\partial r} \right] + P(r) \left[ c_{ss,\pm}(t) - \hat{c}_{ss,\pm}(t) \right], \quad (5.85) \]
for \( r \in (0, R_{p,\pm}), t > 0, n \in \{1, 2, 3\} \), with boundary conditions

\[
\frac{\partial \tilde{c}_{s,\pm}(0, t)}{\partial r} = 0, \quad (5.86)
\]

\[
D_{s,\pm} \left( \tau_{s,\pm,*} \right) \frac{\partial \tilde{c}_{s,\pm}(R_{p,\pm}, t)}{\partial r} = -j_{s,\pm}(t) + Q \left[ c_{ss,\pm}(t) - \tilde{c}_{ss,\pm}(t) \right] . \quad (5.87)
\]

Gains \( P(r) \) and \( Q \) are the ones appearing in Theorem 1; with the parameters of the model and after proper scaling of the domain. With this observer, the estimation error is bounded as follows

\[
\| \tilde{c}_{s,\pm}(\cdot, t) \| < A_{1,\pm} \sqrt{\frac{\exp \left[ -\sigma_1 t \right]}{2 - \exp \left[ -\sigma_1 t \right]} \| \tilde{c}_{s,\pm}(\cdot, 0) \| + \| D_{s,\pm,1} \| | \delta \bar{c}_{s,\pm}(t) | A_{2,\pm} \max_{\tau \in [0,t]} | g(\tau) |}
\]

\[
+ | D_{s,\pm,1} | | \delta \bar{c}_{s,\pm}(t) | A_{3,\pm} \max_{\tau \in [0,t]}}
\]

(5.88)

with

\[
g_{\pm}(t) = \max_{r \in [0,1]} \left| \frac{1}{r^{n-1}} \frac{\partial}{\partial r} \left[ r^{n-1} \frac{\partial c_{s,\pm}}{\partial r}(r, t) \right] \right| \quad (5.89)
\]

and

\[
\delta \bar{c}_{s,\pm}(t) = \bar{c}_{s,\pm}(t) - \bar{c}_{s,\pm,*} . \quad (5.90)
\]

Constants \( A_{1,\pm}, A_{2,\pm} \) and \( A_{3,\pm} \) are the ones in Definition 1, using the with the parameters of this model.

**Remark 5.6.1.** Note that if \( D_{s,\pm} \) is constant, then \( D_{s,\pm,1} = 0 \), thus recovering the convergence properties of the boundary observer for diffusion equations with constant parameters.
5.7 Conclusions

This paper discusses the problem of state estimation for a diffusion equation with a diffusion coefficient depending on the value of the spatial average of the state. The main contribution of this paper is the derivation of bounds in the estimation error that arises in this particular situation. The derivation of these bounds follow recent results on the input-to-state stability of one-dimensional parabolic equations. The main technical challenge is to verify that conditions and assumptions for the ISS results to hold are valid for radial diffusion equations in $n$-dimensional balls.

5.8 Acknowledgment

Chapter 5, in part, is a reprint of the material as it appears in: L. Camacho-Solorio, S. Moura, and M. Krstic, “Robustness of Boundary Observers for Radial Diffusion Equations to Parameter Uncertainty”, American Control Conference (ACC), 2018. The dissertation author was the primary investigator and author of this paper.
Chapter 6

State Estimation for Lithium ion Batteries with Phase Transition Materials

6.1 Abstract

Lithium Iron Phosphate (LiFePO$_4$ or LFP) is a common active material in lithium-ion batteries. It has been observed that this material undergoes phase transitions during the normal charge and discharge operation of the battery. Electrochemical models of lithium-ion batteries can be modified to account for this phenomena at the expense of some added complexity. We explore this problem for the single particle model (SPM) where the underlying dynamic model for diffusion of lithium ions in phase transition materials is a partial differential equation (PDE) with a moving boundary. An observer is derived for the concentration of lithium ions from the SPM via the backstepping method for PDEs in a rigorous way and simulations are provided to illustrate the performance of the observer. Our comments are stated on the gap between the proposed observer and a
complete state-of-charge (SoC) estimation algorithm for lithium-ion batteries with phase transition materials

6.2 Introduction

6.2.1 Motivation

Lithium Iron Phosphate has several attractive features as an active material in lithium-ion batteries such as thermal safety, high energy, and power density [57]. LFP and other common active materials show unique charge-discharge characteristics due to an underlying crystallographic solid-solid phase transition. Electrochemical models for lithium-ion batteries with single phase materials do not allow to capture these unique characteristics and thus a mathematical description of phase transitions needs to be added to these models. Electrochemical models are of interest for the design of accurate estimation algorithms in battery managements systems. Estimation algorithms based on these models provide visibility into operating regimes that induce degradation enabling a larger domain of operation, therefore, increasing the performance of the battery in terms of energy capacity, power capacity, and fast charge rates [1]. Electrochemical model-based estimation is challenging for several reasons. First, measurements of lithium concentrations outside specialized laboratory environments is impractical. Second, the concentration dynamics are governed by partial differential algebraic equations (PDAE). Finally, the only measurable quantities (voltage and current) are related to dynamic states through a nonlinear function.

6.2.2 Relevant Literature

Electrochemical models describe the relevant dynamic phenomena in lithium-ion cells: diffusion, intercalation and electrochemical kinematics. These models predict accurately the internal states of the battery, however, their complexity renders a challenging problem
for estimation algorithms. For this reason, most approaches develop estimation algorithms based on reduced-order models. Among the various reduced-order models, the single particle model (SPM) has been broadly used in the observer design problem, see [58, 15]. The main characteristic of the SPM is the use of a single spherical particle to represent diffusion of lithium ions in the intercalation sites of the porous active materials in the electrodes.

LFP has been extensively used in lithium ion cells due to its thermal stability, cost effectiveness, non-toxic nature, and long cycle life [57]. An electrochemical model for LFP batteries was proposed in [59] based on a core-shell model. The LFP model with phase transition electrode was revisited in [60] based on a more sophisticated core-shell model of diffusion in both phases of LiCoO$_2$ cathode.

The estimation problem for batteries with LFP electrodes has been relatively less studied; a particle filter was derived in [61] and a Sequential Monte Carlo filter was derived in [62]. However, none of the existing estimation algorithms consider the phase transition phenomena in LFP or any other electrode material with this characteristic.

The core-shell model proposed for phase transition electrodes is described by a parabolic PDE with a state-dependent moving boundary. This is the so called Stefan problem, derived originally to model liquid-solid phase transition phenomena [63]. Recently, a control and state estimation technique for the Stefan problem was developed in [64]. There, the authors introduced a backstepping design [65] for this problem and showed the exponential stability of the closed-loop system under some particular (physical) constraints on the moving interface.

### 6.2.3 Outline

This paper is organized as follows. In Section 6.3, the single particle model is introduced for lithium-ion batteries with a phase transition material in the positive electrode. Then, in Section 6.4 an observer is derived for SOC estimation. Simulations are given in
Section 6.5 to evaluate the performance of the observer. Finally, concluding remarks and future work are presented in Section 10.6.

6.3 Electrochemical Model

The electrochemical model for lithium-ion cells with a phase transition material in the positive electrode follows [59]. We restrict the problem to particular initial conditions of the concentration of lithium ions in the particles (i.e. intercalation sites) of the positive electrode and consider only discharge processes. The initial concentration of lithium ions in the particles of the positive electrode follows a core-shell configuration where the core has a constant distribution of lithium ions in a low concentration phase (the $\alpha$ phase), and the shell has a constant distribution of lithium ions in a high concentration phase (the $\beta$ phase). During discharge, the fluxes of lithium ions at the surface of the particles in the positive electrode are positive, thus, increasing the concentration of lithium ions in the shell and moving the boundary between phases is moving to the center, i.e., a shrinking core process as depicted in Figure 6.1.

6.3.1 Single Particle Model

The single particle model is a simple electrochemical model accounting for the several phenomena in lithium-ion cells. The main simplification in this model comes from the assumption that a single diffusion equation in an spherical particle can be used to model the diffusion phenomena of lithium ions in all the intercalation sites of the active material of each electrode. In the SPM, the ionic molar fluxes $j_{n,\pm}(t)$ on both electrodes are proportional the current density $I(t)$ applied to the cell

$$j_{n,\pm}(t) = \mp \frac{I(t)}{a_{n,\pm}F L_{\pm}}, \quad (6.1)$$
where $a_{s,\pm} = 3\epsilon_{s,\pm}/R_{p,\pm}$ is the interfacial area (per unit volume), $\epsilon_{s,\pm}$ is the volume fraction of active material in each electrode, $R_{p,\pm}$ is the averaged radius of the the intercalation sites (particles) in the electrodes, $F$ is the Faraday constant, and $L_{\pm}$ is the thickness of each electrode. The subscripts + and − indicate that the variable corresponds to the positive or negative particle. The concentration dynamics of lithium ions in the negative electrode (single phase) follow the Fick’s law for diffusion

$$
\frac{\partial c_{s,-}}{\partial t}(r,t) = \frac{D_{s,-}}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial c_{s,-}}{\partial r}(r,t) \right],
$$

(6.2)

for $r \in (0, R_{p,-})$, $t > 0$ with boundary conditions

$$
\frac{\partial c_{s,-}}{\partial r}(0,t) = 0, \quad (6.3)
$$

$$
D_{s,-} \frac{\partial c_{s,-}}{\partial r}(R_{p,-},t) = -j_{n,-}(t), \quad (6.4)
$$

and initial condition $c_{0,-} \in L^2(0, R_{p,-})$. Diffusion in the positive particle follows a core-shell model. In the core of the particle, i.e., for $r \in (0, r_p(t))$, lithium ions are in the $\alpha$-phase. The concentration in the core is assumed to be constant and equal to the equilibrium value of the $\alpha$-phase, i.e., $c_{s,+}(r) = c_{s,\alpha}$. In the shell of the particle, i.e. for $r \in (r_p(t), R_{p,+})$, the concentration of lithium ions is in $\beta$-phase. The concentration dynamics of lithium-ions in the shell of the positive particle follows the Fick’s law for diffusion

$$
\frac{\partial c_{s,+}}{\partial t}(r,t) = \frac{D_{s,+}}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial c_{s,+}}{\partial r}(r,t) \right],
$$

(6.5)

for $r \in (r_p(t), R_{p,+})$ with boundary conditions

$$
c_{s,+}(r_p(t), t) = c_{s,\beta},
$$

(6.6)

$$
D_{s,+} \frac{\partial c_{s,+}}{\partial r}(R_{p,+},t) = -j_{n,+}(t),
$$

(6.7)
and initial conditions $c_{0,+} \in L^2(r_p(0), R_{p,+})$. The time-evolution of the moving interface $r_p(t)$ is not given explicitly. Instead, mass balance at the moving interface yields the following state-dependent dynamics:

$$
(c_{s,\beta} - c_{s,\alpha}) \frac{dr_p(t)}{dt} = -D_{s,+} \frac{\partial c_{s,+}}{\partial r}(r_p(t), t).
$$

(6.8)

Overpotentials $\eta_{\pm}(t)$ are found by solving the nonlinear algebraic equation

$$
\begin{align*}
    j_{n,\pm}(t) &= \frac{i_{0,\pm}(t)}{F} \left[ e^{\frac{\alpha_c F \eta_{\pm}(t)}{R_T}} - e^{-\frac{\alpha_c F \eta_{\pm}(t)}{R_T}} \right], \\
    i_{0,\pm}(t) &= Fk_{\pm} [c_{ss,\pm}(t)]^\alpha \left[ c_{e,0} \left( c_{s,max,\pm} - c_{ss,\pm}(t) \right) \right]^\alpha_a,
\end{align*}
$$

(6.9) \hspace{1cm} (6.10)

where $c_{ss,\pm}(t) := c_{s,\pm}(R_{p,\pm}, t)$. The electric potential in each electrode is given by

$$
\phi_{s,\pm}(t) = \eta_{\pm}(t) + U_{\pm}(c_{ss,\pm}(t)) + R_{t,\pm} F j_{n,\pm}(t).
$$

(6.11)

Finally, output voltage is computed as the difference between the electric potential in each electrode

$$
V(t) = \phi_{s,+}(t) - \phi_{s,-}(t).
$$

(6.12)

Equations (6.5) -(6.12) form a complete description of the single particle model with a phase transition electrode, and it provides the following property on the moving interface during the discharge process.

**Remark 6.3.1.** During the single discharge process, the current density $I(t)$ maintains positive, i.e. $I(t) > 0$ for $\forall t > 0$. This current positivity ensures the moving interface being shrinking as shown in [63]. Furthermore, the initial interface position is less than the cell
Figure 6.1: Phase transition in the positive particle during discharge. The particle starts with a large core of low concentration phase $\alpha$ and a small shell of high concentration phase $\beta$. During discharge there is a positive flux of lithium ion in the surface of the positive particle, increasing the concentration and increasing the size of the $\beta$-phase shell.

radius. Hence,

$$\frac{dr_p(t)}{dt} < 0,$$

(6.13)

$$0 \leq r_p(t) < R_{p,+},$$

(6.14)

6.3.2 Mass Conservation

In this model, the total amount lithium ions is conserved. The mathematical description of this property is given in the following lemma.

Lemma 6.3.1. The total amount of lithium $n_{Li}$ in solid phase ( moles per unit area ) defined as

$$n_{Li}(t) = \epsilon_{s,-} L_- \bar{c}_{s,-}(t) + \epsilon_{s,+} L_+ \bar{c}_{s,+}(t),$$

(6.15)

where $\bar{c}_{s,-}(t)$ and $\bar{c}_{s,+}(t)$ are the volumetric averages of the concentrations

$$\bar{c}_{s,-}(t) = \frac{3}{R_{p,-}^3} \int_0^{R_{p,-}} c_{s,-}(r,t)r^2 dr,$$

(6.16)

$$\bar{c}_{s,+}(t) = \frac{3}{R_{p,+}^3} \int_0^{R_{p,+}} c_{s,+}(r,t)r^2 dr,$$

(6.17)
is conserved, namely \( \frac{dn_{\text{Li}}(t)}{dt} = 0 \).

Lemma 6.3.1 was derived in [24] for electrodes with a single phase, and we can show that this result extends to electrodes with phase transition materials.

**Proof.** In our problem formulation there is a single phase in the negative particle and there are two phases in the positive particle, i.e., \( \alpha \)-phase in the core and \( \beta \)-phase in the shell. The concentration in \( \alpha \)-phase at the core is assumed to be constant (at its equilibrium value \( c_{s,\alpha} \)). Under these assumptions, the time derivative of (6.15) is given by

\[
\frac{dn_{\text{Li}}(t)}{dt} = -a_{s,-}L_{-}j_{n,-}(t) - a_{s,+}L_{+}j_{n,+}(t) - \frac{3e_{s,+}L_{+}}{R_{p,+}^{3}} r_{p}^{2}(t)
\times \left[ \frac{dr_{p}(t)}{dt} \left[ c_{s,\beta} - c_{s,\alpha} \right] + D_{s,+} \frac{\partial c_{s,+}}{\partial r} \left( r_{p}(t), t \right) \right].
\]  

(6.18)

Hence, the molar flux equations in (6.1) and the dynamics of the moving interface in (6.8) lead to \( \frac{dn_{\text{Li}}(t)}{dt} = 0 \). In a more general formulation introduced in [66], i.e. when both electrodes have multiple phase transitions not necessarily at the equilibrium, mass conservation of lithium ions is guaranteed with the following interface dynamics

\[
\frac{dr_{i}^{[a,b]}(t)}{dt} = \frac{1}{c_{b} - c_{a}} \left[ D_{a} \frac{\partial c}{\partial r}(r_{i}^{[a,b]}(t) -, t) - D_{b} \frac{\partial c}{\partial r}(r_{i}^{[a,b]}(t) +, t) \right],
\]

(6.19)

where \( r_{i}^{[a,b]} \) is the interface radius between any two phases (phase a and phase b) in any electrode. Each phase has a distinct equilibrium \( c_{a}, c_{b} \) and diffusion coefficient \( D_{a}, D_{b} \). □

### 6.4 State Estimation

Now, an state estimation algorithm for concentration of lithium ions, in both negative and positive electrodes, is provided this section from the single particle model. The state observer for the positive electrode is derived via the backstepping method for
moving boundary PDEs, and the observer for the negative electrode is derived from the mass conservation property.

### 6.4.1 Observer for Phase Transition Positive Electrode

The state observer is a copy of the diffusion system (6.5)-(6.7) in the positive electrode together with output error injection

\[
\frac{\partial \hat{c}_{s,+}(r,t)}{\partial t} = \frac{D_{s,+}}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial \hat{c}_{s,+}(r,t)}{\partial r} \right] + P(r_p(t),r) [c_{ss,+}(t) - \hat{c}_{s,+}(R_{p,+},t)],
\]

for \( r \in (r_p(+t), R_{p,+}) \) with boundary conditions

\[
\hat{c}_{s,+}(r_p(t),t) = c_\beta, \quad D_{s,+} \frac{\partial \hat{c}_{s,+}}{\partial r}(R_{p,+},t) = -j_{n,+}(t) + Q(r_p(t)) [c_{ss,+}(t) - \hat{c}_{s,+}(R_{p,+},t)],
\]

and initial conditions \( \hat{c}_{0,+} \in \mathcal{L}^2(r_p(0), R_{p,+}) \). Observer gains are given by

\[
P(r_p(t),r) = D_{s,+} \frac{r^2 R_{p,+} l(t) s(t)}{2} \frac{I_2(z(t))}{z(t)},
\]

\[
Q(r_p(t)) = \frac{D_{s,+}}{R_{p,+}} \left( \frac{\bar{\lambda}}{2} s(t) + 1 \right),
\]

where \( I_2(\cdot) \) is a modified Bessel function of the second kind and

\[
\bar{\lambda} = \frac{\lambda}{D_{s,+}},
\]

\[
s(t) = R_{p,+} - r_p(t), \quad l(t) = r - r_p(t),
\]

\[
z(t) = \sqrt{\bar{\lambda} [s(t)^2 - l(t)^2]}.
\]
The parameter $\lambda > 0$ is designed to achieve faster convergence of the estimated concentration to true concentration.

### 6.4.2 Stability Analysis of the Estimation Error System

Let $\widetilde{c}_{s,+}(r,t)$ be an estimation error defined by $\widetilde{c}_{s,+}(r,t) := c_{s,+}(r,t) - \overline{c}_{s,+}(r,t)$.

Subtracting (6.20)-(6.22) from (6.5)-(6.7) yields the estimation error dynamics

$$\frac{\partial \widetilde{c}_{s,+}(r,t)}{\partial t} = \frac{D_{s,+}}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial \widetilde{c}_{s,+}(r,t)}{\partial r} \right] - P(r_p(t),r)\overline{c}_{s,+}(R_{p,+},t), \quad (6.28)$$

$$\widetilde{c}_{s,+}(r_p(t),t) = 0, \quad (6.29)$$

$$D_{s,+} \frac{\partial \widetilde{c}_{s,+}}{\partial r}(R_{p,+},t) = -Q(r_p(t))\overline{c}_{s,+}(R_{p,+},t). \quad (6.30)$$

The main result of this paper is presented in the following theorem.

**Theorem 6.4.1.** Consider the estimation error dynamics (6.28)-(6.30) with the observer gains (6.23) and (6.24) under the properties of (6.13) and (6.14). Then, for any initial estimation error $\widetilde{c}_{s,+}(r,0)$, the estimation error is exponentially stable at the origin in the sense of the norm

$$\int_{r_p(t)}^{R_{p,+}} r^2 \overline{c}_{s,+}(r,t)^2 dr. \quad (6.31)$$

The proof of Theorem 6.4.1 is established through the remainder of Section 9.4.
Change of coordinate

First, we introduce the following change of coordinate and state variable to simplify the structure of the estimation error dynamics in a cartesian coordinate:

\[ x = R_{p,+} - r, \]
\[ \tilde{u}(x,t) = r c_{s,+}(r,t). \]  

The estimation error dynamics (6.28)-(6.30) is rewritten by the new coordinate and state as

\[ \frac{\partial \tilde{u}}{\partial t}(x,t) = D_{s,+} + \frac{\partial^2 \tilde{u}}{\partial x^2}(x,t) - \bar{P}(s(t),x)\tilde{u}(0,t), \]
\[ \tilde{u}(s(t),t) = 0, \]
\[ \frac{\partial \tilde{u}}{\partial x}(0,t) = -\bar{Q}(s(t))\tilde{u}(0,t), \]  

where

\[ \bar{P}(s(t),x) = \frac{r}{R_{p,+}} P(r_{p}(t),r), \]
\[ \bar{Q}(s(t)) = \frac{1}{R_{p,+}} - \frac{1}{D_{s,+}} Q(r_{p}(t)). \]  

Backstepping transformation

Consider the following invertible transformation from the estimation error \( \tilde{u}(x,t) \) to the transformed state \( \bar{w}(x,t) \):

\[ \bar{w}(x,t) = \tilde{u}(x,t) + \int_0^x q(x,y)\tilde{u}(y,t)dy, \]
\[ \tilde{u}(x,t) = \bar{w}(x,t) + \int_0^x p(x,y)\bar{w}(y,t)dy, \]  

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where $\overline{x} = s(t) - x$, $\overline{y} = s(t) - y$, and the gain kernel solutions are

$$p(\overline{x}, \overline{y}) = \frac{\lambda I_1\left(\sqrt{\frac{\lambda}{\overline{y}^2 - \overline{x}^2}}\right)}{\sqrt{\lambda \overline{y}^2 - \overline{x}^2}},$$

(6.41)

$$q(\overline{x}, \overline{y}) = -\frac{\lambda J_1\left(\sqrt{\frac{\lambda}{\overline{y}^2 - \overline{x}^2}}\right)}{\sqrt{\lambda \overline{y}^2 - \overline{x}^2}},$$

(6.42)

with a modified Bessel function $I_1(\cdot)$ and a Bessel function $J_1(\cdot)$ of the first kind, respectively. Taking time and spacial derivatives of (6.39) and (6.40), the following target $\tilde{w}$-system is obtained:

$$\frac{\partial \tilde{w}}{\partial t}(x,t) = D_s + \frac{\partial^2 \tilde{w}}{\partial x^2}(x,t) - \lambda \tilde{w}(x,t) + \dot{s}(t) \int_0^x q'(\overline{x}, \overline{y}) \left( \tilde{w}(y,t) + \int_0^y p(\overline{y}, \overline{z}) \tilde{w}(z,t) \, dz \right) \, dy,$$

(6.43)

$$\tilde{w}(s(t), t) = 0,$$

(6.44)

$$\frac{\partial \tilde{w}}{\partial x}(0, t) = 0,$$

(6.45)

where $q'(\overline{x}, \overline{y}) = \frac{\partial q}{\partial \overline{x}}(\overline{x}, \overline{y}) + \frac{\partial q}{\partial \overline{y}}(\overline{x}, \overline{y})$. In other words, the observer gains (6.23) and (6.24) are derived to match the target system (6.43)-(6.45).

**Stability Proof**

To show the exponential stability of (6.43)-(6.45), we consider the time evolution of the following Lyapunov function:

$$W(t) = \frac{1}{2} \int_0^s \tilde{w}(x,t)^2 \, dx.$$  

(6.46)
Taking the time derivative of (6.46) along with (6.43)-(6.45) yields
\[
\dot{W}(t) = -D_{s,+} \int_0^{s(t)} \left( \frac{\partial \tilde{w}}{\partial x} (x,t) \right)^2 dx - \lambda \int_0^{s(t)} \tilde{w}(x,t)^2 dx + \dot{s}(t) \int_0^{s(t)} \tilde{w}(x,t) \left[ \int_0^x q'(x,y) \right. \\
\left. \left( \tilde{w}(y,t) + \int_0^y P(y,z) \tilde{w}(z,t) dz \right) dy \right] dx.
\] (6.47)

The properties on the interface (6.13) and (6.14) leads to \( \dot{s}(t) > 0 \) and \( 0 < s(t) < R_{p,+} \).

With the help of these inequalities and applying Young’s and Cauchy Schwartz inequality, one can show that there exists a constant \( a > 0 \) such that the following inequality holds:
\[
\dot{W}(t) \leq -bW(t) + a\dot{s}(t)W(t),
\] (6.48)

where \( b = \frac{D_{s,+}}{4R_{p,+}^2} + \lambda \). The technique proposed in [64] with \( \dot{s}(t) > 0 \) and \( 0 < s(t) < R_{p,+} \) yields the exponential decay of \( W(t) \) as
\[
W(t) \leq e^{aR_{p,+}W(0)}e^{-bt}.
\] (6.49)

Since the transformation is invertible as seen in (6.39) and (6.40), \( \tilde{w} \)-system and \( \tilde{u} \)-system have the same stability property. In a similar manner, taking back to the original spherical coordinate with the \( \tilde{c}_{s,+}(r,t) \) given by (6.32) and (6.33) concludes Theorem 6.4.1.

### 6.4.3 Observer for Negative Electrode

The observer design for negative electrode presented in this section imposes the following assumption on the known variables through measurements.

**Assumption 6.4.1.** The position and velocity of the interface \( r_p(t), \dot{r}_p(t) \) along with the surface concentration in the positive electrode \( c_{ss}(t) \) are known for any \( t \geq 0 \).

The observer design for lithium ion concentration in the negative electrode is
constructed by the copy of the dynamics (6.2)-(6.4) together with the output injection of
the positive electrode plus an additional term
\[
\frac{\partial \tilde{c}_{s,-}}{\partial t}(r,t) = \frac{D_{s,-}}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial \tilde{c}_{s,-}}{\partial r}(r,t) \right] + P_-(r_p(t))\tilde{c}_{s,+}(R_{p,+},t) + F(r_p(t),\dot{r}_p(t)), \quad (6.50)
\]
for \( r \in (0,R_{p,-}), \ t > 0 \) with boundary conditions
\[
\frac{\partial \tilde{c}_{s,-}}{\partial r}(0,t) = 0, \quad (6.51)
\]
\[
D_{s,-} \frac{\partial \tilde{c}_{s,-}}{\partial r}(R_{p,-},t) = -j_{n,-}(t) + Q_-(r_p(t))\tilde{c}_{s,+}(R_{p,+},t). \quad (6.52)
\]

Observer gains in the negative electrode are computed to conserve the total amount of
lithium ions in solid phase (6.15),
\[
Q_-(r_p(t)) = -\frac{a_{s,+}L_+}{a_{s,-}L_-}Q(r_p(t)), \quad (6.53)
\]
\[
P_-(r_p(t)) = -\frac{\epsilon_{s,+}L_+}{\epsilon_{s,-}L_-} \frac{3}{R_{p,+}^3} \int_{r_p(t)}^{R_{p,+}} P(r_p(t))r^2 dr \right], \quad (6.54)
\]
and the additional term is designed as
\[
F(r_p,\dot{r}_p(t)) = -\frac{\epsilon_{s,+}L_+}{\epsilon_{s,-}L_-} \frac{3r_p^2(t)}{R_{p,+}^3} \left( \dot{r}_p(t) \left[ c_{s,\alpha} - c_{s,\beta} \right] - D_{s,+} \frac{\partial \tilde{c}_{s,+}}{\partial r}(r_p(t),t) \right). \quad (6.55)
\]

Then, one can show that the total amount of the lithium ions in the state observer is
preserved by the same procedure as Section 6.3.2. Hence, the observer error in the negative
electrode approaches to zero uniformly in space with the help of Theorem 6.4.1.
Algorithm 1: Time Update for Increasing Domain (Shrinking Core)

Given some spatial grid \( r = [r_1, r_2, \ldots, r_N] \) and state \( c_s = [c_{s,1}, c_{s,2}, \ldots, c_{s,N}] \) at time \( t_n \):

1. Compute new position for the boundary: \( r_p(t_{n+1}) \)
2. Add this value as a new point to the grid:
   \[ r \leftarrow [r_p(t_{n+1}), r_1, r_2, \ldots, r_N] \]
3. Add a new entry to the state concentration with the value \( c_\beta \):
   \[ c_s \leftarrow [c_\beta, c_{s,1}, c_{s,2}, \ldots, c_{s,N}] \]
4. Define a new grid \( r' = [r'_1, r'_2, \ldots, r'_N] \) such that:
   \[ r'_1 = r_p(t_{n+1}) \text{ and } r'_N = r_N \]
5. Interpolate (linearly) the concentration state to the new grid
6. Compute average concentrations \( \overline{c_s} \) and \( \overline{c} \)
7. Correct for mass conservation with the scaling factor \( \overline{c_s}/\overline{c'_s} \):
   \[ c'_s \leftarrow \frac{\overline{c_s}}{\overline{c'_s}} c'_s \]

6.5 Simulation

Spatial discretization of diffusion dynamics in both electrodes follows a finite volume method over a non-uniform grid, i.e. finer discretization near the endpoints, see for example [67]. The discretization of the boundary dynamics follows a discrete version of (6.8) which is derived properly to guarantee mass conservation. This is done by adding a new point in the discretization grid at every time step according to the dynamics of the moving boundary. To this new point in the grid we associate a new state equal to \( c_\beta \). Then, to avoid an increase of the number of states at every time step, an interpolation is performed from the grid with the additional point to a new grid defined in the larger domain but with the same number of points chosen at the beginning of the simulation. The interpolation is a simple linear interpolation corrected for mass conservation.

6.5.1 Observer Initialization

Observer initialization is the problem of choosing initial concentration estimates in the negative and positive particles for a given initial output voltage estimate \( \tilde{V}(0) \) while
Figure 6.2: Voltage plot for different (constant) current discharge inputs.

Figure 6.3: Normalized concentration of lithium ions in a growing $\beta$-phase region. The plot corresponds to a 5[min] simulation of constant 5[C – rate] discharge. The plot does not show the $\alpha$-phase portion of the concentration since it is assumed to be constant.
satisfying the requirement $\hat{n}_{\text{Li}} = n_{\text{Li}}$. For this purpose, we use the error function defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp[-\xi^2]d\xi. \quad (6.56)$$

In the positive particle, the initial concentration profile is chosen to be smooth transition (smooth approximation of a step function) from $c_\beta$ at $r_{p,0}$ to some value $\hat{c}_{ss}(0)$ at $r = R_{p,+}$, that is

$$\hat{c}_{s,0,+}(r) = c_\beta + A_1 c_{s,\text{max}} \left[ \text{erf}(A_2) + \text{erf} \left( [A_3 + A_2] \frac{r - r_{p,0}}{R_p - r_{p,0}} - A_2 \right) \right] \quad (6.57)$$

where $A_2$, and $A_3$ are positive parameters. The values of $A_2$ and $A_3$ affect the steepness and the position of the transition while $A_1$ affects the amplitude of such transition. Larger values of $A_2$ make the transition steeper and the position of the transition $r_t \in (r_{p,0}, R_{p,+})$ depends on the ratio between $A_2$ and $A_2 + A_3$

$$\frac{A_2}{A_2 + A_3} = \frac{r_t - r_{p,0}}{R_p - r_{p,0}}. \quad (6.58)$$

Note that for large values of $A_2$ and $A_3$, the value of $A_1$ can be found directly from the initial estimate of surface concentration in the positive particle

$$A_1 \simeq \frac{\hat{c}_{ss} - c_{s,\beta}}{c_{s,\text{max}}}. \quad (6.59)$$

For fixed values of $A_2$ and $A_3$ and restricting the initial estimate of concentration in the negative particle to uniform profiles $\hat{c}_{s,0,-} \in (0, c_{s,\text{max}}^{-})$, the observer initialization problem
reduces to solving a pair of algebraic equations

\[ 0 = -n_{\text{Li,s}} + \epsilon_{s,-}L_{-}c_{s,0,-} + \epsilon_{s,+}L_{+}\left[c_{s,a}\left(\frac{r_{p,0}}{R_{p,+}}\right)^3 + \frac{3}{R_{p,+}} \int_{r_{p,0}}^{R_{p,+}} c_{s,0,+}(r)r^2 dr\right], \quad (6.60) \]

\[ 0 = -\tilde{V}(0) + U_{+}(\hat{c}_{s,+}(0)) - U_{-}(\hat{c}_{s,0,-}). \quad (6.61) \]

for the values of \( A_1 \) and \( \hat{c}_{s,0,-} \).

6.5.2 Observer for Constant Discharge

To test the observer we run a numerical example with a constant discharge current of 5 [C-rate]. We are assuming \( c_{s,+} \) is available directly from measurements to be used as output error injection in the observer. In practice, this quantity could be estimated from measurements. Figure 6.4 shows the estimated concentration of lithium ions in \( \beta \)-phase in the positive particle; one can compare this to the true concentration in Figure 6.3. Figure 6.5 shows the averaged concentration in the positive particle, both true value (black) and estimated (blue). Convergence of the estimate to the true value is clear from the plot and in a relative short time. Note that SoC is directly proportional to the averaged concentrations; then the importance to evaluate the estimation of this quantity.

6.6 Conclusions and Future Works

The observer derived in this paper is a first step in a complete SoC estimation algorithm for lithium ion batteries with phase transition materials and is an effort to extend the existing SoC estimation algorithms from SPM to complex electrode settings, as was already achieved for electrodes with multiple active material [21]. It was noted in [59] that two different particles sizes are needed to correctly model LFP electrodes, this correction can be added to our results following [21]. There are several assumptions throughout the
**Figure 6.4:** Estimate of the concentration of lithium ions in the positive particle.

**Figure 6.5:** Averaged concentration of true value (black solid) and estimate (blue dashed) in the positive particle normalized by the maximum concentration. Convergence of the estimate to the true value is observed in a short time scale.
Table 6.1: Phase Transition Model. Parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Negative</th>
<th>Separator</th>
<th>Positive</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$ [m]</td>
<td>$50 \times 10^{-6}$</td>
<td>$25 \times 10^{-6}$</td>
<td>$74 \times 10^{-6}$</td>
</tr>
<tr>
<td>$c_{s,\text{max}}$ [mol/m$^3$]</td>
<td>27760</td>
<td></td>
<td>20950</td>
</tr>
<tr>
<td>$c_{s,\alpha}$ [mol/m$^3$]</td>
<td>$0.0480 \times c_{s,\text{max}}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c_{s,\beta}$ [mol/m$^3$]</td>
<td>$0.8920 \times c_{s,\text{max}}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$R_p$ [m]</td>
<td>$11 \times 10^{-6}$</td>
<td></td>
<td>$52 \times 10^{-6}$</td>
</tr>
<tr>
<td>$D_s$ [m$^2$/s]</td>
<td>$9 \times 10^{-14}$</td>
<td></td>
<td>$8 \times 10^{-18}$</td>
</tr>
<tr>
<td>$\epsilon_s$ [-]</td>
<td>0.33</td>
<td></td>
<td>0.27</td>
</tr>
<tr>
<td>$R_f$ [Ωm$^2$]</td>
<td>$1 \times 10^{-5}$</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>$R_c$ [Ωm$^2$]</td>
<td>0</td>
<td></td>
<td>$6.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>$k$ [m$^{2.5}$/mol$^{0.5}$/s]</td>
<td>$3 \times 10^{-5}$</td>
<td>$3 \times 10^{-17}$</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.2: Phase Transition Model. Physical Constants

<table>
<thead>
<tr>
<th>Other Parameters and Physical Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ [m]</td>
</tr>
<tr>
<td>$F$ [As/mol]</td>
</tr>
<tr>
<td>$R$ [J/Kmol]</td>
</tr>
<tr>
<td>$T$ [K]</td>
</tr>
<tr>
<td>$c_e$ [mol/m$^3$]</td>
</tr>
<tr>
<td>$\alpha_a, \alpha_c$ [-]</td>
</tr>
</tbody>
</table>

$a$ borrowed from [68]  
$b$ assumed

derivation of the observer that make the direct implementation of this algorithms impossible in a SoC estimation scheme. One of the main assumptions is the restriction to only two coexisting phases in a single particle reduced further to a single phase problem by assuming a constant core phase together with the complete knowledge on the position of the phase interface at all times. Another one is the interface position and velocities between the two phases to be known. The relaxation of these assumptions will be addressed in our future work.


6.7 Acknowledgment

Chapter 6, in part, is a reprint of the material as it appears in: S. Koga, L. Camacho-Solorio, M. Krstic, “State Estimation for Lithium-Ion Batteries with Phase Transition Materials”, ASME Dynamic Systems and Control Conference (DSCC), 2017. The dissertation author was one of the primary investigators and co-author of this paper.
Chapter 7

Boundary Observer Design for
Coupled Reaction-Diffusion Systems
with Spatially-Varying Reaction

7.1 Abstract

Following a recent solution to the problem of boundary stabilization of linear coupled reaction-diffusion systems by means of the backstepping method, we present an observer for a coupled pair of reaction-diffusion partial differential equations (PDEs) with boundary measurements. We show that, as in the case of stabilization, the backstepping kernel PDEs are essentially equivalent to the PDEs governing the kernels for stabilization of first-order hyperbolic coupled PDEs. A numerical example is provided for the computation of the kernels. The problem we solve is motivated by diffusion phenomena in lithium-ion batteries with electrodes that comprise multiple active materials. The particular choice of boundary conditions also comes from this application.
7.2 Introduction

Recently, the problem of boundary stabilization for general linear coupled reaction-diffusion systems with \textit{spatially-varying} reaction was solved in [69] by means of the backstepping method [65]. In this paper, we follow the stabilization result to design an observer with boundary measurements for a pair of coupled parabolic equations with a \textit{spatially-varying} reaction coefficient. The problem of observer design [70] and boundary stabilization [71] were recently solved for the case of \textit{constant-coefficients}. The main difficulty arises when trying to solve the PDEs verified by the backstepping kernel equations. For a system of \textit{two} coupled parabolic equations, one needs to find \textit{four} backstepping kernels verifying \textit{four} fully coupled second-order hyperbolic equations in a triangular domain, with complicated boundary conditions. We show that the kernel equations can be written (using some non-trivially-defined intermediate kernels) as a coupled system of \textit{eight}, \textit{first-order} hyperbolic equations. These kernel equations are very similar to those found when applying backstepping to find boundary controllers for first-order hyperbolic coupled systems. A result recently obtained for this problem showed that the resulting kernel equations were well-posed and had piece-wise differentiable solutions [72]. Applying this result to our case allows us to find an observer that guarantees $L^2$ exponential stability for the origin of estimation error system.

Our result shows that the connection between backstepping controllers for coupled parabolic and hyperbolic systems explored in [69] also extends to observers. In addition, the presented result contains some advances with respect to [69]. First, it is based in recently developed results on control of hyperbolic systems, namely [72]; this allows unique kernels to obtain with more regularity, whereas [69] was based in the design presented in [73, 74], which produced non-unique piece-wise-differentiable kernels. In addition, writing the kernel equations as first-order hyperbolic equations is done in a different fashion, allowing to deal with Neumann boundary conditions, whereas the procedure followed in [69] could only
address Dirichlet boundary conditions.

This problem is motivated by diffusion phenomena in lithium-ion batteries with electrodes that comprise multiple active materials. Manufacturers are using multiple active materials in the positive electrode of lithium-ion cells to combine power and energy characteristics or reduce degradation [4, 75]. The recent interest to use electrochemical models for online state-of-charge estimation motivates the design of observers for the PDEs appearing in these models.

The structure of the paper is as follows. In Section 10.3 we introduce the estimation problem. We state our main result in Section 9.4. The solution to the backstepping kernel equations is presented in Section 9.5. Results from the numerical computation of the kernels are shown in Section 9.6. Finally, we conclude the paper with some remarks in Section 9.8.

### 7.3 Problem Statement

#### 7.3.1 Notation

We will use the space $L^2[0,1]$, defined as the space of square-integrable vector functions in the interval $[0,1]$. For simplicity, we write $L^2$. The norm will be written as $\|f\|_{L^2}$ and computed as

$$\|f\|_{L^2} = \int_0^1 |f(x)|^2\,dx,$$

(7.1)

where $|\cdot|$ denotes the regular Euclidean norm. In addition we will use $L^2$ spaces with respect to time, which are analogously defined. Rather than using a more complex notation, we will denote the $L^2$ norm with respect to time equally as $\|\cdot\|_{L^2}$, and since it will only be used for functions only depending on time it should be clear from the context what $L^2$ norm we are referring to.
7.3.2 Coupled Parabolic Reaction-Diffusion Systems

Consider the following linear reaction-diffusion system with spatially-varying reaction
\[
    u_t (x,t) = \Sigma u_{xx} (x,t) + \Lambda (x) u (x,t),
\]
for \( x \in [0, 1], t > 0 \), with \( u(x,t) = [u_1(x,t), u_2(x,t)]^T \), coefficients in (8.15) defined as
\[
    \Sigma = \begin{bmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{bmatrix}, \quad \Lambda (x) = \begin{bmatrix} \lambda_{11} (x) & \lambda_{12} (x) \\ \lambda_{21} (x) & \lambda_{22} (x) \end{bmatrix},
\]
and boundary conditions
\[
    u_x (0, t) = [0, 0]^T, \quad u_x (1, t) = \phi (t) + f (u(1, t)).
\]
The value \( u(1, t) \) is measured and \( \phi (t) = [\phi_1 (t), \phi_2 (t)]^T \) is known. The particular choice of boundary conditions comes from diffusion phenomena in lithium-ion batteries with electrodes that comprise multiple active materials [4, 24]. States are ordered so that \( 0 < \epsilon_1 < \epsilon_2 \). We confine ourselves to the case of strict inequality in diffusion coefficients. An observer was derived previously in [21] for the cases of equal diffusion coefficients or diagonal \( \Lambda (x) \).

7.3.3 Observer and Estimation Error Systems

We consider the linear approximation of \( f (\cdot) \) around some fixed value \( u^* = [u_1^*, u_2^*]^T \),
\[
    f (u(1, t)) = f (u^*) + A (u(1, t) - u^*),
\]
with
\[
    A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}.
\]
Then, the linear approximation of boundary condition (8.20) is
\[ u_x(1,t) = \Phi(t) + Au(1,t), \] (7.9)
with \( \Phi(t) = \phi(t) + f(u^*) - Au^* \).

The proposed state observer is a copy of the reaction-diffusion system (8.15) with boundary conditions (8.18)–(7.9) together with output error injection
\[
\begin{align*}
\tilde{u}_t(x,t) &= \sum \tilde{u}_{xx}(x,t) + \Lambda(x)\tilde{u}(x,t) + P(x)\tilde{u}(1,t), \\
\tilde{u}_x(0,t) &= [0,0]^T, \\
\tilde{u}_x(1,t) &= \Phi(t) + A\tilde{u}(1,t) + (Q + A)\tilde{u}(1,t).
\end{align*}
\] (7.10)
(7.11)
(7.12)

The observer state is the pair \( \tilde{u}(x,t) = [\tilde{u}_1(x,t), \tilde{u}_2(x,t)]^T \), and \( \tilde{u}(1,t) = u(1,t) - \tilde{u}(1,t), \) is the (known) boundary output error. Observer gains \( P(x) \) and \( Q \) are yet to be chosen.

Now, the estimation error system can be found by subtracting (9.7), (9.8) and (9.9) from (8.15), (8.18) and (7.9) respectively, i.e.,
\[
\begin{align*}
\tilde{u}_t(x,t) &= \sum \tilde{u}_{xx}(x,t) + \Lambda(x)\tilde{u}(x,t) - P(x)\tilde{u}(1,t), \\
\tilde{u}_x(0,t) &= 0, \\
\tilde{u}_x(1,t) &= -Q\tilde{u}(1,t),
\end{align*}
\] (7.13)
(7.14)
(7.15)
where \( \tilde{u}(x,t) = u(x,t) - \tilde{u}(x,t) \).

## 7.4 Stability of the Error System

The problem is now to find \( P(x) \) and \( Q \) to guarantee asymptotic convergence of the observer state \( \tilde{u}(x,t) \) to the true state \( u(x,t) \) in the sense of the \( L^2 \) norm. This property is equivalent to the asymptotic stability of the origin in the estimation error system in the sense of the \( L^2 \) norm. Now, we state our main result.

**Theorem 7.4.1.** Consider the system (9.10)-(10.17) with initial condition \( \tilde{u}_0(x) \in L^2 \) and observer gains
\[
\begin{align*}
P(x) &= -K(x,1)\Sigma B - K_s(x,1)\Sigma, \\
Q &= B - K(1,1),
\end{align*}
\] (7.16)
(7.17)
where the kernel matrix $K(x,s)$ is a solution of the following hyperbolic system of PDEs
\[ \Sigma K_{xx} - K_{ss} \Sigma = -KC(s) - \Lambda(x)K, \quad (7.18) \]
in the domain $\mathcal{T} = \{(x,s) : 0 \leq x \leq s \leq 1\}$ with boundary conditions
\[ 0 = K(x,x)\Sigma - \Sigma K(x,x), \quad (7.19) \]
\[ \Lambda(x) + C(x) = -\Sigma K_x(x,x) - K_s(x,x)\Sigma - \Sigma \frac{d}{dx}[K(x,x)], \quad (7.20) \]
\[ 0 = K_x(0,s), \quad (7.21) \]
\[ 0 = K(0,0), \quad (7.22) \]
and
\[ B = \begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix}, \quad (7.23) \]
\[ C(x) = \begin{bmatrix} c_{11} & 0 \\ c_{21}(x) & c_{22} \end{bmatrix}, \quad (7.24) \]
with $b_1, b_2 \geq 0$ and $c_{11}, c_{22} > 0$. Then, the origin $\tilde{u} \equiv 0$ is asymptotically (and exponentially) stable in the $L^2$ norm.

In Theorem 9.4.1, the main question is if the kernel equations (9.15)–(9.19) do indeed have a solution, as implicitly assumed in the theorem’s statement. The next result answers this question.

**Theorem 7.4.2.** The kernel equations (9.15)–(9.19) possess a piecewise differentiable solution in the domain $\mathcal{T}$. In addition, the transformation defined by
\[ g(x) = f(x) - \int_x^1 K(x,s)f(s)ds, \quad (7.25) \]
is an invertible transformation. Both, the transformation and its inverse map $L^2$ functions into $L^2$ functions, verifying
\[ \|g\|_{L^2} \leq k_1\|f\|_{L^2}, \quad (7.26) \]
\[ \|f\|_{L^2} \leq k_2\|g\|_{L^2}. \quad (7.27) \]

In the next sections we prove Theorem 9.4.1 and Theorem 9.4.2, in Section 9.4.2 and 9.5 respectively.
7.4.1 Target System and Backstepping Transformation

We prove that, with the particular choice of $P(x)$ and $Q$ in (9.13)–(9.14), the origin of the estimation error system is asymptotically stable by applying the backstepping method. The main idea in the backstepping method is to map (9.10)–(10.17) into an stable target system which has to be adequately chosen. We select the following target system

$$w_t(x,t) = \Sigma w_{xx}(x,t) - C(x)w(x,t),$$

(7.28)

for $x \in [0,1]$, $t > 0$ with target state $w(x,t) = [w_1(x,t), w_2(x,t)]^T$ and boundary conditions

$$w_x(0,t) = 0,$$

(7.29)

$$w_x(1,t) = -Bw(1,t).$$

(7.30)

The backstepping transformation that maps $w$ into $\tilde{u}$ is defined as

$$\tilde{u}(x,t) = w(x,t) - \int_x^1 K(x,s)w(s,t)ds,$$

(7.31)

where the kernel matrix $K(x,s)$ is given by

$$K(x,s) = \begin{bmatrix} K_{11}(x,s) & K_{12}(x,s) \\ K_{21}(x,s) & K_{22}(x,s) \end{bmatrix}.$$

(7.32)

Now, we prove the stability property needed for the target system.

**Proposition 7.4.3.** The origin $w \equiv 0$ of the system (7.28) with boundary conditions (7.29), (10.27) and initial conditions $w_0 \in \mathcal{L}^2$ is exponentially stable in the $\mathcal{L}^2$ norm.

**Proof.** Consider the Lyapunov functional

$$V(t) = \frac{1}{2} \int_0^1 w^T \Pi w dx,$$

(7.33)

with

$$\Pi = \begin{bmatrix} \pi_{11} & 0 \\ 0 & 1 \end{bmatrix}.$$
Taking the time derivative of (9.45) and using integration by parts

\[ \dot{V}(t) = -|\sqrt{\Pi \Sigma B} w(1,t)|^2 - \int_0^1 w_x^T \Pi \Sigma w_x dx - \int_0^1 w^T \Pi C(x) w dx. \]  

(7.35)

From Young's inequality,

\[ - \int_0^1 c_{21}(x) w_1 w_2 dx \leq \frac{c_{21}^2}{2c_{22}} \int_0^1 w_1^2 dx + \frac{c_{22}}{2} \int_0^1 w_2^2 dx \]  

(7.36)

where \( c_{21} := \max_{x \in [0,1]} |c_{21}(x)|. \)

Then, using \( \pi_{11} \geq \frac{1}{2} + \frac{c_{21}^2}{2c_{11}c_{22}} \) we arrive to

\[ \dot{V}(t) \leq -|\sqrt{\Pi \Sigma B} w(1,t)|^2 - \int_0^1 w_x^T \Pi \Sigma w_x dx - \frac{\gamma}{2} \int_0^1 w^T \Pi w dx, \]  

(7.37)

with \( \gamma = 2 \min(1/\pi_{11}, 1) \min(c_{11}, c_{22}) \). Using Poincaré inequality

\[ \dot{V}(t) \leq - (\beta \epsilon_1 + \gamma) V(t), \]  

(7.38)

with \( \beta = \min(b_1, b_2, 1/2) \). Finally, applying Gronwall’s inequality the proposition is proved. \( \square \)

### 7.4.2 Proof of Theorem 9.4.1

Assume for the moment that Theorem 9.4.2 holds and that there is a solution to the kernel equations (9.15)–(9.19) such that the transformation (9.37) is invertible and both the transformation and its inverse map \( L^2 \) functions into \( L^2 \) functions. Consider now the target system equation (7.28) with boundary conditions (7.29)–(10.27) and initial conditions \( w_0(x) \) given by applying the inverse backstepping transformation to the initial estimation error \( \tilde{u}_0(x) \), i.e.,

\[ w_0(x) = \tilde{u}_0(x) - \int_x^1 I(x,s) \tilde{u}_0(s) ds, \]  

(7.39)

where \( I(x,s) \) is the kernel matrix of the inverse transformation. Since \( w_0 \in L^2 \), we have \( w_0 \in L^2 \), then Proposition 7.4.3 holds and Theorem 9.4.1 is proved.
7.4.3 Kernel Equations

To find the equations that the kernel matrix \( K(x, s) \) must verify we take time and space derivatives in (9.37), substitute the estimation error system and target system, and integrate by parts twice. Kernel equations are analog to those found in [72]. An important feature of the kernel equations is their cascade structure which can be recognized by expanding (9.15), i.e.,

\[
\begin{align*}
e_2K_{xx}^{22} - e_2K_{ss}^{22} &= - \left[ c_{22} + \lambda_{22}(x) \right] K^{22} - \lambda_{21}(x) K^{12}, \quad (7.40) \\
e_1K_{xx}^{12} - e_2K_{ss}^{12} &= - \left[ c_{22} + \lambda_{11}(x) \right] K^{12} - \lambda_{12}(x) K^{22}, \quad (7.41) \\
e_1K_{xx}^{11} - e_1K_{ss}^{11} &= - \left[ c_{11} + \lambda_{11}(x) \right] K^{11} - \lambda_{12}(x) K^{21} - c_{21}(s) K^{12}, \quad (7.42) \\
e_2K_{xx}^{21} - e_1K_{ss}^{21} &= - \left[ c_{11} + \lambda_{22}(x) \right] K^{21} - \lambda_{21}(x) K^{11} - c_{21}(s) K^{22}. \quad (7.43)
\end{align*}
\]

Equations (7.40)–(7.41) form a system that is independent from the other two entries of the kernel matrix. The solution of (7.40)–(7.41) then appears in the system (7.42)–(7.43) via \( c_{21}(s) \). Boundary condition (9.16) gives

\[
K^{12}(x, x) = K^{21}(x, x) = 0, \quad (7.44)
\]

Three entries in (9.17) are boundary conditions

\[
\begin{align*}
\frac{d}{dx} \left[ K^{22}(x, x) \right] &= - \frac{c_{22} + \lambda_{22}(x)}{2e_2}, \quad (7.45) \\
2e_1K_x^{12}(x, x) + (e_1 + e_2) K_s^{12}(x, x) &= - \lambda_{12}(x), \quad (7.46) \\
\frac{d}{dx} \left[ K^{11}(x, x) \right] &= - \frac{c_{11} + \lambda_{11}(x)}{2e_1}, \quad (7.47)
\end{align*}
\]

and the remaining entry in (9.17) is the definition of \( c_{21}(x) \), i.e.,

\[
c_{21}(x) = -2e_2K_x^{21}(x, x) - (e_1 + e_2) K_s^{21}(x, x) - \lambda^{21}(x). \quad (7.48)
\]

The last two boundary conditions, (9.18)–(9.19) imply that entries of matrices \( K_x(0, s) \) and \( K(0, 0) \) are all zero.
7.5 Well Posedness of Kernel Equations (Proof of Theorem 9.4.2)

Define \( L(x,s) \) and \( R(x,s) \) in the following way
\[
L(x,s) = \sqrt{\Sigma} K_x(x,s) - K_s(x,s) \sqrt{\Sigma}, \tag{7.49}
\]
\[
R(x,s) = \sqrt{\Sigma} K_x(x,s) + K_s(x,s) \sqrt{\Sigma}. \tag{7.50}
\]

Replacing (9.76) and (9.77) in (9.15) we obtain
\[
\sqrt{\Sigma} L_x + L_s \sqrt{\Sigma} = -KC(s) - \Lambda(x) K, \tag{7.51}
\]
\[
\sqrt{\Sigma} R_x - R_s \sqrt{\Sigma} = -KC(s) - \Lambda(x) K. \tag{7.52}
\]

Thus, the original \( 2 \times 2 \) system is replaced by a pair of \( 2 \times 2 \) systems of first-order hyperbolic equations. The cascade structure now appears in the systems (9.78)--(9.79). Equations (9.78)--(9.79) can be solved using the method of characteristics as follows:

- Functions \( L^{22}(x,s) \) and \( R^{22}(x,s) \) satisfy
\[
\sqrt{\epsilon_1} L^{22}_x + \sqrt{\epsilon_2} L^{22}_s = -[c_{22} + \lambda_{22}(x)] K^{22} - \lambda_{21}(x) K^{12}, \tag{7.53}
\]
\[
\sqrt{\epsilon_2} R^{22}_x - \sqrt{\epsilon_2} R^{22}_s = -[c_{22} + \lambda_{22}(x)] K^{22} - \lambda_{21}(x) K^{12}, \tag{7.54}
\]

with boundary conditions
\[
L^{22}(0,s) = -R^{22}(0,s), \tag{7.55}
\]
\[
R^{22}(x,x) = -\frac{c_{22} + \lambda_{22}(x)}{2 \sqrt{\epsilon_2}}. \tag{7.56}
\]

The characteristic lines are straight lines with slopes 1 for (7.53), and \(-1\) for (7.54) and are shown in Fig. 7.1.

- Functions \( L^{12}(x,s) \) and \( R^{12}(x,s) \) satisfy
\[
\sqrt{\epsilon_1} L^{12}_x + \sqrt{\epsilon_2} L^{12}_s = -[c_{22} + \lambda_{11}(x)] K^{12} - \lambda_{12}(x) K^{22}, \tag{7.57}
\]
\[
\sqrt{\epsilon_1} R^{12}_x - \sqrt{\epsilon_2} R^{12}_s = -[c_{22} + \lambda_{11}(x)] K^{12} - \lambda_{12}(x) K^{22}, \tag{7.58}
\]
Figure 7.1: Characteristic lines for functions $L^{22}(x,s)$, $R^{22}(x,s)$, $L^{11}(x,s)$, and $R^{11}(x,s)$. Function $K^{ij}(s,s)$ is used in the diagram to represent any of $K^{22}(s,s)$, $K^{12}(s,s)$, $K^{21}(s,s)$, or $K^{11}(s,s)$ with boundary conditions

$$R^{12}(x,x) = -\frac{\lambda_{12}(x)}{\sqrt{\epsilon_2} + \sqrt{\epsilon_1}},$$  \hspace{1cm} (7.59)$$

$$L^{12}(0,s) = -R^{12}(0,s),$$ \hspace{1cm} (7.60)$$

$$L^{12}(x,x) = \frac{\lambda_{12}(x)}{\sqrt{\epsilon_2} - \sqrt{\epsilon_1}}.$$ \hspace{1cm} (7.61)$$

The characteristic lines are straight lines with slopes $\sqrt{\epsilon_2/\epsilon_1}$ for (7.57), and $-\sqrt{\epsilon_2/\epsilon_1}$ for (7.58) and are shown in Fig. 7.2. Note that the geometry of the problem, i.e., domain shape and slope of the characteristic lines, impose the need of two boundary conditions (7.60) and (7.61) to compute $L^{12}$. 

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Figure 7.2: Characteristic lines for functions $L_{12}^1(x,s)$ and $R_{12}^1(x,s)$. The line $\sqrt{\epsilon_2}x = \sqrt{\epsilon_1}s$ divides the domain in two regions, each with a different boundary condition for $L_{12}^1(x,s)$.

- Functions $L_{21}^1(x,s)$ and $R_{21}^1(x,s)$ satisfy

\[
\sqrt{\epsilon_2}L_{x}^{21} + \sqrt{\epsilon_1}L_{s}^{21} = - [c_{11} + \lambda_{22}(x)]K^{21} - \lambda_{21}(x)K^{11} - c_{21}(s)K^{22}, \quad (7.62)
\]

\[
\sqrt{\epsilon_2}R_{x}^{21} - \sqrt{\epsilon_1}R_{s}^{21} = - [c_{11} + \lambda_{22}(x)]K^{21} - \lambda_{21}(x)K^{11} - c_{21}(s)K^{22}, \quad (7.63)
\]

with boundary conditions

\[
R_{21}^1(x,x) = \left[\frac{\sqrt{\epsilon_2} - \sqrt{\epsilon_1}}{\sqrt{\epsilon_2} + \sqrt{\epsilon_1}}\right]L_{21}^1(x,x), \quad (7.64)
\]

\[
L_{21}^1(0,s) = -R_{21}^1(0,s). \quad (7.65)
\]

The characteristic lines are straight lines with slopes $\sqrt{\epsilon_1/\epsilon_2}$ for (7.62), and $-\sqrt{\epsilon_1/\epsilon_2}$ for (7.63) and are shown in Fig. 7.3. Function $c_{21}(s)$ defined in (7.48), can be computed
Figure 7.3: Characteristic lines for functions $L^{21}(x, s)$ and $R^{21}(x, s)$. 

from $L^{21}(s, s)$ (or $R^{21}(s, s)$ using (7.64)) as

$$c_{21}(s) = -\lambda_{21}(s) + \left[ \frac{\epsilon_1 - \epsilon_2}{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}} \right] L^{21}(s, s).$$  \hspace{1cm} (7.66)

• Functions $L^{11}(x, s)$ and $R^{11}(x, s)$ satisfy

$$\sqrt{\epsilon_1} L^{11}_x + \sqrt{\epsilon_1} L^{11}_s = -[c_{11} + \lambda_{11}(x)] K^{11} - \lambda_{12}(x) K^{21} - c_{21}(s) K^{12}, \hspace{1cm} (7.67)$$

$$\sqrt{\epsilon_1} R^{11}_x - \sqrt{\epsilon_1} R^{11}_s = -[c_{11} + \lambda_{11}(x)] K^{11} - \lambda_{12}(x) K^{21} - c_{21}(s) K^{12}, \hspace{1cm} (7.68)$$

with boundary conditions

$$R^{11}(x, x) = -\frac{c_{11} + \lambda_{11}(x)}{2\sqrt{\epsilon_1}}, \hspace{1cm} (7.69)$$

$$L^{11}(0, s) = -R^{11}(0, s). \hspace{1cm} (7.70)$$
The characteristic lines are straight lines with slopes 1 for (7.67), and \(-1\) for (7.68) and are shown in Fig. 7.1.

Note that elements of the kernel matrix \(K(x,s)\) appear in the right hand side of equations (9.78) and (9.79). This is not a problem because we can always write \(K(x,s)\) in terms of \(L(x,s)\) and \(R(x,s)\) by integrating (9.76) and (9.77). For instance, since \(K(x,x)\) is given by boundary conditions we can write

\[
K_{11}^{11}(x,s) = -\frac{1}{2\sqrt{\epsilon_1}} \int_{\mathcal{L}(x)} \left[ R_{11}^{11}(\xi,s) + L_{11}^{11}(\xi,s) \right] d\xi + K_{11}^{11}(s,s), \tag{7.71}
\]

\[
K_{12}^{12}(x,s) = -\frac{1}{2\sqrt{\epsilon_1}} \int_{\mathcal{L}(x)} \left[ R_{12}^{12}(\xi,s) + L_{12}^{12}(\xi,s) \right] d\xi + K_{12}^{12}(s,s), \tag{7.72}
\]

\[
K_{21}^{21}(x,s) = -\frac{1}{2\sqrt{\epsilon_2}} \int_{\mathcal{L}(x)} \left[ R_{21}^{21}(\xi,s) + L_{21}^{21}(\xi,s) \right] d\xi + K_{21}^{21}(s,s), \tag{7.73}
\]

\[
K_{22}^{22}(x,s) = -\frac{1}{2\sqrt{\epsilon_2}} \int_{\mathcal{L}(x)} \left[ R_{22}^{22}(\xi,s) + L_{22}^{22}(\xi,s) \right] d\xi + K_{22}^{22}(s,s). \tag{7.74}
\]

Integration in (7.71)–(7.74) is perform along straight lines parallel to the \(x\)-axis and this is illustrated in Figures 7.1-7.3. Finally, kernel equations (9.78)–(9.79), with boundary conditions (7.55)–(7.56), (7.60)–(7.61), (7.65)–(7.64), (7.69)–(7.70) are similar to the equations and boundary conditions verified by the kernels in [72] except for the presence of the integrals (7.71)–(7.74). However, the integrals do not complicate the proof in [72], thus following a similar approach the result follows and one obtains bounded and piece-wise differentiable kernels. Since the kernels are bounded and the transformation is of Volterra type, it is automatically invertible as in (7.39) with bounded inverse kernels.

A closed form solution of elements in the kernel matrix \(K(x,s)\) is not available, but numerical computation is always possible.

### 7.6 Numerical Computation of the Kernels
Figure 7.4: Kernel element $K^{22}(x,s)$.

Figure 7.5: Kernel element $K^{12}(x,s)$. 
Figure 7.6: Kernel element $K^{21}(x,s)$.

Figure 7.7: Kernel element $K^{11}(x,s)$. 
This set of plots shows results from the numerical computation of the kernel matrix $K(x,s)$. To find $K(x,s)$, we first compute $L(x,s)$ and $R(x,s)$ using the method of characteristics together with the method of successive approximations and finally compute $K(x,s)$ using (7.71)–(7.74). For this example, $\epsilon_1 = 1$, $\epsilon_2 = 3$, $\lambda_{11}(x) = 1$, $\lambda_{12}(x) = x$, $\lambda_{21}(x) = x$, $\lambda_{22}(x) = 1$, $c_{11} = 5$, and $c_{22} = 11$.

## 7.7 Conclusion

This paper presents an observer for a pair of coupled parabolic systems with spatially-varying reaction. The result is more general than a recently published work on observers for systems of coupled parabolic systems with constant coefficients. The result shows that the connection between backstepping controllers for coupled parabolic and hyperbolic systems explored extends to observers. Furthermore, with respect to the stabilization result, this paper presents an advancement in the formulation of the backstepping kernel equations. Future work includes extending the result for a general system of $n$ coupled reaction-diffusion systems and for ball-shaped domains in general dimension. All these extension are motivated by state estimation for lithium-ion batteries with electrodes that comprise multiple active materials.

## 7.8 Acknowledgment

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Chapter 8

Observer Design for the Pointwise Expected Value of a Randomly Switching Diffusion-Reaction Equation

8.1 Abstract

The pointwise expected value of the solution of a randomly switching reaction-diffusion PDE is by itself the solution of a deterministic system of coupled reaction-diffusion equations; provided that the random switching is Markovian and that the PDE satisfies some regularity conditions. Following recent results on boundary observers for systems of coupled reaction-diffusion equations, an observer is constructed for the asymptotic estimation of the expected value of the randomly switching reaction-diffusion PDE. Although only the case where the PDE switches between two states is developed here, the same results hold for an arbitrary, but finite, number of switching states. In general, the observer gains are to be
computed numerically from the solution of a system of coupled second order hyperbolic PDEs. Several phenomena described by randomly switching reaction-diffusion PDEs, for example: neurotransmitters diffusion that take into account switching between quiescent and firing states, thermostats and failure in lithium-ion batteries.

8.2 Introduction

Boundary observers and controllers can be obtained for reaction-diffusion equations with constant or spatially and time varying parameters [65, 53]; provided that the problem is deterministic. Here, we construct an observer for the pointwise expected value of a randomly switching reaction-diffusion equation with Neumann-type boundary conditions. The switching function is an stochastic process, satisfying the Markov properties and taking values in a finite set. For simplicity, we restrict the problem to the case where the switching function takes only two possible values. For each value of the switching function, the state of the PDE satisfies a particular boundary value problem; that is, a reaction-diffusion equation with specific parameter values and specific boundary conditions (both of Neumann-type). The result builds upon two recent results on reaction-diffusion systems. On one side, in [76] a deterministic system of coupled reaction-diffusion equations was derived for the statistical moments of parabolic equations with random switching. On the other, boundary observers and controllers have been constructed for systems of coupled reaction-diffusion equations [77, 69, 78, 71]. These observers and controllers are based on the backstepping method for PDEs. The main advantage of backstepping [65], is that, once the well-posedness of the kernel equations has been established, analytical and numerical results are often simple to obtain.

The literature on stochastic and deterministic switching system is vast. For a broad exposition of the fundamental results on analysis and control of switched dynamical systems
the reader might refer to the books [79, 80, 81, 82]. Existing stability results include systems as intricate as nonlinear systems under stochastic switching [83, 84]. The literature on the analysis and stability of switching systems is not restricted to finite dimensional systems, but includes also switched infinite dimensional systems. Stability of switching PDEs has been studied in [85], [86]. In particular, stability has been studied for switched hyperbolic systems [87], for reaction-diffusion system [88], and optimal control problems in [89]. State and parameter estimation has been studied for switched hyperbolic systems in [90].

Possible applications of the observer include: neurotransmitters diffusion that take into account switching between quiescent and firing states, models of insect respiration, and thermostats [76]. In addition, since boundary observers for radial diffusion equations [52] have been derived for state and parameters estimation in lithium-ion batteries (from electrochemical models) to serve as estimation algorithms in battery management system [53, 21, 91, 92, 23, 15], the ability to estimate the expected values of randomly switching diffusion equations might allow us to include models of failure in those estimation algorithms. In fact, from all possible failure modes of lithium-ion batteries, several might occur abruptly and randomly, for example: particle fracture in the electrodes, appearance of holes in separator due to dendrite formation or external forcing, gas generation and bloating of cell casting due to high external temperatures, and internal short circuit between electrodes due to external load on the cell [93].

8.2.1 Organization

The structure of the paper is as follows. In Section 10.3 we introduce the problem. The observer for the expected value of the switching PDE and convergence properties of the observer are included in Section 10.4. Section 8.5 and 8.6 describe and bound the measurement error, arising from the fact that expected values of boundary are not available as measurements. Results from a numerical example are included in Section 9.7. Finally,
we conclude the paper with some remarks in Section 10.6.

8.3 Problem Statement

8.3.1 Switching Reaction-Diffusion Equation

The switching function \( s(t) : [0,T] \mapsto \mathcal{B} \) is defined as a two-state continuous-time Markov process taking values in the binary set \( \mathcal{B} = \{1,2\} \). A continuous-time Markov process is completely characterized by a generator matrix and an initial distribution [94]. The initial probability distribution of \( s(t) \) is \( q_0 = [q_{01}, q_{02}]^T \), with

\[
q_{01} = \mathbb{P}(s(0) = 1),
\]

\[
q_{02} = \mathbb{P}(s(0) = 2),
\]

satisfying: \( q_{01}, q_{02} \in [0,1] \) and \( q_{01} + q_{02} = 1 \). The generator matrix \( G \in \mathbb{R}^{2 \times 2} \) describes transition rates of \( s(t) \). For the binary set \( \mathcal{B} \), the generator matrix is of the form

\[
G = \begin{bmatrix}
-\alpha & \alpha \\
\beta & -\beta
\end{bmatrix},
\]

for some \( \alpha, \beta \in [0,\infty) \). The map between the initial probability distribution and the (conditional) probability distribution at later times, \( q(t) = [q_1(t), q_2(t)]^T \), is given by a transition matrix \( \Phi(t) \), that is

\[
q(t) = \Phi^T(t)q_0.
\]
For the two-state problem, the transition matrix $\Phi(t)$ can be found explicitly

$$
\Phi(t) = \frac{1}{\gamma} \begin{bmatrix}
\beta & \alpha \\
\beta & \alpha
\end{bmatrix} + \frac{e^{-\gamma t}}{\gamma} \begin{bmatrix}
\alpha & -\alpha \\
-\beta & \beta
\end{bmatrix},
$$

with $\gamma = \alpha + \beta$.

**Remark 8.3.1.** Associated to the stochastic process $s(t)$, there is a sequence of switching times $\{t_1, t_2, \ldots, t_N\}$. Since $\mathbb{B}$ is finite, and $\alpha, \beta < \infty$, there is a finite number of switching times in $[0, T]$ and the time intervals $\{(0, t_1], (t_1, t_2], \ldots, (t_N, T]\}$ have all a positive length [95, Theorem 4, Chapter II.5].

Consider a pair of differential operators $\mathcal{A}_1, \mathcal{A}_2 : \mathcal{H}^2(0,1) \mapsto \mathcal{L}^2(0,1)$, defined as

$$
\mathcal{A}_i[u](x,t) = \epsilon_i \partial_{xx} u(x,t) + \lambda_i(x) u(x,t),
$$

for $i \in \{1, 2\}$, with $\epsilon_2 \geq \epsilon_1 > 0$, $\lambda_1(x), \lambda_2(x) \in C^0([0,1])$, together with a pair of Neumann-type boundary conditions

$$
\partial_x u(0,t) = f_i(t),
$$

$$
\partial_x u(1,t) = g_i(t).
$$

Associated to the stochastic process $s(t)$, define a linear Markov switching diffusion-reaction system

$$
\partial_t u(x,t) = \mathcal{A}_{s(t)}[u](x,t),
$$
for \( x \in (0,1), \ t \in (0,T] \), with boundary conditions

\[
\partial_x (0, t) = f_s(t)(t), \quad \tag{8.10}
\]
\[
\partial_x (1, t) = g_s(t)(t), \quad \tag{8.11}
\]

for \( t \in (0,T] \), and initial condition \( u_0(x) \in \mathcal{L}^2([0,1]) \). A continuous and piecewise deterministic solution \( u(x,t) \in C^0 \left([0,T]; \mathcal{L}^2(0,1)\right) \) can be defined, in a week sense, for the system (8.9)-(8.11).

**Definition 8.3.1** (Piecewise definition of the solution). For the first time interval, i.e., \( t \in (0,t_1] \), the system (8.9)-(8.11) is a deterministic initial-boundary value problem with a unique continuous solution \( u(x,t) \in C^0 \left([0,t_1]; \mathcal{L}^2(0,1)\right) \), [96, Theorem 4.1]. If a continuous solution exists on the interval \( (0,t_k] \), for \( k < N \), then in the next interval, i.e., \( t \in (t_k,t_{k+1}] \), the system is a deterministic initial-boundary value problem with initial condition \( u(x,t_k) \in C^2([0,1]) \) and a unique continuous solution \( u(x,t) \in C^0 \left([t_k,t_{k+1}]; \mathcal{L}^2(0,1)\right) \). Then, inductively, a continuous and piecewise deterministic solution for the switching reaction-diffusion system can be found on \( (0,T] \).

**Remark 8.3.2.** The stochastic process \( u(x,t) \) is predictable [97, p. 297] with respect to \( s(t) \). That is, formally, for any given \( t_* > 0 \), the value \( u(x,t_*) \) is a function on the history (path) \( \{s(t) : 0 \leq t < t_*\} \). This is true since \( u(x,t) \) is adapted [76] with respect to \( s(t) \) and continuous.
\[ \begin{align*}
\frac{\partial u}{\partial t}(x, t) &= \epsilon_1 \frac{\partial^2 u}{\partial x^2}(x, t) + \lambda_1(x)u(x, t), \\
\frac{\partial u}{\partial x}(0, t) &= f_1(t), \quad \frac{\partial u}{\partial x}(1, t) = g_1(t), \\
\frac{\partial u}{\partial x}(0, t) &= f_2(t), \quad \frac{\partial u}{\partial x}(1, t) = g_2(t), \\
u_0(x)
\end{align*} \]

Figure 8.1: The stochastic process \( u(x, t) \) is piecewise deterministic. The process might start in any of the two states in \( B \), for example \( s(0) = 2 \), and propagate the initial condition \( u_0(x) \) according to the operator \( A_2 \) with the second set of boundary conditions. At some time \( t_1 > 0 \), the switching function changes its value, that is \( s(t_1) = 1 \). Now, the value \( u(x, t_1) \) serves as the initial condition for a second propagation interval according to the operator \( A_1 \) and the first set of boundary conditions. This process continues according to the particular realization of the switching function \( s(t) \).

### 8.3.2 Pointwise Expected Value

Following [76], define a pair of deterministic functions

\[ \begin{align*}
v_1(x, t) &= \mathbb{E}\left[ \mathbb{1}_{s(t)=1} u(x, t) \right], \\
v_2(x, t) &= \mathbb{E}\left[ \mathbb{1}_{s(t)=2} u(x, t) \right],
\end{align*} \]

such that, the pointwise expectation of \( u(x, t) \) is simply

\[ \mathbb{E}[u(x, t)] = v_1(x, t) + v_2(x, t). \]

**Lemma 8.3.1.** The function \( v(x, t) = [v_1(x, t), v_2(x, t)]^T \), defined in (8.12), (8.13), satisfies a deterministic initial-boundary value problem, that is, a system of coupled reaction-diffusion
\begin{equation}
\partial_t (x,t) = \Sigma \partial_{xx} v(x,t) + \left( \Lambda(x) + G^T \right) v(x,t),
\end{equation}

for \( x \in (0,1), t \in (0,T] \), with coefficients

\begin{equation}
\Sigma = \begin{bmatrix}
\epsilon_1 & 0 \\
0 & \epsilon_2
\end{bmatrix}, \Lambda(x) = \begin{bmatrix}
\lambda_1(x) & 0 \\
0 & \lambda_2(x)
\end{bmatrix},
\end{equation}

with \( G \) defined in (8.3), boundary conditions

\begin{align}
\partial_x v_1(0,t) &= q_1(t)f_1(t), \\
\partial_x v_2(0,t) &= q_2(t)f_2(t),
\end{align}

and

\begin{align}
\partial_x v_1(1,t) &= q_1(t)g_1(t), \\
\partial_x v_2(1,t) &= q_2(t)g_2(t),
\end{align}

and initial conditions

\begin{align}
v_{1,0}(x) &= q_1(0)u_0(x), \\
v_{2,0}(x) &= q_2(0)u_0(x).
\end{align}

Proof. This lemma follows from Theorem 1 in [76]. The assumptions in the theorem are satisfied for our problem; following the arguments in the Appendix of the same reference [76].
We will assume, in the next section, that the expected value of the the \( \mathbb{E}[u(1,t)] \), is known and construct a deterministic boundary observer to estimate \( \mathbb{E}[u(x,t)] \) in the sense of the \( L^2 \)-norm.

### 8.4 Observer

From the law of total expectation, and using continuity of \( u(x,t) \), it is possible to compute \( v(1,t) \) from \( \mathbb{E}[u(1,t)] \) as

\[
v_1(1,t) = q_1(t)\mathbb{E}[u(1,t)], \tag{8.23}
\]
\[
v_2(1,t) = q_2(t)\mathbb{E}[u(1,t)]. \tag{8.24}
\]

The proposed state observer is a copy of the reaction-diffusion system (8.15) with boundary conditions (8.18)–(8.20) together with an output error term

\[
\partial_t (x,t) = \Sigma \partial_{xx} \tilde{v}(x,t) + \left( \Lambda(x) + G^T \right) \tilde{v}(x,t) + P(x)\tilde{v}(1,t), \tag{8.25}
\]

for \( x \in (0,1), t > 0 \), and boundary conditions

\[
\partial_x \tilde{v}(0,t) = [q_1(t)f_1(t), q_2(t)f_2(t)]^T, \tag{8.26}
\]
\[
\partial_x \tilde{v}(1,t) = [q_1(t)g_1(t), q_2(t)g_2(t)]^T + Q\tilde{v}(1,t),
\]

with \( \tilde{v}(1,t) = v(1,t) - \bar{v}(1,t) \). The estimation error, defined as \( \bar{v}(x,t) = v(x,t) - \bar{v}(x,t) \), is the solution of the estimation error system

\[
\partial_t \bar{v}(x,t) = \Sigma \partial_{xx} \bar{v}(x,t) + \left( \Lambda(x) + G^T \right) \bar{v}(x,t) - P(x)\bar{v}(1,t), \tag{8.27}
\]
with boundary conditions

\[
\partial_x \tilde{v}(0, t) = 0, \tag{8.28}
\]
\[
\partial_x \tilde{v}(1, t) = -Q \tilde{v}(1, t). \tag{8.29}
\]

The problem is now to find \(P(x)\) and \(Q\) to guarantee asymptotic convergence of the observer state \(\hat{v}(x, t)\) to the true state \(v(x, t)\) in the sense of the \(L^2\) norm, that is,

\[
\|v(\cdot, t) - \hat{v}(\cdot, t)\|_2 \to 0 \tag{8.30}
\]
as \(t \to 0\). This property is equivalent to the asymptotic stability of the origin in the estimation error system in the sense of the \(L^2\) norm.

**Theorem 8.4.1.** Under the assumption that \(E[u(1, t)]\) is available as a measurement and \(v(1, t)\) computed from (8.23), (8.24). For the the estimation error system with initial condition \(\tilde{v}_0(x) \in L^2(0, 1)\) and observer gains

\[
P(x) = -K(x, 1) \Sigma B - K_s(x, 1) \Sigma, \tag{8.31}
\]
\[
Q = B - K(1, 1), \tag{8.32}
\]

where the kernel matrix \(K(x, s)\) is a solution of the following hyperbolic system of PDEs

\[
\Sigma \partial_{xx} K - \partial_{ss} K \Sigma = -KC(s) - \Lambda(x) K, \tag{8.33}
\]
in the domain \(\mathcal{T} = \{(x, s): 0 \leq x \leq s \leq 1\}\) with boundary conditions

\[
0 = K(x, x) \Sigma - \Sigma K(x, x), \tag{8.34}
\]
\[
\Lambda(x) + C(x) = -\Sigma \partial_x K(x, x) - \partial_s K(x, x) \Sigma - \Sigma \frac{d}{dx}[K(x, x)], \tag{8.35}
\]
\[
0 = \partial_x K(0, s), \tag{8.36}
\]
\[
0 = K(0, 0). \tag{8.37}
\]
with \( b_1, b_2 \geq 0 \) and \( c_{11}, c_{22} > 0 \). Then, the origin \( \tilde{v} \equiv 0 \) is asymptotically (and exponentially) stable in the \( \mathcal{L}^2 \)-norm.

**Proof.** The proof follows directly from Theorem 1 in [77].

The remaining problem is to quantify the error between measurements \( u(1, t) \) of some particular realization and the requirement boundary value \( \mathbb{E}[u(1, t)] \).

### 8.5 Measurement Error

To quantify the error between the expected boundary value \( \mathbb{E}[u(1, t)] \), required in the observer, and the boundary measurement \( u(1, t) \) taken from some particular realization of the stochastic switching diffusion-reaction system, we use a representation of \( u(x, t) \) and \( \mathbb{E}[u(x, t)] \) in terms of the eigenfunctions of the operators \( \mathcal{A}_1 \) and \( \mathcal{A}_2 \) with homogeneous Neumann boundary conditions [98]. In this context, with an abuse of notation, the equality sign between a function and the eigenfunction representation indicates convergence in the sense of the \( \mathcal{L}^2 \)-norm. For some particular realization \( \{s_p(t), u_p(x, t)\} \)

\[
\begin{align*}
  u_p(x, t) &= \int_0^1 u_0(\xi)M(x, \xi, \tau)d\tau - \epsilon \int_0^t \left[ 1\{s_p(\tau)=1\} f_1(\tau) M_1(x, 0, t-\tau) 
  \right. \\
  &\quad + \left. 1\{s_p(\tau)=2\} f_2(\tau) M_2(x, 0, t-\tau) \right] d\tau + \epsilon \int_0^t \left[ 1\{s_p(\tau)=1\} g_1(\tau) M_1(x, 1, t-\tau) 
  \right. \\
  &\quad + \left. 1\{s_p(\tau)=2\} g_2(\tau) M_2(x, 1, t-\tau) \right] d\tau, 
\end{align*}
\]  

(8.40)
with

\[ M(x,\xi,\tau) = \mathbb{1}_{s(\tau)=1} M_1(x,\xi,\tau) + \mathbb{1}_{s(\tau)=2} M_2(x,\xi,\tau), \quad (8.41) \]

and

\[ M_1(x,\xi,t) = \sum_{n=1}^{\infty} \frac{\phi_{1,n}(x)\phi_{1,n}(\xi)}{||\phi_{1,n}(\cdot)||_2^2} \exp[-\sigma_{1,n}t], \quad (8.42) \]

\[ M_2(x,\xi,t) = \sum_{n=1}^{\infty} \frac{\phi_{2,n}(x)\phi_{2,n}(\xi)}{||\phi_{2,n}(\cdot)||_2^2} \exp[-\sigma_{2,n}t], \quad (8.43) \]

where \( \phi_n(x) \) and \( \sigma_n \) are the eigenfunction and eigenvalues of the Sturm-Liouville problem

\[ \epsilon_1 \phi_1''(x) + \lambda_1(x) \phi_1'(x) = -\sigma_1 \phi_1(x), \quad (8.44) \]

with boundary conditions \( \phi'(0) = 0, \phi'(1) = 0 \), and

\[ \epsilon_2 \phi_2''(x) + \lambda_2(x) \phi_2'(x) = -\sigma_2 \phi_2(x), \quad (8.45) \]

with boundary conditions \( \phi'(0) = 0, \phi'(1) = 0 \). Similarly, the representation of the pointwise expected value \( \mathbb{E}[u(x,t)] \) is

\[ \mathbb{E}[u(x,t)] = \int_0^1 u_0(\xi) \overline{M}(x,\xi,\tau) d\tau - \epsilon \int_0^t [q_1(t) f_1(\tau) M_1(x,0,t-\tau) + q_2(t) f_2(\tau) M_2(x,0,t-\tau)] d\tau + \epsilon \int_0^t [q_1(t) g_1(\tau) M_1(x,1,t-\tau) + q_2(t) g_2(\tau) M_2(x,1,t-\tau)] d\tau, \quad (8.46) \]

with

\[ \overline{M}(x,\xi,\tau) = q_1(t) M_1(x,\xi,\tau) + q_2(t) M_2(x,\xi,\tau). \quad (8.47) \]
Thus, the mismatch between measurements and boundary values is

\[ E[u(x,t)] - u_p(x,t) = e_p(t) \int_0^1 u_0(\xi) A_0(x,\xi,t) d\xi + \int_0^t e_p(\tau) [A_2(x,t,\tau) - A_1(x,t,\tau)] d\tau, \]  

(8.48)

with

\[ e_p(t) = q_1(t) - \mathbb{1}_{\{s_p(t)=1\}}, \]  

(8.49)

and

\[ A_0(x,\xi,t) = M_1(x,\xi,t) - M_2(x,\xi,t), \]  

(8.50)

\[ A_1(x,t,\tau) = \epsilon_1 f_1(\tau) M_1(x,0,t-\tau) - \epsilon_2 f_2(\tau) M_2(x,0,t-\tau), \]  

(8.51)

\[ A_2(x,t,\tau) = \epsilon_1 g_1(\tau) M_1(x,1,t-\tau) - \epsilon_2 g_2(\tau) M_2(x,1,t-\tau). \]  

(8.52)

Therefore

\[ |E[u(1,t)] - u_p(1,t)| \leq \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{1-\delta}^{1} \left| e_p(t) \right| \left| \int_0^1 u_0(\xi) A_0(x,\xi,t) d\xi \right| + \left| \int_0^t e_p(\tau) \times [A_2(x,t,\tau) - A_1(x,t,\tau)] d\tau \right| dx. \]  

(8.53)

Then, the observer is only useful if the right hand of the inequality is independent of the initial conditions.

**Proposition 8.5.1.** The error between the measurements \( u_p(1,t) \) and the expected value \( E[u(1,t)] \) is asymptotically independent of the initial conditions provided that

\[ \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{1-\delta}^{1} \int_0^1 A_0(x,\xi,t)^2 d\xi dx \to 0 \text{ as } t \to \infty \]  

(8.54)
with $A_0$ defined in (8.50). If, in addition, the realization of $s_p(t)$ of $s_p(t)$ is available as a measurement, it is possible to compute a corrected measurement $\hat{u}_p(1, t)$ as follows

$$
\hat{u}_p(1, t) = u_p(1, t) + \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{1-\delta}^1 \int_0^t e_p(\tau) \left[ A_2(x, t, \tau) - A_1(x, t, \tau) \right] d\tau dx
$$

with $A_1$ and $A_2$ defined in (8.51), (8.52). Then, the error $|\mathbb{E}[u(1, t)] - \hat{u}_p(1, t)|$, tends to zero asymptotically.

**Proof.** The proof of the first statement in the lemma follows directly from the inequality (8.53) and the Cauchy-Schwarz inequality. The second statements comes from the fact that if the value of the stochastic process $s(t)$ is available as a measurement, then $e_p(t)$ is also known, thus (8.53) and the first statement imply that, asymptotically, the measurement error tends to zero.

\[\Box\]

### 8.6 Switching Boundary Conditions

For the case where coefficients of the PDE are constants over the switching process, that is, $\epsilon_1 = \epsilon_2$ and $\lambda_1 = \lambda_2$, initial conditions have the same effect in all possible realizations. In turn, this implies that the effect of the initial condition in $\mathbb{E}[u(x, t)]$ is the same as in any particular realization. To understand this argument, consider a particular realization $\{s_p(t), u_p(x,t)\}$, and the representation

$$
u_p(x,t) = \int_0^1 u_0(\xi) M(x, \xi, t) d\xi - \epsilon \int_0^t \left[ \mathbb{1}_{\{s_p(\tau)=1\}} f_1(\tau) + \mathbb{1}_{\{s_p(\tau)=2\}} f_2(\tau) \right] M(x, 0, t - \tau) d\tau $$

$$+ \epsilon \int_0^1 \left[ \mathbb{1}_{\{s_p(t)=1\}} g_1(t) + \mathbb{1}_{\{s_p(t)=2\}} g_2(t) \right] M(x, 1, t - \tau) d\tau, \quad (8.56)$$
with

$$M(x, \xi, t) = \sum_{n=1}^{\infty} \frac{\phi_n(x)\phi_n(\xi)}{\|\phi_n(\cdot)\|^2_2} \exp[-\sigma_n t], \quad (8.57)$$

where \( \phi_n(x) \) and \( \sigma_n \) are the eigenfunction and eigenvalues of the Sturm-Liouville problem

$$\epsilon \phi''(x) + \lambda(x) \phi'(x) = -\sigma \phi(x), \quad (8.58)$$

with boundary conditions \( \phi'(0) = 0, \phi'(1) = 0 \). The first term in (8.56) is the same for any particular realization. This implies that, for any particular realization \( s_p(t) \), the difference \( u_p(x, t) - \mathbb{E}[u(x, t)] \) is not a function of the initial conditions. In other words, for any particular realization \( s_p(t) \), the measurement \( u_p(1, t) \) would provide the same information about the initial conditions as \( \mathbb{E}[u(1, t)] \) would, that is

$$\mathbb{E}[u(x, t)] - u_p(x, t) = \int_0^t e_p(\tau)[B_2(x, t, \tau) - B_1(x, t, \tau)]d\tau, \quad (8.59)$$

with

$$B_1(x, t, \tau) = \epsilon [f_1(\tau) - f_2(\tau)] M(x, 0, t - \tau), \quad (8.60)$$
$$B_2(x, t, \tau) = \epsilon [g_1(\tau) - g_2(\tau)] M(x, 1, t - \tau). \quad (8.61)$$

and

$$|\mathbb{E}[u(1, t)] - u_p(1, t)| \leq \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{1-\delta}^{1} \left| \int_0^t e_p(\tau)[B_2(x, t, \tau) - B_1(x, t, \tau)]d\tau \right|dx. \quad (8.62)$$

**Proposition 8.6.1.** For switching boundary conditions, the error between \( \mathbb{E}[u(x, t)] \) and \( u_p(x, t) \) is independent of the initial conditions. If, in addition, the realization \( s_p(t) \) of \( s(t) \)
Figure 8.2: A particular realization of the stochastic process $u(x,t)$; where measurements $u(1,t)$ are taken is known as a measurement, it is possible to compute a corrected measurement

$$\tilde{u}_p(x,t) = u_p(x,t) + \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{1-\delta}^{1} \int_{0}^{t} e_p(\tau) \left[ B_2(x,t,\tau) - B_1(x,t,\tau) \right] d\tau dx,$$  \hspace{1cm} (8.63)

such that

$$\mathbb{E}[u(1,t)] - \tilde{u}_p(1,t) = 0$$  \hspace{1cm} (8.64)

for all $t > 0$.

Proof. The proof of the first statement follows directly form the inequality (8.62). The second statements follows from the fact that knowledge of $s(t)$ implies knowledge of $e_p(t)$ together with inequality (8.62).

\vspace{1cm}

8.7 Example
Figure 8.3: Closed loop estimate of the pointwise expected value using measurements $u(1,t)$. The true expected value is included to illustrate the effectiveness of the observer and to show the remaining error due to the difference between $\mathbb{E}[u(1,t)]$ and $u(1,t)$.

Figure 8.4: The open loop estimate of the expected value is the results of solving the deterministic system of coupled reaction diffusion equations without output error terms.
To illustrate the performance of the observer, we consider a pair of diffusion equations with switching Neumann boundary conditions

\[ \partial_t u(x,t) = \epsilon \partial_{xx} u(x,t) \]  

(8.65)

with \( \epsilon = 10^{-4} \), and boundary conditions

\[ \partial_x u(0,t) = f_1(t), \]  

(8.66)

\[ \partial_x u(1,t) = 0, \]  

(8.67)

where

\[ f_1(t) = 0, \quad f_2 = \frac{1}{2} t + 50\sin(t). \]  

(8.68)

The generator matrix for the stochastic Markov process \( s(t) \) is

\[ G = 10^{-4} \begin{bmatrix} -1 & 1 \\ 500 & -500 \end{bmatrix}, \]  

(8.69)

and the initial distribution is \( q(t) = [0.5, 0.5] \). A particular realization of this process \( u(x,t) \) is shown in Figure 2 for \( t \in [0,100] \). The observer parameters are chosen as \( c_1 = c_2 = 10 \) and \( b_1 = b_2 = 0 \) and we assume that the value of the switching function \( s(t) \) is not available from measurements.

The measurement error for this example is bounded as follows

\[ |\mathbb{E}[u(1,t)] - u(1,t)| \leq \left| \int_0^t e_p(\tau) \left[ \frac{1}{2} \tau + 50\sin(\tau) \right] d\tau \right|. \]  

(8.70)

In Figure 3, the expected value of the diffusion equation (8.65) with switching boundary
conditions (8.66), (8.67), computed as the mean value of 5000 realization of the stochastic process, is shown in blue. In the same figure, the observer state, derived from Section III, is shown in orange. Figure 4, compares the expected value against an open loop estimate, that is, the solution of a system of coupled reaction diffusion equations without output error terms.

8.8 Acknowledgment

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Chapter 9

Boundary Observers for Coupled Diffusion-Reaction Systems with Prescribed Convergence Rate

9.1 Abstract

Following recent results on the boundary stabilization of coupled first-order hyperbolic equations by means of integral transformations, here an analogous result is presented for the problem of state estimation of coupled linear reaction-diffusion PDEs with Neumann boundary conditions from boundary measurements. For this purpose, an observer is constructed with a prescribed convergence rate. The stability of the estimation error system is derived by mapping the estimation error system to a stable target system using a pair of integral transformations. The kernels in the integral transformations are matrices of functions whose entries satisfy a system of coupled second-order hyperbolic equations, defined on a triangle and a square. The well-posedness of both kernel systems is established by noticing a resemblance with the kernel systems appearing in the problem of boundary
stabilization of coupled first-order hyperbolic equations. Our method is applicable as well to the dual problem of boundary stabilization of coupled linear reaction-diffusion PDEs. A numerical scheme, based on power series approximations of the kernels is formulated, taking into account the fact that the kernels are piecewise differentiable.

9.2 Introduction

The problems of stabilization and estimation for coupled linear parabolic equations have been addressed recently, by means of the backstepping method for PDEs [65], in a series of publications. First, the stabilization and estimation problems for coupled reaction-diffusion equations, with constant parameters and equal diffusion coefficients, were solved in [99], [70] and [100]. The extension to allow distinct diffusion coefficients was proposed later for coupled reaction-diffusion equations with constant coefficients in [101, 71]. Then, boundary stabilization for coupled reaction-diffusion equations, with a spatially varying reaction, was solved in [69], in a relative general way. The generality allowed for subsequent results on the boundary estimation of coupled reaction-diffusion equations, with a spatially varying reaction, in [77], and on the boundary stabilization problem for coupled reaction-advection-diffusion equations with spatial variation in all parameters in [78]. Likewise, the problem of boundary stabilization and output regulation for one-dimensional coupled parabolic PIDEs with spatially varying coefficients and with Dirichlet, Neumann, and Robin boundary conditions was addressed in [102] and in [103], respectively. More recently, stabilization for a pair of coupled diffusion-reaction equations with unknown parameters was studied in [104]. The estimation and stabilization problems are closely related. In the estimation problem, one commonly designs an observer which guarantees some stability property for the origin of the estimation error system. The stability of the estimation error system then implies the convergence of the state estimate
to the unknown state.

Briefly speaking, in the backstepping method, one seeks for an invertible transformation to map a, possibly unstable, PDE to a carefully selected stable target system. The transformation is typically an integral transformation and the main difficulty arises when trying to solve the PDEs verified by the kernels in the integral transformation. In [69, 78] Volterra integral transformation (of second kind) was employed for a system of \( n \) coupled (advection)-reaction-diffusion equations. The kernels in [69, 78] satisfy \( n^2 \) coupled second-order hyperbolic equations in a triangular domain and were solved by deriving an equivalent system of \( 2n^2 \) coupled first-order hyperbolic equations, noticing a resemblance with the kernel equations appearing in the boundary stabilization problem of coupled systems of first-order hyperbolic equations [105, 73]. A similar approach was followed in [77], but making use of a more recent solution of the boundary stabilization problems of coupled systems of first-order hyperbolic equations [72].

9.2.1 Contribution

The contribution of this paper is twofold, we provide a pair of integral transformations to decouple the equation in the estimation error system and device a numerical method to compute the kernel equations.

First, motivated again by advances on the problem of boundary stabilization for coupled first-order hyperbolic equations [106] where a decoupling technique is applied, we propose a new solution to the state estimation problem for coupled reaction-diffusion equations from boundary measurements. We show that a pair of integral transformations allows us to map the estimation error system into a simple stable target system, with uncoupled equations. Previous methods [101, 71, 69, 77, 78, 102, 103] lead to target systems with coupled equations, convoluting the assignment of an exact convergence rate or the formulation of robustness with respect to measurement disturbances [107, 96]. Compared
with [99, 70, 100], the result in this paper is not restricted to systems with equal diffusivity.
The case with equal diffusion coefficients is less involved; in particular, a solution to the
kernel equations can be found following the same method used in the problems with a
single PDE. The result in this paper is not restricted to the problem of state estimation
from boundary measurements. Actually, due to the similarity of the kernel equations in the
problems of boundary stabilization and boundary estimation, this result is also applicable
to problem of boundary stabilization of coupled linear reaction-diffusion PDEs. We derive
and solve the equations for the kernels of each transformation; the first one over a triangular
domain and the second one over a square of unit area. The solutions are constructed by the
method of characteristics; where nontrivial partitions of the domains are required. We show
that for both transformations, the kernel equations are second-order coupled hyperbolic,
with a coupling between some of the kernels at the boundaries.

Second, we provide a simple numerical method to solve the kernel equations. The
numerical scheme is based on polynomial approximations of the kernels; taking into account
the fact that the kernels are piecewise differentiable. The problem of approximating solution
of kernel equations by polynomials was studied previously in [108], where the authors
formulate the approximation problem as an optimization problem.

9.2.2 Outline

The structure of the paper is as follows. In Section 10.3 the estimation problem
is introduced. The main result in presented in Section 9.4. The solution to the kernel
equations is derived in Section 9.5. A numerical scheme to compute the kernels is presented
in Section 9.6; together with an example of the numerical computation 9.7. Finally, we
conclude the paper with some remarks in Section 9.8.
9.3 Problem Statement

9.3.1 Coupled Parabolic Reaction Diffusion Systems

Consider a linear reaction diffusion equation

\[
    u_t(x,t) = \Sigma(x) u_{xx}(x,t) + \Lambda(x) u(x,t),
\]

with coefficients

\[
    \Sigma = \begin{bmatrix}
        \epsilon_1 & 0 & \cdots & 0 \\
        0 & \epsilon_2 & \cdots & 0 \\
        \vdots & \vdots & \ddots & \vdots \\
        0 & 0 & \cdots & \epsilon_n
    \end{bmatrix},
\]

\[
    \Lambda(x) = \begin{bmatrix}
        \lambda_{11}(x) & \lambda_{12}(x) & \cdots & \lambda_{1n}(x) \\
        \lambda_{21}(x) & \lambda_{22}(x) & \cdots & \lambda_{2n}(x) \\
        \vdots & \vdots & \ddots & \vdots \\
        \lambda_{n1}(x) & \lambda_{n2}(x) & \cdots & \lambda_{nn}(x)
    \end{bmatrix}.
\]

for \( x \in (0,1), \ t \in (0,T) \), with \( \lambda_{ij} \in C^1(0,1) \) for all \( i,j \in \{1,2,\ldots,n\} \) and \( \epsilon_i > 0 \), for all \( i \in \{1,2,\ldots,n\} \). The state \( u(x,t) \in \mathbb{R}^n \) is defined as

\[
    u(x,t) = [u_1(x,t), u_2(x,t), \ldots, u_n(x,t)]^T.
\]

The boundary conditions are of Neumann type

\[
    u_x(0,t) = f_0(t),
\]

\[
    u_x(1,t) = f_1(t) + Au(1,t),
\]
and initial conditions \( u_0 \in \mathcal{L}^2(0,1) \), and \( A_1 \in \mathbb{R}^{n \times n} \). The states are ordered so that
\[ \epsilon_n > \cdots > \epsilon_2 > \epsilon_1 > 0 \]
The well-posedness of the system follows from standard results on linear parabolic equations [109, Subsection 7.1.3], [110]. In particular, we consider solutions which, as functions of the spatial variable, belong to the space \( \mathcal{L}^2(0,1) \). Equation (10.105) and boundary conditions (9.5)-(9.6) constitute a dynamic system with state \( u \in C([0,T]; \mathcal{L}^2(0,1)) \), known inputs \( f_0 \in \mathcal{L}^2([0,T]), f_1 \in \mathcal{L}^2([0,T]) \), and output measurement \( y \in \mathcal{L}([0,t]), \) with \( y(t) = u(1,t) \). The estimation problem is to obtain an estimate \( \hat{u} \) of \( u \), from boundary measurements \( f_0, f_1 \) and \( y \). A boundary observer that provides a solution to this problem, with prescribed convergence rate, is provided in the next section.

**Remark 9.3.1.** The diffusion of lithium ions in the porous electrodes of lithium-ion batteries (with multiple active materials) [21], is described by a system of (radial) diffusion equations, i.e., a system with \( \Lambda = 0 \), with a nonlinear coupling at the boundary. Linearization of the boundary coupling results in a boundary condition of the form (9.6), where \( f_1(t) \) is related to the charge (or discharge) current, the matrix \( A \) relates the flux lithium ions in all the materials within the electrode to satisfy a potential equilibrium assumption.

**9.3.2 Observer and Estimation Error Systems**

The proposed state observer is a copy of the reaction-diffusion system (10.105) with boundary conditions (9.5)-(9.6) together with boundary output error feedback

\[
\hat{u}_t(x,t) = \Sigma \hat{u}_{xx}(x,t) + \Lambda(x)\hat{u}(x,t) + P(x)[u(1,t) - \hat{u}(1,t)] \tag{9.7}
\]

for \( x \in (0,1), t \in (0,T] \), with boundary conditions

\[
\hat{u}_x(0,t) = f_0(t), \tag{9.8}
\]

\[
\hat{u}_x(1,t) = f_1(t) + Au(1,t) + Q[u(1,t) - \hat{u}(1,t)], \tag{9.9}
\]
and initial conditions $\tilde{u}_0 \in \mathcal{L}^2(0,1)$. The observer state is $\hat{u} \in C([0,T];\mathcal{L})$ and $u(1,t) - \hat{u}(1,t)$ is the boundary output error. Observer gains $P(x)$ and $Q$ are yet to be chosen. The estimation error system can be found by subtracting (9.7), (9.8) and (9.9) from (10.105), (9.5) and (9.6) respectively, to obtain

$$\tilde{u}_t(x,t) = \Sigma \tilde{u}_{xx}(x,t) + \Lambda(x)\tilde{u}(x,t) - P(x)\tilde{u}(1,t),$$  \hspace{1cm} (9.10)
$$\tilde{u}_x(0,t) = 0,$$  \hspace{1cm} (9.11)
$$\tilde{u}_x(1,t) = -Q\tilde{u}(1,t),$$  \hspace{1cm} (9.12)

where $\tilde{u}(x,t) = u(x,t) - \hat{u}(x,t)$, is the estimation error. The problem is then to find observer gains $P(x)$ and $Q$ that guarantee exponential stability of the estimation error system

$$P(x) = -K(x,1)\Sigma B - K_s(x,1)\Sigma,$$  \hspace{1cm} (9.13)
$$Q = B - K(1,1),$$  \hspace{1cm} (9.14)

where the matrix $K(x,s) \in \mathbb{R}^{n \times n}$ is a solution of the following hyperbolic system of PDEs

$$\Sigma K_{xx} - K_{ss}\Sigma = -KC - \Lambda(x)K,$$  \hspace{1cm} (9.15)

in the domain $\mathcal{T} = \{(x,s): 0 < x < s < 1\}$ with boundary conditions

$$0 = K(x,x)\Sigma - \Sigma K(x,x),$$  \hspace{1cm} (9.16)
$$\Lambda(x) + C = -\Sigma K_x(x,x) - K_s(x,x)\Sigma - \Sigma \frac{d}{dx}[K(x,x)],$$  \hspace{1cm} (9.17)
$$H(s) = K_x(0,s),$$  \hspace{1cm} (9.18)
$$0 = K(0,0),$$  \hspace{1cm} (9.19)
where $B$ and $C$ are, user defined, diagonal matrices

$$B = \begin{bmatrix}
  b_1 & 0 & \cdots & 0 \\
  0 & b_2 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & b_n
\end{bmatrix}, \quad C = \begin{bmatrix}
  c_1 & 0 & \cdots & 0 \\
  0 & c_2 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & c_n
\end{bmatrix}, \quad (9.20)$$

with $b_1, b_2, \ldots, b_n \geq 0$ and $c_1, c_2, \ldots, c_n > 0$. The matrix $H(s)$ in (9.18) is lower triangular

$$H(s) = \begin{bmatrix}
  0 & 0 & \cdots & 0 \\
  h_{21}(s) & \ddots & \cdots & \vdots \\
  \vdots & \ddots & 0 & 0 \\
  h_{n1}(s) & \cdots & h_{n,n-1}(s) & 0
\end{bmatrix}, \quad (9.21)$$

where each non-zero element $h_{ij}(s)$ is defined piecewise

$$h_{ij}(s) = \begin{cases}
  K_{ij}^x(0,s) & \text{for } 0 \leq s \leq 1 - \sqrt{\frac{\epsilon_j}{\epsilon_i}}, \\
  \bar{K}_{ij}^x(0,s) & \text{for } 1 - \sqrt{\frac{\epsilon_j}{\epsilon_i}} \leq s \leq 1,
\end{cases} \quad (9.22)$$

and the matrix $\bar{K}(x,s)$ is a solution of a second hyperbolic system of PDEs

$$\Sigma \bar{K}_{xx} - \bar{K}_{ss} \Sigma = C \bar{K} - \bar{K} C \quad (9.23)$$

defined in the square $\mathcal{S} = \{(x,s) : 0 < x < 1, 0 < s < 1\}$ with boundary conditions

$$\bar{K}_s(x,1) = \bar{K}_s(x,0) = \bar{K}_x(1,s) = \bar{K}(x,0) = 0, \quad (9.24)$$

$$\bar{K}_x(0,s) = H(s). \quad (9.25)$$
The main results in the paper, stated in the next theorem, provides a solution to the estimation problem.

### 9.4 Stability of the Estimation Error System

**Theorem 9.4.1.** The origin of the estimation error system (9.10)-(10.17), with initial condition \( \tilde{u}_0 \in L^2(0,1) \) and observer gains computed from (9.13) and (9.14) is exponentially stable, that is, for any prescribed \( \sigma > 0 \), there exists a positive constant \( \kappa \), such that

\[
\|\tilde{u}(\cdot,t)\|_{L^2} \leq \kappa \exp[-\sigma t],
\]

(9.26)

for all \( t > 0 \).

In the proof of Theorem 9.4.1, the main question is if the kernel PDEs (9.15)–(9.19) and (9.23)–(9.25) do indeed have a solution, as implicitly assumed in the theorem’s statement, The next result answers this question.

**Theorem 9.4.2.** Both systems of kernel equations (9.15)–(9.19) and (9.23)–(9.25) possess a continuous piecewise differentiable solution, \( K(x,s) \) and \( \tilde{K}(x,s) \), in their respective domains of definition, \( T \) and \( S \). In addition, the transformations \( T, \tilde{T} \) defined by

\[
T[f](x) = f(x) - \int_x^1 K(x,s)f(s)ds,
\]

\[
\tilde{T}[f](x) = f(x) - \int_0^1 \tilde{K}(x,s)f(s)ds,
\]

(9.27) \hspace{1cm} (9.28)

are invertible and both, the transformations and their inverses \( T^{-1} \) and \( \tilde{T}^{-1} \), map \( L^2(0,1) \)
functions into $\mathcal{L}^2(0,1)$ functions, verifying

\begin{align*}
  k_1 \| f \|_{\mathcal{L}^2} &\leq \| T[f] \|_{\mathcal{L}^2} \leq k_2 \| f \|_{\mathcal{L}^2}, & (9.29) \\
  k_3 \| f \|_{\mathcal{L}^2} &\leq \| \tilde{T}[f] \|_{\mathcal{L}^2} \leq k_4 \| f \|_{\mathcal{L}^2}. & (9.30)
\end{align*}

for some $k_1,k_2,k_3,k_4 > 0$

The proof of Theorem 9.4.1 is presented in Subsection 9.4.2. The proof of Theorem 9.4.2 is delivered in Section 9.5; in particular, Lemma 9.5.3 and Lemma 9.5.4.

### 9.4.1 Target System

To prove that the choice of $P(x)$ and $Q$ in (9.13) and (9.14) the origin of the estimation error system is exponentially stable two integral transformations are employed. The first transformation defined in (9.37), maps the estimation error system (9.10)-(10.17) to a first target system (9.31)-(9.34). The first transformation is a second-kind Volterra integral transformation, and alone, it will map the estimation error system to a target system with coupled boundary conditions along with set of kernel equations with some arbitrary terms in the boundary conditions [78]. Here, the first target system includes a boundary feedback term $\mathcal{H}: \mathcal{L}^2(0,1) \mapsto \mathbb{R}$, defined precisely such that a second transformation (9.40) exists, which will map the first target system (9.31)-(9.34) to a set of $n$ uncoupled and stable diffusion reaction equations (9.42)-(9.44) and the kernel systems for both transformations include no arbitrary terms. The first target system is

\begin{equation}
  w_t(x,t) = \sum w_{xx}(x,t) - Cw(x,t),
\end{equation}

(9.31)
for \( x \in (0,1), t \in (0,T] \), with target state

\[
w(x,t) = [w_1(x,t), w_2(x,t), \ldots, w_n(x,t)]^T,
\]

and boundary conditions

\[
w_x(0,t) = \mathcal{H}[w](x,t),
\]

\[
w_x(1,t) = -Bw(1,t).
\]

In (9.31), matrices \( B \) and \( C \) are user-defined diagonal matrices. The term \( \mathcal{H} \) in (9.33) is a linear bounded operator acting on the state \( w \) and applied in the boundary as feedback. The operator \( \mathcal{H} \) has the form

\[
\mathcal{H}[w](t) = \int_0^1 H(s)w(s,t)ds.
\]

Matrix \( H(s) \) is lower triangular, defined in (9.21). The transformation \( T : L^2(0,1) \to L^2(0,1) \) that maps the first target system into the estimation error system is defined as

\[
\tilde{u}(x,t) = T[w](x,t),
\]

\[
= w(x,t) - \int_x^1 K(x,s)w(s,t)ds,
\]

where the kernel matrix \( K(x,s) \) is given by

\[
K(x,s) = \begin{bmatrix}
K^{11}(x,s) & K^{12}(x,s) & \ldots & K^{1n}(x,s) \\
K^{21}(x,s) & K^{22}(x,s) & \ldots & K^{2n}(x,s) \\
\vdots & \vdots & \ddots & \vdots \\
K^{n1}(x,s) & K^{n2}(x,s) & \ldots & K^{nn}(x,s)
\end{bmatrix}.
\]
Figure 9.1: Maps between the estimation error systems and the first and second target systems.

The second transformation $\tilde{T} : L^2(0,1) \rightarrow L^2(0,1)$ is

$$v(x,t) = \tilde{T}[w],$$

$$= w(x,t) - \int_0^1 \tilde{K}(x,s)w(s,t)ds,$$

where $\tilde{K}$ is a lower triangular matrix

$$\tilde{K}(x,s) = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
\tilde{K}^{21}(x,s) & \ddots & \ddots & \vdots \\
\vdots & \ddots & 0 & 0 \\
\tilde{K}^{n1}(x,s) & \cdots & \tilde{K}^{n,n-1}(x,s) & 0
\end{bmatrix},$$

which maps the second target system into the first target system. The second target system

$$v_t(x,t) = \Sigma v_{xx}(x,t) - Cv(x,t),$$

with boundary conditions

$$v_x(0,t) = 0, \quad (9.43)$$

$$v_x(1,t) = -Bv(1,t), \quad (9.44)$$

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Now, we prove the stability property needed for the second target system.

**Proposition 9.4.3.** The origin $v \equiv 0$ of the system (9.42) with boundary conditions (9.43), (9.44) and initial conditions $v_0 \in \mathcal{L}^2(0,1)$ is exponentially stable in the $\mathcal{L}^2$ norm.

**Proof.** The stability of the system (9.42)-(9.44), can be verified with the Lyapunov functional

$$V(t) = \frac{1}{2} \int_0^1 v(x,t)^T v(x,t) dx. \quad (9.45)$$

Taking the time derivative of $V(t)$ along the solutions of (9.42) - (9.44), and applying integrations by parts twice lets to

$$\frac{dV}{dt}(t) = -\sum_{i=1}^n \epsilon_i \left( b_i v(1,t)^2 + \int_0^1 \left( \frac{\partial v_i}{\partial x} (x,t) \right)^2 dx \right)$$

$$- \sum_{i=1}^n c_i \int_0^1 v_i(x,t)^2 dx, \quad (9.46)$$

For each $i \in \{1, \ldots, n\}$, Wirtinger’s inequality implies

$$\int_0^1 (v_i(x,t) - v_i(1,t))^2 dx \leq \frac{4}{\pi^2} \int_0^1 \left( \frac{\partial v_i}{\partial x} (x,t) \right)^2 dx, \quad (9.47)$$

Then, using Young’s inequality in the left hand side of (9.47) results in

$$\frac{\gamma}{\gamma+1} \int_0^1 v_i(x,t)^2 dx - \gamma v_i^2(1,t) \leq \frac{4}{\pi^2} \int_0^1 \left( \frac{\partial v_i}{\partial x} (x,t) \right)^2 dx, \quad (9.48)$$

for any $\gamma > 0$. In particular, by choosing $\gamma = 4b_i/\pi^2$, the inequalities in (9.48) become

$$\frac{\pi^2 b_i}{\pi^2 + 4b_i} \int_0^1 v_i(x,t)^2 dx \leq b_i v_i^2(1,t) + \int_0^1 \left( \frac{\partial v_i}{\partial x} (x,t) \right)^2 dx. \quad (9.49)$$
Substituting (9.49) into (9.46) lets to

\[
\frac{dV}{dt}(t) \leq - \sum_{i=1}^{n} \left( \epsilon_{i} \frac{\pi^{2} b_{i}}{\pi^{2} + 4b_{i}} + c_{i} \right) \int_{0}^{1} v_{i}(x,t)^{2} dx,
\]

(9.50)

therefore

\[
\frac{dV}{dt}(t) \leq -2\sigma V(t),
\]

(9.51)

with

\[
\sigma = \min_{i \in \{1, \ldots, n\}} \left\{ \frac{\epsilon_{i} \pi^{2} b_{i}}{\pi^{2} + 4b_{i}} + c_{i} \right\}.
\]

(9.52)

Finally, by comparison principle

\[
\|v(\cdot, t)\|_{L^{2}} \leq \|v_{0}\|_{L^{2}} \exp[-\sigma t].
\]

(9.53)

\[\square\]

\[\square\]

**9.4.2 Proof of Theorem 9.4.1**

*Proof.* Assume for the moment that Theorem 9.4.2 holds and that there is a solution to both kernel systems, (9.15)-(9.19) and (9.23)-(9.25), such that the transformations \( T \) and \( \tilde{T} \) are invertible and both, transformations and their inverses, map \( L^{2}(0,1) \) functions into \( L^{2}(0,1) \) functions. Consider now the second target system in (9.42)-(9.44), with initial conditions \( v_{0}(x) \) given by applying \( \tilde{T}^{-1} \) to the initial condition of the first target system
\( w_0(x) \), that is

\[
\begin{align*}
  v_0(x) &= \hat{T}^{-1}[w_0](x), \\
  &= w_0(x) - \int_0^1 \hat{I}(x,s)w_0(s)ds,
\end{align*}
\]

(9.54) \hspace{1cm} (9.55)

where \( \hat{I}(x,s) \) is the kernel of the inverse transformation. Assume for that \( w_0 \in L^2(0,1) \), thus have \( v_0 \in L^2(0,1) \), and

\[
\|w(\cdot,t)\|_2 \leq \frac{k_3}{k_4} \|w_0\|_2 \exp[-\sigma t].
\]

(9.56)

Consider now the first target system in (9.31)-(9.34), with initial conditions \( w_0(x) \) given by applying \( T^{-1} \) to \( \tilde{u}_0(x) \), that is

\[
\begin{align*}
  w_0(x) &= T^{-1}[\tilde{u}_0](x), \\
  &= \tilde{u}_0(x) - \int_0^1 I(x,s)\tilde{u}_0(s)ds,
\end{align*}
\]

(9.57) \hspace{1cm} (9.58)

where \( \tilde{I}(x,s) \) is the kernel of the inverse transformation. Since \( u_0 \in L^2(0,1) \), we do have \( w_0 \in L^2(0,1) \), and from (9.56), it follows that

\[
\|\tilde{u}(\cdot,t)\|_2 \leq \frac{k_1k_3}{k_2k_4} \|\tilde{u}_0\|_2 \exp[-\sigma t],
\]

(9.59)

and Theorem 9.4.1 is proved. \( \square \)

In the next section, we construct the solution to both kernel systems and verify the invertibility of both transformations. The result is the proof for Theorem 9.4.2.

**Remark 9.4.1.** The well-posedness of the second target system (9.42)-(9.44) follows also from standard results on linear parabolic equations. This, along with the fact that transformations \( T \) and \( \hat{T} \) (and their inverses) map functions in \( L^2(0,1) \) to \( L^2(0,1) \), results
in the well-posedness of observer system (9.7)-(9.9). In particular, we consider solutions \( \hat{u}(x,t) \) which, as functions of the spatial variable, belong to the space \( L^2(0,1) \).

### 9.5 Solution to the Kernel Equations

#### 9.5.1 Kernel Equations for First Transformation

To find the equations that the elements in the kernel matrix \( K(x,s) \) must verify, one take time and space derivatives in (9.37), substitute the estimation error system and target system, and integrate by parts twice. There is a natural classification for the coefficients of \( K(x,s) \) induced by the geometry of the domain and the boundary conditions. This classification consists of three groups: coefficients in the diagonal of the matrix \( K(x,s) \), coefficients in its upper triangular part, and coefficients in its lower triangular part.

The **coefficients in the diagonal** of \( K(x,s) \) satisfy the equation

\[
\epsilon_i K_{xx}^{ii}(x,s) - \epsilon_i K_{ss}^{ii}(x,s) = -\epsilon_i K^{ii}(x,s) - \sum_{l=1}^{n} \lambda_{il}(x) K_{li}^{ii}(x,s),
\]

for \( i \in \{1,2,\ldots,n\} \), with boundary conditions

\[
\frac{d}{dx} \left[ K^{ii}(x,x) \right] = -\frac{c_i + \lambda_{ii}(x)}{2\epsilon_i},
\]

\( K_{x}^{ii}(0,s) = 0 \),

\( K^{ii}(0,0) = 0 \).

The **coefficients in the upper triangular part** of \( K(x,s) \) satisfy the equation

\[
\epsilon_i K_{xx}^{ij}(x,s) - \epsilon_j K_{ss}^{ij}(x,s) = -\epsilon_j K^{ij}(x,s) - \sum_{l=1}^{n} \lambda_{il}(x) K_{lj}^{ij}(x,s),
\]

for \( i \neq j \).
for $i \in \{1, 2, \ldots, n-1\}$ and $i < j$, with boundary conditions

$$K_x^{ij}(x,x) = \frac{\lambda_{ij}(x)}{\epsilon_j - \epsilon_i}, \quad (9.65)$$

$$K_s^{ij}(x,x) = \frac{\lambda_{ij}(x)}{\epsilon_i - \epsilon_j}, \quad (9.66)$$

$$K^{ij}(x,x) = 0, \quad (9.67)$$

$$K^{ij}(0,s) = 0, \quad (9.68)$$

$$K^{ij}(0,0) = 0. \quad (9.69)$$

The coefficients in the lower triangular part of $K(x,s)$ satisfy the equation

$$\epsilon_i K_x^{ij}(x,s) - \epsilon_j K_s^{ij}(x,s) = -c_j K^{ij}(x,s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{lj}(x,s), \quad (9.70)$$

for $i \in \{2, 3, \ldots, n\}$ and $j < i$, with boundary conditions

$$K_x^{ij}(x,x) = \frac{\lambda_{ij}(x)}{\epsilon_j - \epsilon_i}, \quad (9.71)$$

$$K_s^{ij}(x,x) = \frac{\lambda_{ij}(x)}{\epsilon_i - \epsilon_j}, \quad (9.72)$$

$$K^{ij}(x,x) = 0, \quad (9.73)$$

$$K^{ij}(0,s) = h_{ij}(s), \quad (9.74)$$

$$K^{ij}(0,0) = 0. \quad (9.75)$$

### 9.5.2 Well Posedness of Kernel Equations in First Transformation

**Lemma 9.5.1.** Assume each $h_{ij}(s)$ is known, bounded and continuous along the segment $1 - \sqrt[4]{\epsilon_j/\epsilon_i} \leq s \leq 1$. Then, there exists a unique solution $K(x,s)$, satisfying equations

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(9.15) with boundary conditions (9.16)-(9.19). The solution is continuous and piecewise differentiable.

Proof. Define auxiliary variables $L(x,s)$ and $R(x,s)$ as follows

$$L(x,s) = \sqrt{\Sigma}K_x(x,s) - K_s(x,s)\sqrt{\Sigma}, \quad (9.76)$$

$$R(x,s) = \sqrt{\Sigma}K_x(x,s) + K_s(x,s)\sqrt{\Sigma}. \quad (9.77)$$

Then, replacing (9.76) and (9.77) in (9.15) we obtain

$$\sqrt{\Sigma}L_x + L_s\sqrt{\Sigma} = -KC - \Lambda(x)K, \quad (9.78)$$

$$\sqrt{\Sigma}R_x - R_s\sqrt{\Sigma} = -KC - \Lambda(x)K. \quad (9.79)$$

Boundary conditions for (9.78) and (9.79) can be derived by substituting (9.76) and (9.77) in (9.16)-(9.19). The fact that $K(x,s)$ still appears in the right hand side of equations (9.78) and (9.79) is not a problem since $K(x,s)$ can computed from $L(x,s)$ and $R(x,s)$ integrating (9.76) and (9.77) along horizontal lines and using the known values of $K(x,s)$ in the diagonal, that is

$$K_{ij}(x,s) = K_{ij}(s,s) - \frac{1}{2\sqrt{\epsilon_i}} \int_x^s [R_{ij}(z,s) + L_{ij}(z,s)] dz, \quad (9.80)$$

Equations (9.78) and (9.79) are analog to those found in [72, 106]. The classification introduced for the elements of $K(x,s)$ remains unchanged after the change of variables and is useful to construct a solution for (9.78) and (9.79) using the method of characteristics.
The **diagonal coefficients** of $L(x,s)$ and $R(x,s)$ satisfy the equations

\[
\sqrt{\epsilon_i} L^{ii}_x(x,s) + \sqrt{\epsilon_i} L^{ii}_s(x,s) = -c_i K^{ii}(x,s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{ii}(x,s), \tag{9.81}
\]

\[
\sqrt{\epsilon_i} R^{ii}_x(x,s) - \sqrt{\epsilon_i} R^{ii}_s(x,s) = -c_i K^{ii}(x,s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{ii}(x,s), \tag{9.82}
\]

for $i \in \{1,2,\ldots,n\}$, with boundary conditions

\[
L^{ii}(0,s) = -R^{ii}(0,s), \tag{9.83}
\]

\[
R^{ii}(x,x) = -\frac{c_i + \lambda_{ii}(x)}{\sqrt{\epsilon_i}}. \tag{9.84}
\]

Equations (9.81) and (9.82) with boundary conditions (9.83) and (9.84) can be solved using the method of characteristics. That is, writing 9.81 and 9.82 as integral equations along the characteristic lines; straight lines with slope 1 for (9.81) and slope $-1$ for (9.82). The geometry of the problem, that is, the characteristic lines, the boundary and the domain, is shown in Figure 9.2.

The **coefficients of the upper triangular part** of matrices $L(x,s)$ and $R(x,s)$ satisfy the equations

\[
\sqrt{\epsilon_i} L^{ij}_x(x,s) + \sqrt{\epsilon_j} L^{ij}_s(x,s) = -c_j K^{ij}(x,s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{ij}(x,s), \tag{9.85}
\]

\[
\sqrt{\epsilon_i} R^{ij}_x(x,s) - \sqrt{\epsilon_j} R^{ij}_s(x,s) = -c_j K^{ij}(x,s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{ij}(x,s), \tag{9.86}
\]
for \( i \in \{1, 2, \ldots, n-1\} \), and \( i < j \), with boundary conditions

\[
L_{ij}^i(x, x) = \frac{\lambda_{ij}(x)}{\sqrt{\epsilon_j} - \sqrt{\epsilon_i}}, \quad (9.87)
\]

\[
L_{ij}^0(0, s) = -R_{ij}^0(0, s), \quad (9.88)
\]

\[
R_{ij}^i(x, x) = -\frac{\lambda_{ij}(x)}{\sqrt{\epsilon_i} + \sqrt{\epsilon_j}}. \quad (9.89)
\]

Equations (9.85) and (9.86), with boundary conditions (9.87)-(9.89), can be solved using the method of characteristics. That is, writing (9.85) and (9.86) as integral equations along the characteristic lines; straight lines with slope \( \sqrt{\epsilon_j/\epsilon_i} \) for (9.85) and \( -\sqrt{\epsilon_j/\epsilon_i} \) for (9.86). The boundary condition (9.89) provides enough information to solve for \( R_{ij}^i(x, s) \) in the whole domain. However, to solve for \( L_{ij}^i(x, s) \), boundary information from two segments of the boundary is needed. Specifically, to compute \( L_{ij}^i(x, s) \) in the set \( A_{ij}^i = \{(x, s) \in \)
\( \mathcal{T} : \sqrt{\epsilon_j x} \leq \sqrt{\epsilon_i s} \), boundary conditions (9.88), given at the left side of the triangle, are needed. On the other hand, to compute \( L^{ij}(x, s) \) in the set \( \mathcal{A}^{ij}_2 = \{(x, s) \in \mathcal{T} : \sqrt{\epsilon_i s} \leq \sqrt{\epsilon_j x} \} \), boundary conditions (9.87), given at the diagonal of the triangle, are needed. This implies a discontinuity in the function \( L^{ij}(x, s) \) at the line \( \sqrt{\epsilon_i s} = \sqrt{\epsilon_j x} \), but results only in a discontinuity for the first derivatives of the elements \( K^{ij}(x, s) \), as can be seen from the definition (9.76). The geometry of the problem, that is, the characteristic lines, the boundary, and the partition of the domain in sets \( \mathcal{A}^{ij}_1 \) and \( \mathcal{A}^{ij}_2 \), is shown in Figure 9.3.

![Figure 9.3: Domain, boundary and characteristic lines for the upper diagonal coefficients of matrices \( L(x, s) \) and \( R(x, s) \).](image)

The **coefficients in the lower triangular part** of the matrices \( L(x, s) \) and \( R(x, s) \)
satisfy the equations

\[
\sqrt{\epsilon_i} L_{x}^{ij}(x, s) + \sqrt{\epsilon_j} L_{s}^{ij}(x, s) = -c_j K^{ij}(x, s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{lj}(x, s), \quad (9.90)
\]

\[
\sqrt{\epsilon_i} R_{x}^{ij}(x, s) - \sqrt{\epsilon_j} R_{s}^{ij}(x, s) = -c_j K^{ij}(x, s) - \sum_{l=1}^{l=n} \lambda_{il}(x) K^{lj}(x, s), \quad (9.91)
\]

for \( i \in \{2,3,\ldots,n\} \) and \( j < i \), with boundary conditions

\[
L^{ij}(x, x) = \frac{\lambda_{ij}(x)}{\sqrt{\epsilon_j} - \sqrt{\epsilon_i}}, \quad (9.92)
\]

\[
L^{ij}(0, s) = 2\sqrt{\epsilon_i} h_{ij}(s) - R^{ij}(0, s), \quad (9.93)
\]

\[
R^{ij}(x, x) = -\frac{\lambda_{ij}(x)}{\sqrt{\epsilon_i} + \sqrt{\epsilon_j}}, \quad (9.94)
\]

Equations (9.90) and (9.91) with boundary conditions (9.92)-(9.94) can be solved using the method of characteristics. That is, writing (9.90) and (9.91) as integral equations along the characteristic lines. The characteristic lines are straight lines with slope \( \sum \epsilon_j/\epsilon_i \) for (9.90) and \( -\sum \epsilon_j/\epsilon_i \) for (9.91). Boundary condition (9.94) provides enough information to compute \( R^{ij}(x, s) \) in the whole domain. Setting up boundary conditions for the lower triangular coefficients of \( L(x, s) \) is less clear. Boundary conditions have to provide enough information to solve the system in the whole domain and, at the same time, avoid any inconsistency due to overdetermination. For example, in [77], boundary conditions for the lower triangular coefficients of \( L(x, s) \) are given at the left and diagonal sides of the boundary. This results in a system that appears overdetermined, but a term is added to the target system specifically to absorb the redundancy in boundary conditions. The path followed in [78] leads to a system, for the lower triangular coefficients of \( L(x, s) \), with boundary conditions given at the diagonal side of the boundary. This results in a system that appears undetermined, but an arbitrary boundary condition is added to avoid it. Here, boundary conditions (9.92)-(9.93) are given at the diagonal and left
sides of the boundaries; respectively. Boundary conditions (9.92) allow us to compute
$L^{ij}(x,s)$ in the set $B^{ij}_1 = \{(x,s) \in T : \sqrt{\epsilon_i} s + \sqrt{\epsilon_j} \leq \sqrt{\epsilon_j} x + \sqrt{\epsilon_i}\}$. The segment of the
left boundary that coincides with the piece $B^{ij}_1$ is precisely the segment where $h_{ij}(s)$
is defined in terms of $K_x(0,s)$; hence, avoiding inconsistency due to overdetermination.
Boundary conditions (9.93) allow us to compute $L^{ij}(x,s)$ in the remaining set, that is,
$B^{ij}_2 = \{(x,s) \in T : \sqrt{\epsilon_j} x + \sqrt{\epsilon_i} \leq \sqrt{\epsilon_i} s + \sqrt{\epsilon_j}\}$. The segment of the left boundary that
coincides with $B^{ij}_2$ is precisely the segment where $h_{ij}(s)$ is defined in terms of $\bar{K}_x(0,s)$;
hence, providing useful boundary information. Thus, the piecewise definition of $h_{ij}(s)$ in
(9.22) serves the double purpose of avoiding overdetermination and providing boundary
conditions to avoid underdetermination. Again, there is a discontinuity in the function
$L^{ij}(x,s)$ at the line $\sqrt{\epsilon_i} s + \sqrt{\epsilon_j} = \sqrt{\epsilon_j} x + \sqrt{\epsilon_i}$, but results only in a discontinuity for the first
derivatives of the elements $K^{ij}(x,s)$, as can be seen from definition (9.76). The geometry
of the problem, that is, the characteristic lines, the boundary, and the partition of the
domain in sets $B^{ij}_1$ and $B^{ij}_2$, is shown in Figure 9.4.

Using the method of successive approximation, it can be verified that the integral
equations for all the coefficients of $L(x,s)$ and $R(x,s)$ have a unique solution. Equation
(9.80) is used to recover $K(x,s)$ from $L(x,s)$ and $R(x,s)$.

Next, we construct a solution in the system (9.23)-(9.25).

9.5.3 Kernel Equations for Second Transformation

For each coefficient $\bar{K}^{ij}(x,s)$, we divide the domain in $M_{ij} + 1$ polygons ($M_{ij}$ of
which are triangles and 1 quadrilateral), with

$$M_{ij} = 2 \left( \left\lfloor \frac{1}{2} \left( \sqrt{\epsilon_i} - 1 \right) \right\rfloor + 1 \right), \quad (9.95)$$
Figure 9.4: Domain, boundary and characteristic lines for the lower diagonal coefficients of matrices \( L(x,s) \) and \( R(x,s) \).

where \( \lceil \cdot \rceil \) stands for the ceiling function. We denote these polygons \( C^{ij}_{k} \); for \( k \in \{0, 1, \ldots, M_{ij}\} \).

The sets \( C^{ij}_{0} \) and \( C^{ij}_{M_{ij}} \) are triangles defined as

\[
C^{ij}_{0} = \left\{ (x,s) \in S : 0 \leq s \leq \frac{\epsilon_j}{\epsilon_i} x \right\}, \tag{9.96}
\]

\[
C^{ij}_{M_{ij}} = \left\{ (x,s) \in S : 1 + (x - 1) \sqrt{\frac{\epsilon_j}{\epsilon_i}} \leq s \leq 1 \right\}. \tag{9.97}
\]

For \( 0 < k < M_{ij} \), the sets \( C^{ij}_{k} \) are polygons defined as

\[
C^{ij}_{k} := \left\{ (x,s) \in S : s^{ij}_{k}(x) \leq s \leq s^{ij}_{k}(x), \right. \\
\left. s \leq 1 + (x - 1) \sqrt{\frac{\epsilon_j}{\epsilon_i}} \right\}, \tag{9.98}
\]
Figure 9.5: Partition of the domain for the kernel in the second transformation

\[
1 - \sqrt{\frac{\epsilon_j}{\epsilon_i}}
\]

with

\[
s_k^{ij}(x) = \begin{cases} 
(k-1)\sqrt{\frac{\epsilon_j}{\epsilon_i}} + x\sqrt{\frac{\epsilon_j}{\epsilon_i}} & \text{for } k \text{ odd}, \\
{k}\sqrt{\frac{\epsilon_j}{\epsilon_i}} - x\sqrt{\frac{\epsilon_j}{\epsilon_i}} & \text{for } k \text{ even},
\end{cases}
\]

(9.99)

\[
s_k^{ij}(x) = \begin{cases} 
(k+1)\sqrt{\frac{\epsilon_j}{\epsilon_i}} + x\sqrt{\frac{\epsilon_j}{\epsilon_i}} & \text{for } k \text{ odd}, \\
{k}\sqrt{\frac{\epsilon_j}{\epsilon_i}} + x\sqrt{\frac{\epsilon_j}{\epsilon_i}} & \text{for } k \text{ even}.
\end{cases}
\]

(9.100)

Note that \( S = \bigcup_{k=0}^{M_{ij}} C_k \); Figure 9.5 shows this partition. The partition is not arbitrary, but follows naturally from the boundary conditions, the characteristics lines of the equation to solve and the the shape of the domain \( S \) itself. The solution \( \tilde{K}^{ij}(x,s) \), over all the domain \( S \), is defined in a piecewise fashion according to this partition. That is, one has to solve equation (9.23) with boundary conditions (9.24)-(9.25) separately on each set and impose continuity conditions in the boundaries between those sets; sequentially, i.e., starting from
\(C_{ij}^0\) until \(C_{M_{ij}}^{ij}\). In the triangle \(C_{ij}^0\), the element \(\tilde{K}^{ij}(x, s)\) satisfies

\[
\epsilon_i \tilde{K}^{ij}_{xx}(x, s) - \epsilon_j \tilde{K}^{ij}_{ss}(x, s) = [c_i - c_j] \tilde{K}^{ij}(x, s),
\]

with boundary conditions

\[
\tilde{K}^{ij}(x, 0) = \tilde{K}^{ij}_x(x, 0) = \tilde{K}^{ij}(1, s) = 0.
\]

Thus, in the piece \(C_{ij}^0\), the unique solution is simply \(\tilde{K}^{ij}(x, s) = 0\).

For \(k\) odd and \(0 < k < M_{ij}\), the sets \(C_{ij}^k\) are either triangles or a quadrilateral if \(k = M_{ij} - 2\). In these sets the function \(\tilde{K}^{ij}(x, s)\) satisfies the equation

\[
\epsilon_i \tilde{K}^{ij}_{xx}(x, s) - \epsilon_j \tilde{K}^{ij}_{ss}(x, s) = [c_i - c_j] \tilde{K}^{ij}(x, s),
\]

with a boundary condition

\[
\tilde{K}^{ij}_x(0, s) = h_{ij}(s).
\]

In addition, the continuity requirement at the intersection between \(C_{ij}^k\) and \(C_{ij}^{k-1}\) implies that \(\tilde{K}^{ij}(x, s)\) is given along the segment defined by \(\tilde{K}^{ij}_x(x)\); assuming a unique solution has been found in the previous piece \(C_{ij}^{k-1}\).

For \(k\) even and \(0 < k < M_{ij}\), the sets \(C_{ij}^k\) are all triangles, and in these sets the function \(K^{ij}(x, s)\) satisfies the equation

\[
\epsilon_i K^{ij}_{xx}(x, s) - \epsilon_j K^{ij}_{ss}(x, s) = [c_i - c_j] K^{ij}(x, s),
\]

and a boundary condition

\[
K^{ij}_x(0, s) = 0.
\]
In addition, the continuity requirement at the intersection between $C^k_{ij}$ and $C^k_{ij-1}$ implies that $\tilde{K}^{ij}(x,s)$ is given along the segment defined by $s^k_{ij}(x)$; assuming a unique solution has been found in the previous piece $C^k_{ij-1}$.

Finally, in the triangle $C^M_{ij}$ the function $\tilde{K}^{ij}(x,s)$ satisfies

$$\epsilon_i \tilde{K}^{ij}_{xx}(x,s) - \epsilon_j \tilde{K}^{ij}_{ss}(x,s) = [c_i - c_j] \tilde{K}^{ij}(x,s),$$

(9.107)

with the boundary condition

$$\tilde{K}^{ij}_s(x,1) = 0.$$  

(9.108)

In addition, the continuity requirement at the intersections between $C^M_{ij}$ and $C^M_{ij-1}$ and between $C^M_{ij}$ and $C^M_{ij-2}$ implies that $\tilde{K}^{ij}(x,s)$ is given along the segment defined by $s = 1 + (x-1)\sqrt{\frac{\epsilon_j}{\epsilon_i}}$, from the assumption that a unique solution has been found in the previous set $C^M_{ij-1}$.

Note that finding the solution $\tilde{K}(x,s)$ at $C_M_{ij}$ completes the piecewise definition of $H(s)$, i.e.

$$h_{ij}(s) = \begin{cases} K^M_{ij}(0,s) & \text{for } 0 \leq s \leq 1 - \sqrt{\frac{\epsilon_j}{\epsilon_i}}, \\ \tilde{K}^{ij}_x(0,s) & \text{for } 1 - \sqrt{\frac{\epsilon_j}{\epsilon_i}} \leq s \leq 1. \end{cases}$$

(9.109)

Therefore, the boundary condition used to solve system (9.15)-(9.19) is not longer arbitrary.

### 9.5.4 Well Posedness of Kernel Equations in Second Transformation

**Lemma 9.5.2.** If each $h_{ij}(0,s)$ is bounded and continuous on the segment $0 \leq s \leq 1 - \sqrt{\epsilon_j/\epsilon_i}$. Then, there exists a unique solution $\tilde{K}^{ij}(x,s)$ satisfying equations (9.23) and
boundary conditions (9.24)–(9.25). The solution is defined piecewise and is continuous over all the domain.

Proof. Since the unique solution at $C_{ij0}^k$ is $\tilde{K}^{ij}(x,s) = 0$, to find a (continuous) solution in the whole domain, it is sufficient to proof that a unique solution can be found at $C_{ijk}^k$ given a solution in all previous sets $C_{ijk}^{k-1}, C_{ijk}^{k-2}, \ldots, C_{ij0}^k$.

Define again auxiliary variables $\tilde{L}(x,s)$ and $\tilde{R}(x,s)$ as follows

\begin{align}
\tilde{L}(x,s) &= \sqrt{\Sigma} \tilde{K}_x(x,s) - \tilde{K}_s(x,s) \sqrt{\Sigma}, \\
\tilde{R}(x,s) &= \sqrt{\Sigma} \tilde{K}_x(x,s) + \tilde{K}_s(x,s) \sqrt{\Sigma}.
\end{align}

(9.110) (9.111)

In the case $k$ is odd and $0 < k < M_{ij}$, the functions $\tilde{L}^{ij}(x,s)$ and $\tilde{R}^{ij}(x,s)$ satisfy the first order equations

\begin{align}
\sqrt{\epsilon_i} \tilde{L}^{ij}_x(x,s) + \sqrt{\epsilon_j} \tilde{L}^{ij}_s(x,s) &= [c_i - c_j] \tilde{K}^{ij}(x,s) \\
\sqrt{\epsilon_i} \tilde{R}^{ij}_x(x,s) - \sqrt{\epsilon_j} \tilde{R}^{ij}_s(x,s) &= [c_i - c_j] \tilde{K}^{ij}(x,s)
\end{align}

(9.112) (9.113)

with boundary conditions

\begin{align}
\tilde{L}^{ij}(0,s) &= 2\sqrt{\epsilon_i} h(s) - \tilde{R}^{ij}(0,s), \\
\tilde{R}^{ij}(x,s_k^{ij}(x)) &= \sqrt{\epsilon_i} \tilde{K}^{ij}_x \left( x, s_k^{ij}(x) \right) + \sqrt{\epsilon_j} \tilde{K}^{ij}_s \left( x, s_k^{ij}(x) \right).
\end{align}

(9.114) (9.115)

The fact that there is a shared boundary between $C_{ij}^k$ and $C_{ij}^{k-1}$, i.e. $s_k^{ij}(x) = s_{k-1}^{ij}(x)$, and the assumption that $\tilde{K}^{ij}(x,s)$ is known at $C_{ij}^{k-1}$, imply that the right hand side of (9.115) is known and bounded. Equations (9.112) and (9.113) with boundary conditions (9.114) and (9.115) can be solved using the method of characteristics. That is, writing (9.112) and (9.113) as integral equations along the characteristic lines. The characteristic lines are
straight lines with slope $\sqrt{\epsilon_j/\epsilon_i}$ for (9.112) and $-\sqrt{\epsilon_j/\epsilon_i}$ for (9.113). The geometry of the problem, that is, the characteristic lines, the boundary, and the domain $C^{ij}_k$ (for $k$ odd and $0 < k < M_{ij}$) is depicted in Figure 9.6.

In the case $k$ is even and $0 < k < M_{ij}$, functions $\tilde{L}^{ij}(x,s)$ and $\tilde{R}^{ij}(x,s)$ satisfy the same first-order hyperbolic equations

\[
\sqrt{\epsilon_i}\tilde{L}^{ij}_x(x,s) + \sqrt{\epsilon_j}\tilde{L}^{ij}_s(x,s) = [c_i - c_j]\tilde{K}^{ij}(x,s) \tag{9.116}
\]

\[
\sqrt{\epsilon_i}\tilde{R}^{ij}_x(x,s) - \sqrt{\epsilon_j}\tilde{R}^{ij}_s(x,s) = [c_i - c_j]\tilde{K}^{ij}(x,s) \tag{9.117}
\]

with boundary conditions

\[
\tilde{L}^{ij}(x,\tilde{s}^{ij}_k(x)) = \sqrt{\epsilon_i}\tilde{K}^{ij}_x(x,\tilde{s}^{ij}_k(x)) - \sqrt{\epsilon_j}\tilde{K}^{ij}_s(x,\tilde{s}^{ij}_k(x)), \tag{9.118}
\]

\[
\tilde{R}^{ij}(1,s) = -\tilde{L}^{ij}(1,s). \tag{9.119}
\]

The fact that there is a shared boundary between $C^{ij}_k$ and $C^{ij}_{k-1}$, i.e. $\tilde{s}^{ij}_k(x) = \tilde{s}^{ij}_{k-1}(x)$, and the assumption that $\tilde{K}^{ij}(x,s)$ is known at $C^{ij}_{k-1}$, imply that the right hand side of (9.118) is known and bounded. Equations (9.116) and (9.117) with boundary conditions (9.118) and (9.119) can be solved using the method of characteristics. That is, writing (9.116) and (9.117) as integral equations along the characteristic lines. The characteristic lines are straight lines with slope $\sqrt{\epsilon_j/\epsilon_i}$ for (9.116) and $-\sqrt{\epsilon_j/\epsilon_i}$ for (9.117). The geometry of the problem, that is, the characteristic lines, the boundary, and the domain $C^{ij}_k$ (for $k$ even and $0 < k < M_{ij}$) is depicted in Figure 9.7.

Finally, for $k = M_{ij}$, functions $\tilde{L}^{ij}(x,s)$ and $\tilde{R}^{ij}(x,s)$ satisfy the same first-order hyperbolic
equations
\[
\sqrt{\epsilon_i} \tilde{L}^{ij}_{x}(x,s) + \sqrt{\epsilon_j} \tilde{L}^{ij}_{s}(x,s) = [c_i - c_j] \tilde{K}^{ij}(x,s) \tag{9.120}
\]
\[
\sqrt{\epsilon_i} \tilde{R}^{ij}_{x}(x,s) - \sqrt{\epsilon_j} \tilde{R}^{ij}_{s}(x,s) = [c_i - c_j] \tilde{K}^{ij}(x,s) \tag{9.121}
\]
and boundary conditions
\[
\tilde{L}^{ij}(x,1) = \tilde{R}^{ij}(x,1), \tag{9.122}
\]
\[
\tilde{R}^{ij} \left( x, 1 + (x - 1) \sqrt{\frac{\epsilon_j}{\epsilon_i}} \right) = \sqrt{\epsilon_i} \tilde{R}^{ij}_{x} \left( x, 1 + (x - 1) \sqrt{\frac{\epsilon_j}{\epsilon_i}} \right) + \sqrt{\epsilon_j} \tilde{R}^{ij}_{s} \left( x, 1 + (x - 1) \sqrt{\frac{\epsilon_j}{\epsilon_i}} \right). \tag{9.123}
\]

In this case, \( C_{M_{ij}}^{ij} \) shares a boundary with two previous sets: \( C_{M_{ij} - 1}^{ij} \) and \( C_{M_{ij} - 2}^{ij} \). The assumption that \( \tilde{K}^{ij}(x,s) \) is known at \( C_{M_{ij} - 1}^{ij} \) and \( C_{M_{ij} - 2}^{ij} \), imply that the right hand side of (9.122) is known and bounded. Equations (9.120) and (9.121) with boundary conditions (9.122) and (9.123) can be solved using the method of characteristics. The characteristic lines are straight lines with slope \( \sqrt{\epsilon_j/\epsilon_i} \) for equation (9.120) and \( -\sqrt{\epsilon_j/\epsilon_i} \) for equation (9.121). The geometry of the problem, that is, the characteristic lines, the boundary, and the domain \( C_{M_{ij}}^{ij} \) is depicted in Figure 9.8.

The fact that \( \tilde{K}^{ij}(x,s) \) appears in the right hand side of the equations is not a problem, since for \( 0 < k < M_{ij} \)

\[
\tilde{K}^{ij}(x,s) = \bar{K}^{ij}(x,\tilde{x}_k^{ij}(x)) + \frac{1}{2 \sqrt{\epsilon_j}} \int_{\tilde{x}_k^{ij}(x)}^{s} \left[ \bar{R}^{ij}(x,\xi) + \tilde{L}^{ij}(x,\xi) \right] d\xi, \quad \text{for } (x,s) \in A_i^{ij} \tag{9.124}
\]
and for $k = M_{ij}$

$$
\tilde{K}^{ij}(x, s) = \tilde{K}^{ij} \left( x, 1 + (x-1) \frac{\sqrt{\epsilon_j}}{\epsilon_i} \right) + \frac{1}{2 \sqrt{\epsilon_j}} \int_{1+(x-1)}^{x} \sqrt{\epsilon_i} \left[ \tilde{R}^{ij}(x, \xi) + \tilde{L}^{ij}(x, \xi) \right] d\xi,
$$

(9.125)

for $(x, s) \in A_{M_{ij}}^{ij}$

(9.126)

Using the method of successive approximations, it can be verified that the integral equations derived from the method of characteristics have a unique solution. Equations (9.124) and (9.126) are used to recover $\tilde{K}(x, s)$ from the solutions $\tilde{L}(x, s)$ and $\tilde{R}(x, s)$.

Lemma 9.5.3. There is a unique solution $K(x, s)$, $\tilde{K}(x, s)$ to the equations (9.15) and (9.23) with boundary conditions (9.16)-(9.19) and (9.24)-(9.25). The solution is defined piecewise and is continuous over all the domain.

Proof. Note that the $n$ elements in a given column $j \in \{1, 2, \ldots, n\}$ of $K(x, s)$ together with the $j - 1$ non-zero elements in the same column $j$ of $\tilde{K}(x, s)$ form a system that is independent of all other elements in both matrices. Thus, the problem can be solved in a column-wise fashion. In particular, for the last column, all elements of $\tilde{K}(x, s)$ are zero and
Figure 9.7: Polygon $\mathcal{C}_k^{ij}$ for $k$ even

Figure 9.8: Polygon $\mathcal{C}_{M_{ij}}^{ij}$. Note that solving $\tilde{K}^{ij}$ in section $\mathcal{C}_{M_{ij}}^{ij}$ provides the value of $h_{ij}(s)$ along the segment.
the elements $K^{i,n}(x,s)$ for $i \in \{1,2,\ldots,n\}$ can be solved following Lemma 9.5.1 without the need to solve for $\tilde{K}(x,s)$. For any other column $j \in \{1,2,\ldots,n-1\}$, the problem can be solve sequentially as follows. For a fix column $j^* \in \{1,2,\ldots,n-1\}$, all elements $K^{i,j^*}(x,s), i \in \{1,2,\ldots,n\}$ can be found in the subset $B_{1}^{n,j^*}$ (see Figure 9.4), without need to solve for any element in $\tilde{K}^{i,j^*}(x,s)$, following to Lemma 9.5.1. In particular, the solution $K^{n,j^*}$, restricted to the subset $B_{1}^{n,j^*}$, provides the boundary conditions needed to solve for $\tilde{K}^{n,j^*}(x,s)$, its whole domain of definition $S$, following Lemma 9.5.2. Since $\tilde{K}^{n,j^*}(x,s)$ is available, one can solve for all elements $K^{i,j^*}(x,s), i \in \{1,2,\ldots,n\}$ in the subset $B_{1}^{n-1,j^*}$, following Lemma 9.5.1. In particular, the solution $\tilde{K}^{n,j^*}$ restricted to the subset $B_{1}^{n-1,j^*}$ provides all information needed to solve for $\tilde{K}^{n-1,j^*}(x,s)$ its whole domain of definition $S$, following Lemma 9.5.2. Note that $B_{1}^{n,j^*} \subset B_{1}^{n-1,j^*} \subset \ldots \subset B_{1}^{1,j^*}$. The procedure is repeated until the solution is found for all non zero terms $\tilde{K}^{i,j^*}(x,s), i \in \{1,2,\ldots,j^*-1\}$ in $S$. Finally, the solution $\tilde{K}^{i,j^*}(x,s), i \in \{1,2,\ldots,j^*-1\}$ in $S$, provides all the boundary conditions needed to compute $K^{i,j^*}(x,s), i \in \{1,2,\ldots,n\}$ in $T$.

### 9.5.5 Inversion of the Transformations

**Lemma 9.5.4.** There exists an integral transformation, mapping the function $w$ to $v$, i.e. an inverse transformation of $\tilde{T}$, in the form

$$v(x,t) = \tilde{T}^{-1}[w], \quad (9.127)$$

$$= w(x,t) + \int_{0}^{1} \tilde{I}(x,s)w(s,t)ds, \quad (9.128)$$

**Proof.** The structure of $\tilde{K}(x,s)$ implies the invertibility of transformation $\tilde{T}$. This is verified with an induction argument by noticing that

$$v_{1}(x,t) = w_{1}(x,t), \quad (9.129)$$
and
\[ v_i(x,t) = w_i(x,t) + \sum_{l=1}^{i-1} \int_0^1 \tilde{K}^{il}(x,s) w_i(s,t) ds. \]  
(9.130)

for \( i \in \{2, \ldots, n\} \). The inverse has, in fact, the same structure as the direct transformation, that is

\[ v(x,t) = \tilde{T}^{-1}[w], \]
\[ = w(x,t) + \int_0^1 \tilde{I}(x,s) w(s,t) ds, \]
(9.132)

where \( \tilde{I}(x,s) \) is lower triangular,

\[ \tilde{I}(x,s) = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
\tilde{I}^{21}(x,s) & \ddots & \ddots & \vdots \\
\vdots & \ddots & 0 & 0 \\
\tilde{I}^{n1}(x,s) & \cdots & \tilde{I}^{n,n-1}(x,s) & 0 
\end{bmatrix}, \]
(9.133)

where each \( \tilde{I}^{ij}(x,s) \) is simply computed from \( \tilde{K}^{ij}(x,s) \).

\[ \Box \]

### 9.6 A Numerical Method to Compute Kernels

The numerical approximation of the kernels is based on a piecewise polynomial approximation that captures the piecewise differential nature of the kernels. For the approximation of coefficients in \( K(x,s) \), the domain is divided according to the intersection of the sets \( A_{ij}^1, A_{ij}^2, B_{1j}^i \) and \( B_{2j}^i \), defined in Section 9.5 (Figures 9.3 and 9.4) corresponding to all the coefficients within the same column; due to the column-wise coupling in equations (9.60), (9.64) and (9.70). For the approximation of coefficients in \( \tilde{K}(x,s) \), the domain is divided according to the sets \( C_{k}^{ij} \) defined in Section 9.5 (Figure 9.5), with an additional
partition of the set \( C_{M_{ij}}^{ij} \). The extra partition is required since the boundary conditions at the diagonal side of \( C_{M_{ij}}^{ij} \) have a discontinuity, due to the fact that the diagonal side of \( C_{M_{ij}}^{ij} \) coincides with two other sets, \( C_{M_{ij}-1}^{ij} \) and \( C_{M_{ij}-2}^{ij} \); see Figure 9.9. For each coefficient in \( K(x,s) \) or \( \tilde{K}(x,s) \), an index \( p \in \{1,\ldots,p_{\max}\} \) is employed to indicate the polynomial approximation in a particular piece the domain \( T \) or \( S \). The numbers of pieces \( p_{\max} \) is not the same for all coefficients. For the coefficient \( \tilde{K}_{ij}^{ij}(x,s) \), the number of pieces in the partition of \( S \) is

\[
p_{\max}^{ij} = \begin{cases} 
M_{ij} + 2 & \text{if } \left[ \frac{1}{2} \left( \sqrt{\epsilon_i/\epsilon_j} - 1 \right) \right] > 1/2 \sqrt{\epsilon_i/\epsilon_j}, \\
M_{ij} + 1 & \text{if } \left[ \frac{1}{2} \left( \sqrt{\epsilon_i/\epsilon_j} - 1 \right) \right] < 1/2 \sqrt{\epsilon_i/\epsilon_j}, \\
M_{ij} & \text{if } \left[ \frac{1}{2} \left( \sqrt{\epsilon_i/\epsilon_j} - 1 \right) \right] = 1/2 \sqrt{\epsilon_i/\epsilon_j},
\end{cases}
\]

with \( M_{ij} \) defined in (9.95). For the coefficients in \( K(x,s) \), the numbers of pieces is the same for all the elements within the same column, but the column-wise intersection of the sets defined in Section 9.5 is rather complicated for large values of \( n \). For a particular example of the partition of \( T \), with \( n = 3 \), see Figures 9.10, 9.11 and 9.12.
Figure 9.9: The triangle $C_{M_{ij}}^{ij}$ shares the diagonal side with two other polygons. This implies that the boundary data for $\hat{K}^{ij}(x,s)$ is discontinuous. The discontinuity is represented in the diagrams in blue and red color. The discontinuity force us to further divide the domain $C$ in two or three pieces.
Figure 9.10: Partition of the domain $\mathcal{T}$ for the piecewise polynomial approximation of the coefficients in the first column of $K(x,s)$; for a particular example with $n = 3$. The partition is the intersection of the sets defined in Section 9.5 corresponding to all coefficients in the first column, together with the extra partition induced from the additional discontinuity in functions $h_{21}(s)$ and $h_{31}(s)$ on the segments $(1 - \sqrt{\epsilon_1/\epsilon_2}, 1)$ and $(1 - \sqrt{\epsilon_1/\epsilon_3}, 1)$. 
Figure 9.11: Partition of the domain $\mathcal{T}$ for the piecewise polynomial approximation of the coefficients in the second column of $K(x,s)$; for a particular example with $n = 3$. The partition is the intersection of the sets defined in Section 9.5 corresponding to all coefficients in the second column, together with the extra partition induced from the additional discontinuity in $h_{32}(s)$ on the segment $(1 - \sqrt{\epsilon_2/\epsilon_3}, 1)$.  

\[ [K^{12}, K^{22}, K^{32}]^T \]
Figure 9.12: Partition of the domain $\mathcal{T}$ for the piecewise polynomial approximation of the coefficients in the third column of $K(x,s)$; for a particular example with $n = 3$. The partition is the intersection of the sets defined in Section 9.5 corresponding to all coefficients in the third column.
For each piece $p \in \{1, \ldots, p_{\text{max}}\}$, the $m$-th order triangular polynomial approximation of $K_{ij}(x,y)$ and $\tilde{K}_{ij}(x,y)$ has the form

$$p_K_{ij}^m(x,s) = \sum_{a=0}^{m} \sum_{b=0}^{m-a} p_{d_{ab}}^{ij} x^a s^b,$$

$$p_{\tilde{K}}_{ij}^m(x,s) = \sum_{a=0}^{m} \sum_{b=0}^{m-a} p_{\tilde{d}_{ab}}^{ij} x^a s^b,$$

where the values of coefficients $p_{d_{ab}}^{ij}, p_{\tilde{d}_{ab}}^{ij} \in \mathbb{R}$, are found from equations and boundary or continuity conditions. For the numerical approximation it is convenient to use the second-order hyperbolic equations (9.60), (9.64), (9.70), and (9.101), rather than the first-order equivalent equations (9.81), (9.82), (9.85), (9.86), (9.90), (9.91), (9.112) and (9.113).

**Remark 9.6.1.** To approximate the kernels by polynomials of $m$-th order, we need to assume $\lambda_{ij}(x) \in C^m(0,1)$; in particular,

9.6.1 Algebraic System of Equations for Coefficients in the Polynomial Approximation

For each piece $p$, there are $(m+1)(m+2)/2$ unknown constants in the polynomial approximation of each kernel function $K_{ij}(x,s)$. Thus, for each piece $p$, there is a total of $n(m+1)(m+2)/2$ unknown constants, corresponding to all the kernels in a given column of the matrix $K(x,s)$; whose values have to be determined. For this purpose, define $pD^j$ as the column vector of dimension $n(m+1)(m+2)/2$ whose elements are the coefficients $p_{d_{ab}}^{ij}$ of the polynomial approximations of all the kernels in a given column $j \in \{1, \ldots, n\}$ and a given piece of the domain $p \in \{1, \ldots, p_{\text{max}}\}$, arranged in some particular order, for example

$$pD^j = \begin{bmatrix} p_{d_{00}^{1j}}, p_{d_{10}^{1j}}, p_{d_{01}^{1j}}, \ldots, p_{d_{0m}^{1j}}, \ldots, p_{d_{0m}^{nj}} \end{bmatrix}^T.$$
The problem of approximating $K(x,s)$ with a triangular polynomial of order $m$ is now the problem of finding the values of $pD^j$; for all the columns $j \in \{1,\ldots,n\}$ in $K(x,s)$ and for all pieces $p \in \{1,\ldots,p^{\text{max}}\}$ of the domain. Each second order hyperbolic equation in (9.60), (9.64) or (9.70) provides $(m-1)m/2$ algebraic equations. To see this, note that the differential operation in the left-hand side of the equations, applied to the polynomial approximation of order $m$, leads to a $(m-2)$-th order polynomial, that is

$$
\epsilon_i \frac{\partial^2 pK^i_{m}}{\partial x^2}(x,s) - \epsilon_j \frac{\partial^2 pK^j_{m}}{\partial s^2}(x,s) = \sum_{a=0}^{m-2} \sum_{b=0}^{m-2-a} \left( \epsilon_i(a+2)(a+1)p^{d^i_{a+2,b}} - \epsilon_j(b+2)(b+1)p^{d^j_{a,b+2}} \right)x^a s^b. \tag{9.138}
$$

The algebraic operation in the right hand side of the equations in (9.60), (9.64) and (9.70), applied to a $(m-2)$-th order polynomial approximation of the kernels, results in a second $(m-2)$-th order polynomial

$$
c_{jp}K_{m-2}^i(x,s) - \sum_{l=1}^{n} \lambda^{ij}_{l}(x)K_{m-2}^l(x,s) = \sum_{a=0}^{m-2} \sum_{b=0}^{m-2-a} \left( c_{jp}d^i_{a,b} - \sum_{l=1}^{n} \sum_{r=0}^{a} \lambda^{il}_{r}p^{d^j_{a-r,b}} \right)x^a s^b, \tag{9.139}
$$

where $p^{\lambda^i_{rj}} \in \mathbb{R}$ are the coefficients of some $m$-th order polynomial approximation of $\lambda^{ij}(x)$; around some point $x_0$ in the piece $p$. Since equations in (9.60), (9.64) and (9.70) hold for all points $(x,s)$ in the domain, the coefficients of each power $x^a s^b$ have to coincide for both polynomials in (9.138) and (9.139). Thus, for all $a+b \leq m-2$, and for all $i \in \{1,2,\ldots,n\}$,

$$
\epsilon_i(a+2)(a+1)p^{d^i_{a+2,b}} - \epsilon_j(b+2)(b+1)p^{d^j_{a,b+2}} - c_{jp}d^i_{a,b} - \sum_{l=1}^{n} \sum_{r=0}^{a} \lambda^{il}_{r}p^{d^j_{a-r,b}} = 0. \tag{9.140}
$$

These are $n(m-1)m/2$ linear algebraic equations which can be arrange in a $nm(m-1)/2$ by $n(m+2)(m+1)/2$ matrix $pM^j_{\text{PDE}}$; following the order chosen for $pD^j$. Note that $n(2m+1)$
more equations are needed to equate the number of equations and unknowns; these will be provided by boundary and continuity conditions. Since continuity conditions are actually boundary conditions at the boundaries between pieces, there is no need to distinguish between both in the polynomial approximation. Continuity of a kernel function is a Dirichlet-type condition, and continuity of a derivative of a kernel function is a Neumann-type boundary condition. Dirichlet-type conditions provide \( m + 1 \) algebraic equations while Neumann-type conditions provide \( m \) algebraic equations. For example, a Neumann-type condition at \( x = 0 \), that is \( \partial_x pK^{ij}(0,s) = p\alpha^{ij}(s) \), for \( s \in (0,1) \), applied to the \( m \)-th order polynomial approximation \( pK_m^{ij}(x,s) \) is

\[
\sum_{b=0}^{m-1} a_p d_{1b}^i s^b = \sum_{b=0}^{m-1} p\alpha^{ij}_b s^b,
\tag{9.141}
\]

where \( p\alpha^{ij}_b \) are the coefficients of some \((m-1)\)-th order polynomial approximation of \( p\alpha^{ij}(s) \); around a point \( s_0 \) in the piece \( p \). Equation (9.141) is true for all values \( s \in (0,1) \), therefore

\[
a_p d_{1b}^i = p\alpha^{ij}_b \text{ for all } b \in \{0, \ldots, m-1\}. \tag{9.142}
\]

On the other hand, a Dirichlet-type condition at some line of the form \( s = m_{slp}x \), that is \( pK^{ij}(x,m_{slp}x) = p\beta^{ij}(x) \), for \( x \in (0,1) \), applied to the \( m \)-th order polynomial approximation of \( pK_m^{ij}(x,s) \), is

\[
\sum_{r=0}^{m} \left( \sum_{r=a+b} m_{slp}^b d_{ab}^j \right) x^r = \sum_{r=0}^{m} p\beta^{ij}_r x^r,
\tag{9.143}
\]
where \(p^{\beta_{ij}}_r\) are the coefficients of some polynomial approximation of \(\beta_{ij}(x)\); around some point \(x_0\) in the piece \(p\). Equation (9.143) holds for all values of \(x \in (0, 1)\), therefore

\[
\sum_{r=a+b}^m m_{slp}^b p^{\beta_{ij}}_r = p^{\beta_{ij}}_r \text{ for all } r \in \{0, \ldots, m\}.
\] (9.144)

Together, one Neumann-type and one Dirichlet-type conditions provide \(2m+1\) algebraic equations of the form (9.142) or (9.144). It is then possible to arrange the \(2m+1\) equations for each of the \(n\) kernels in a given column \(j \in \{1, \ldots, n\}\) of \(K(x,s)\), for particular piece \(p \in \{1, \ldots, p^{\text{max}}\}\) of the domain, in a matrix \(pM^j_{BC}\) of dimensions \(n(2m+1) \times n(m+2)(m+1)/2\). Thus a system of algebraic equations for \(pD^j\) is obtained

\[
\begin{bmatrix}
pM^j_{PDE} \\
pM^j_{BC}
\end{bmatrix}
pD^j =
\begin{bmatrix}
0 \\
p\alpha^j \\
p\beta^j
\end{bmatrix},
\] (9.145)

where \(p\alpha^j\) and \(p\beta^j\) are column vectors with elements \(p\alpha^j_b\) for \(b \in \{0, \ldots, m-1\}\), \(i \in \{1, \ldots, n\}\) and \(p\beta^j_r\) for \(r \in \{0, \ldots, m\}\), \(i \in \{1, \ldots, n\}\). Note that continuity conditions enforce a particular order. That is, functions \(p\alpha^j\) and \(p\beta^j\) might actually correspond to a polynomial approximation of \(K_{ij}(x,s)\) in an contiguous piece of the domain. Thus, one can either solve the approximation problem sequentially, following this order, or simultaneously for all coefficients in the problem (including those for \(K(x,s)\)). The construction of a polynomial approximation for \(K(x,s)\) follows the same approach. In this case, equations are not coupled and therefore, a matrix \(pM^j_{PDE}\) can be derived for the unknown constants \(p\tilde{d}^j_{ab}\) of a single coefficient of the matrix \(\tilde{K}(x,s)\).

**Remark 9.6.2.** The approximation of \(K(x,s)\) and \(\tilde{K}(x,s)\) by polynomials of \(m\)-th order, requires \(\lambda_{ij}(x) \in C^m(0,1)\); in particular, equations (9.139). This requirement is related to the smoothness of the solutions to the kernel equations. Indeed, following the steps in
[105, Theorem A.1], the property $\lambda_{ij}(x) \in C^m(0,1)$ results in solutions $K(x,s)$ and $\tilde{K}(x,s)$, which are piecewise $C^m(T)$ and $C^m(S)$, respectively.

9.7 Example

9.7.1 Kernel Functions

For a pair of coupled reaction-diffusion equation, a total of five kernel functions have to be computed, that is

$$K(x,s) = \begin{bmatrix} K^{11}(x,s) & K^{12}(x,s) \\ K^{21}(x,s) & K^{22}(x,s) \end{bmatrix},$$

$$\tilde{K}(x,s) = \begin{bmatrix} 0 & 0 \\ \tilde{K}^{21}(x,s) & 0 \end{bmatrix},$$

Figures 9.14 to 9.17 show plots of the piecewise polynomial approximation of the four elements in the kernel matrix $K(x,s)$. Similarly, Figure 9.13 shows a plot of the polynomial approximation of the non-zero element in the kernel matrix $\tilde{K}(x,s)$. The order of polynomial approximation is $m = 10$, and the parameters in the problem are the following

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix}, \ A(x) = \begin{bmatrix} 1 & x \\ x & 1 \end{bmatrix}, \ C = \begin{bmatrix} 5 & 0 \\ 0 & 11 \end{bmatrix}.$$
Figure 9.13: Piecewise polynomial approximation of the kernel $K^{21}(x,s)$.

Figure 9.14: Piecewise polynomial approximation of the kernel $K^{11}(x,s)$. 
Figure 9.15: Piecewise polynomial approximation of the kernel $K^{21}(x, s)$.

Figure 9.16: Piecewise polynomial approximation of the kernel $K^{12}(x, s)$. 
Figure 9.17: Piecewise polynomial approximation of the kernel $K^{22}(x, s)$

Figure 9.18: Evolution of the second state $u_2(x, t)$. 
Figure 9.19: Estimation error $\tilde{u}_2(x,t)$ for the second state.

Figure 9.20: Evolution of the norm of the state $u(x,t) = [u_1(x,t), u_2(x,t)]$. The norm grows unbounded because the equilibrium $u(x,t) = 0$ is unstable.

Figure 9.21: Evolution of the norm of the estimation error $\tilde{u}(x,t) = [\tilde{u}_1(x,t), \tilde{u}_2(x,t)]$. The norm of the estimation error decays to zero due to the exponential convergence of the estimate $\tilde{u}(x,t)$ to the state $u(x,t)$.
9.7.2 Observer

To evaluate the performance of the observer, we consider an unstable pair of coupled diffusion-reaction equations in the form (10.105)-(9.6), with parameters $\Sigma$ and $\Lambda(x)$ in (9.148), together with

\[
A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad f(t) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
\]

(9.149)

Functions $g_1(t)$ and $g_2(t)$ are chosen as piecewise constant functions taking values from the set $\{-10, 0, 10\}$. The evolution of the second state $u_2(x,t)$, for a particular choice of non-zero initial conditions, is shown in Figure 9.18. The state norm is shown in Figure 9.20; the unbounded growth of the norm is a result of the equilibrium $u(x,t) = 0$ being unstable and of non-zero boundary and initial conditions. The observer for this example has the form (9.7)-(9.9), where gains $P$ and $Q$ are computed from (9.13) and (9.14); with the matrix $B$ set to zero and the matrix $C$ chosen in (9.148). To find $P$ and $Q$ we used the numerical approximation of $K(x,s)$ computed previously in Section 9.7.1. The evolution of the estimation error of the second state, i.e., $\tilde{u}_2(x,t)$, is shown in Figure 9.19. The norm of the estimation error $\tilde{u}(x,t)$ is shown in Figure 9.21; the decay of the norm of the estimation error system is a result of the exponential convergence of the estimate $\tilde{u}(x,t)$ to the state $u(x,t)$.

9.8 Conclusion

This paper details the design of observers for coupled parabolic systems, studying as well its in an input-to-state stability property with respect to measurement disturbances. The converge of estimate follows from the stability of the estimation error system; derived by mapping the estimation error system to an stable target system using a pair of integral
transformations. The target system is a set of \( n \) decoupled equations, providing a simple setting to verify input-to-state stability with respect to measurement disturbances. The simple target system is not only advantageous for input-to-state stability analysis, but also allows the user to precisely assign designer-chosen convergence rates. The well-posedness of the kernel systems, associated to the pair of integral transformations, is derived by the method of characteristics and successive approximations. The methodology followed in this paper would be applicable to the dual problem of boundary stabilization of coupled parabolic equations. A numerical method based on power series approximations of the kernels, taking into account the fact that the kernels are piecewise differentiable, is outlined to precisely compute the solutions to the kernels systems and the observer gains. Future work include the adaptive estimation problem, for unknown constant reaction terms, as well as the use of the numerical method for kernel equations arising in the estimation and stabilization problems for other classes of PDEs.
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Chapter 10

State Estimation for a Coupled ODE and Radial Diffusion Equation from a Wellbore Reservoir Drilling Model

10.1 Abstract

The problem of state estimation for a coupled ODE-PDE system is addressed here by means of the backstepping method for PDEs. The ODE is a finite-dimensional, linear, and time-invariant system and the PDE is a linear radial diffusion equation with Neumann and Robin boundary conditions. The coupling appears at one of the boundaries of the PDE and is bidirectional. More precisely, the ODE state appears in one of the boundary conditions of the PDE and the value of the PDE state at the boundary is an input to the ODE. Measurements of the ODE output are available, while the state of the PDE is out of sight. The estimate is defined as the state of an observer; constructed as a copy of the coupled system ODE-PDE with output error feedback. This study is motivated by the influx estimation problem from a wellbore-reservoir model used in managed pressured
drilling applications. The convergence of the estimate derives from the stability properties of the estimation error system. Observer gains are selected specifically to guarantee the exponential stability of the estimation error system. To guarantee the existence and invertibility of the backstepping transformation the well-posedness of a cascade system of a DAE and a hyperbolic PDE is derived; with well-posedness guarantee if and only if an observability assumption is satisfied.

10.2 Introduction

The problem of state estimation for a coupled ODE-PDE system is addressed here by means of the backstepping method for PDEs [65]. The ODE is a finite dimensional, linear, and time-invariant system and the PDE is a linear radial diffusion equation with Neumann and Robin boundary conditions. The coupling appears at one of the boundaries of the PDE and is bidirectional. More precisely, the ODE state appears in one of the boundary conditions of the PDE and the value of the PDE state at the boundary is an input to the ODE. Measurements of the ODE output are available, while the state of the PDE is out-of-sight. The estimate is defined as the state of an observer; constructed as a copy of the coupled system ODE-PDE with output error injection. The convergence of the estimate follows the stability properties of the estimation error system. Observer gains are selected specifically to guarantee the exponential stability of the estimation error system. To guarantee the existence and the invertibility of the backstepping transformation the well-posedness of a cascade hyperbolic PDE-DAE system is derived.

The purpose of this study is to provide a solution to the state estimation problem for a wellbore-reservoir model used in managed pressured drilling (MPD) operations [111]. An ODE is used to described pressure dynamics of a fluid along the wellbore and a radial diffusion equation is used to described the diffusion of the fluid in a porous reservoir. The
bidirectional coupling between the ODE and the PDE arises from conservation laws and the continuity of physical quantities in the model.

Control and estimation problems for cascaded PDE-ODE systems including transport, heat, and wave PDEs were studied in [112], [113, Part IV], [114], [115], and [116]. An observer for cascaded hyperbolic PDE-ODE system was derived in [117], to estimate flow, pressure and down hole rate of circulation loss in oil well drilling application. A cascaded stabilization cascaded ODE-Schroedinger equation was studied in [118]. State and output feedback for a coupled diffusion ODE system was developed in [119] and state and output feedback for sandwiched ODE-PDE-ODE system was developed in [120].

10.3 Problem Statement

In this section, we construct an observer and derive observability conditions for a coupled ODE-PDE system. The ODE is a linear time invariant $n$-dimensional system

$$\frac{dx}{dt}(t) = Ax(t) + Bu(a,t), \quad (10.1)$$

$$y(t) = Cx(t), \quad (10.2)$$

with $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times 1}$, $C \in \mathbb{R}^{1 \times n}$, for $t \in (0,T]$ and initial conditions $x_0 \in \mathbb{R}^n$. The PDE is a radial-diffusion equation

$$\partial_t u(r,t) = \frac{\epsilon}{r^{m-1}} \partial_r \left( r^{m-1} \partial_r u(r,t) \right), \quad (10.3)$$
for \( r \in (a, b), \ t \in (0, T] \), with diffusion coefficient \( \epsilon > 0 \) and some integer parameter \( m > 0 \), related to the geometry of the underlying physical problem. Boundary conditions are

\[
\begin{align*}
\partial_r u(a, t) &= \beta u(a, t) + Dx(t), \\
\partial_r u(b, t) &= 0,
\end{align*}
\]

with \( \beta > 0 \), and initial conditions \( u_0 \in C(a, b) \). The system is understood as a dynamic system with combined state \( x \in C([0, T]; \mathbb{R}^n) \), \( u \in C([0, T]; \mathcal{L}^2(a, b)) \), and output \( y \in C([0, T]; \mathbb{R}) \). The estimation objective is to compute an estimate \( \hat{x}, \hat{u} \) from measurements \( y(t) \in \mathbb{R} \) with exponential convergence in the sense of a norm. The proposed observer is a copy of (10.1)-(10.5) with output error feedback, that is

\[
\begin{align*}
\frac{d\hat{x}}{dt}(t) &= A\hat{x}(t) + B\hat{u}(a, t) + L(\hat{y}(t) - y(t)), \\
\hat{y}(t) &= C\hat{x}(t),
\end{align*}
\]

for \( t \in (0, T] \), with observer gain \( L = [l_1, l_2, \ldots, l_n] \), initial conditions \( \hat{x}_0 \in \mathbb{R}^n \), and

\[
\partial_r \hat{u}(r, t) = \frac{\epsilon}{r^{m-1}} \partial_r \left( r^{m-1} \partial_r \hat{u}(r, t) \right) + l_{n+1}(r) (\hat{y}(t) - y(t)),
\]

for \( r \in (a, b), \ t \in (0, T] \), boundary conditions

\[
\begin{align*}
\partial_r \hat{u}(a, t) &= \beta \hat{u}(a, t) + Dx(t) + l_{n+2}(y(t) - \hat{y}(t)), \\
\partial_r \hat{u}(b, t) &= l_{n+3}(y(t) - \hat{y}(t)),
\end{align*}
\]

with observer gains \( l_{n+1} \in \mathcal{L}^2(a, b), \ l_{n+2} \in \mathbb{R}, \ l_{n+3} \in \mathbb{R} \), and initial conditions \( \hat{u}_0 \in \mathcal{L}^2(0, 1) \). The estimation error is defined as the difference between the state \( x, u \) and the observer
The estimation error $\tilde{x}$, $\tilde{u}$ is a solution of the estimation error system

$$\frac{d\tilde{x}}{dt}(t) = A\tilde{x}(t) + B\tilde{u}(a,t) - LC\tilde{x}(t),$$

(10.13)

$$\tilde{y}(t) = C\tilde{x}(t),$$

(10.14)

for $t \in (0,T]$, with initial conditions $\tilde{x}_0 = x_0 - \hat{x}_0$, and

$$\partial_t\tilde{u}(r,t) = \frac{\epsilon}{r^{m-1}}\partial_r\left(r^{m-1}\partial_r\tilde{u}(r,t)\right) - l_{n+1}(r)C\tilde{x}(t),$$

(10.15)

for $r \in (a,b)$, $t \in (0,T]$, and boundary conditions

$$\partial_r\tilde{u}(a,t) = \beta\tilde{u}(a,t) + D\tilde{x}(t) - l_{n+2}C\tilde{x}(t),$$

(10.16)

$$\partial_r\tilde{u}(b,t) = -l_{n+3}C\tilde{x}(t),$$

(10.17)

with initial conditions $\tilde{u}_0 = u_0 - \hat{u}_0$. Exponential convergence of the estimate $\hat{x}$, $\hat{u}$ to the state $x$, $u$ is equivalent to the exponential stability of zero solution of the estimation error system. The main result, in Theorem 1, provides a way to compute observer gains $L$, $l_{n+1}$, $l_{n+2}$, and $l_{n+3}$, to guarantee exponential stability of the estimation error system. Before the statement of the main result, an additional observability condition is required.

**Assumption 10.3.1.** The finite dimensional subsystem (10.1), (10.2) is observable, that is, $\text{rank}(\mathcal{O}) = n$, with $\mathcal{O} = \begin{bmatrix} C & CA & \cdots & CA^{n-1} \end{bmatrix}^T$.

Assumption 1 guarantees the existence of a linear and invertible transformation
The transformation $T_O$ is an invertible matrix, satisfying

$$T_O A_O = A T_O, \quad T_O B_O = B, \quad C_O = C T_O,$$

(10.18)

where $A_O, B_O, C_O$ are in observer canonical form, that is

$$A_O = \begin{bmatrix}
  a_1 & 1 & 0 & \cdots & 0 \\
  a_2 & 0 & 1 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  a_{n-1} & 0 & 0 & \cdots & 1 \\
  a_n & 0 & 0 & \cdots & 0 \\
\end{bmatrix}, \quad B_O = \begin{bmatrix}
  b_1 \\
  b_2 \\
  \vdots \\
  b_n \\
\end{bmatrix},$$

(10.19)

$$C_O = \begin{bmatrix}
  1 & 0 & \cdots & 0 \\
\end{bmatrix}.$$

(10.20)

**Assumption 10.3.2** (Observability of the Coupled System). None of the eigenvalues $\lambda_k \in \mathbb{R}, \ k \in \mathbb{N}$ of the radial Laplacian operator with Neumann boundary conditions, that is

$$\begin{cases}
  \epsilon \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \phi(r) \right) = -\lambda_k r^{m-1} \phi(r), \\
  \phi_n'(a) = 0, \\
  \phi_n'(b) = 0,
\end{cases}$$

(10.21)

are, simultaneously, solutions to the polynomial equation $D(\lambda_k) = 0$, with

$$D(\xi) = b_n + b_{n-1} \xi + b_{n-2} \xi^2 + \cdots + b_2 \xi^{n-2} + b_1 \xi^{n-1},$$

(10.22)

and at least one $b_i, i \in \{1, 2, \cdots, n\}$ is different from zero.
10.4 Main Result

Before the main result, we describe briefly the methodology followed to define observer gains that guarantee the stability of the estimation error system.

10.4.1 Methodology

Following the backstepping method for PDEs [65], we seek a pair of transformations $T_O : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $T_u : L^2(0,1) \times \mathbb{R}^n \rightarrow L^2(0,1)$, that map the states $\bar{x}, \bar{u}$ satisfying (10.13)–(10.14), (10.15)–(10.17), to states $\bar{z}, \bar{w}$ satisfying the target system

$$\frac{d\bar{z}}{dt}(t) = F\bar{z}(t) + B_O \bar{w}(a,t), \quad (10.23)$$

with initial condition $\bar{z}_0 = T_O^{-1} \bar{x}_0$ and $F \in \mathbb{R}^{n \times n}$ is in companion form, that is

$$F = \begin{bmatrix} f_1 & 1 & 0 & \cdots & 0 \\ f_2 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_{n-1} & 0 & 0 & \cdots & 1 \\ f_n & 0 & 0 & \cdots & 0 \end{bmatrix}, \quad (10.24)$$

and

$$\partial_t \bar{w}(r,t) = \frac{\epsilon}{r^{m-1}} \partial_r \left( r^{m-1} \partial_r \bar{w}(r,t) \right) - \sigma \bar{w}(r,t), \quad (10.25)$$
for \( r \in (a,b) \), \( t \in (0,T] \), and boundary conditions

\[
\begin{align*}
\partial_r w(a,t) &= (\beta - \frac{\sigma}{2\epsilon}(b-a))w(a,t), \\
\partial_r w(b,t) &= 0,
\end{align*}
\]  
(10.26)  
(10.27)

with initial conditions \( w_0 \in C(a,b) \), satisfying \( \bar{u}_0 = T_w(w_0,z_0) \). The finite-dimensional transformation \( T_O \) is defined by (10.18), (10.19), while \( T_u \) is the sum of a second-kind Volterra integral transformation acting on \( w \) and a linear spatially-varying transformation acting \( z \), that is

\[
\begin{align*}
\bar{x}(t) &= T_O \bar{z}(t), \\
\bar{u}(r,t) &= w(r,t) - \int_a^r K(r,s)w(s,t)ds + (\gamma(r) - \gamma(a)) \bar{z}(t),
\end{align*}
\]  
(10.28)  
(10.29)

Substitution of (10.28), (10.29) in the error (10.13)-(10.17) and target systems results in a hyperbolic equation and boundary condition for the kernel \( K \) and a differential-algebraic system of equation and boundary condition for \( \gamma \). Thus, existence of a transformation \( T_u \) in the form (10.29) is guaranteed by the existence of a solution to the hyperbolic PDE and DAE systems, which is proven addressed in Lemma 10.4.1 and Lemma 10.4.2. Invertibility is given by invertibility of \( T_O \), the triangular structure of the pair (29)-(30) and the fact that the part of the operator \( T_u \) acting on \( w \) is a second-kind Volterra integral. To ensure stability of the target system, the eigenvalues of \( F \) are selected with negative real part and \( \sigma \) is chosen positive, satisfying

\[
\sigma \leq \frac{2\epsilon \beta}{b-a}.
\]  
(10.30)

Once the eigenvalues of \( F \) and the value of \( \sigma \) are chosen, there is a unique value for the observer gains \( L, l_n \) permitted for consistency of the transformations. These are the
observer gains that guarantee the convergence of the estimate to the unknown system state $x, u$, and are presented next in Theorem 1.

10.4.2 Main Result

Theorem 10.4.1. Let the premises in Assumption 1 and 2 hold. Consider the estimation error system in (10.13), (10.14), (10.15)-(10.17), and a similarity transformation $T_\Omega \in \mathbb{R}^{n \times n}$ that maps (10.1), (10.2) to observer canonical form (10.18), (10.19). Let the ODE observer gain $L \in \mathbb{R}^{n \times 1}$ be chosen such that the eigenvalues $\mu_i, i \in \{1, \ldots, n\}$ of the companion (10.24) matrix $F \in \mathbb{R}^{n \times n}$, defined as

$$F = A_\Omega - L_\Omega C_\Omega,$$

$$L = T_\Omega L_\Omega,$$  \hspace{1cm} (10.31) \hspace{1cm} (10.32)

have negative real part, and the PDE observer gains $l_{n+1} \in L^2(a,b)$, $l_{n+2} \in \mathbb{R}$, and $l_{n+3} \in \mathbb{R}$ computed from

$$l_{n+1}(r) = \epsilon\gamma''_1(r) + \epsilon \frac{n-1}{r} \gamma'_1(r) - \sum_{i=1}^{n} (\gamma_i(r) - \gamma_i(a)) f_i,$$  \hspace{1cm} (10.33)

for $r \in (a, b)$, and

$$l_{n+2} = \gamma'_1(a) - d_1,$$  \hspace{1cm} (10.34)

$$l_{n+3} = \gamma'_1(b),$$  \hspace{1cm} (10.35)

where $\gamma_i(r), i \in \{1, \ldots, n\}$, is the solution of a differential-algebraic system of equations

$$\epsilon \partial_s K(r,a) + \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b-a) - \frac{m-1}{a} \right) K(r,a) + \sum_{i=1}^{n} (\gamma_i(r) - \gamma_i(a)) b_i = 0,$$  \hspace{1cm} (10.36)
for \( r \in (a,b) \), and

\[
\begin{align*}
\epsilon \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_2(r) \right) &= \gamma_1(r), \\
\epsilon \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_3(r) \right) &= \gamma_2(r), \\
&\vdots \\
\epsilon \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_n(r) \right) &= \gamma_{n-1}(r),
\end{align*}
\]

(10.37)

for \( r \in (a,b) \), with boundary conditions

\[
\begin{align*}
\gamma'_i(a) &= d_i, \\
\gamma'_i(b) &= 0,
\end{align*}
\]

(10.38)

(10.39)

for all \( i \in \{2,\ldots,n\} \), where \( b_i \) are the coefficients of \( B_\mathcal{O} \) and \( d_i \) are the coefficients of \( D_\mathcal{O} = DT_\mathcal{O} \). In equation (10.36), \( K \in \mathcal{L}^2(\mathcal{T}) \) is the solution to a second-order hyperbolic equation

\[
\begin{cases}
\frac{1}{r^{m-1}} \partial_r \left( r^{m-1} \partial_r K(r,s) \right) - \partial_s \left( s^{m-1} \partial_s \left( \frac{K(r,s)}{s^{m-1}} \right) \right) = -\frac{\sigma}{\epsilon} K(r,s), \\
\text{with boundary conditions:} \\
K(r,r) = \frac{\sigma}{2\epsilon} (r-b), \\
\partial_r K(b,s) = 0,
\end{cases}
\]

(10.40)

with \( \sigma \) positive, chosen as

\[
\mu \leq \sigma \leq \frac{2\epsilon \beta}{b-a},
\]

(10.41)

\[
\mu = \min_{i \in \{1,2,\ldots,n\}} \{ |\mu_i| \}.
\]

(10.42)
This choice of observer gains guarantees that estimation error system is exponentially stable, that is

\[
\|\tilde{x}(t)\|_2 \leq \kappa_1 \exp(-\mu t) (\|\tilde{x}_0\|_2 + \|\tilde{u}_0\|_{H^1}),
\]

(10.43)

\[
\|\tilde{u}(\cdot, t)\|_{L^2} \leq \kappa_2 \exp(-\mu t) (\|\tilde{x}_0\|_2 + \|\tilde{u}_0\|_{H^1}).
\]

(10.44)

for some positive \(\kappa_1, \kappa_2\).

The well-posedness of the DAE and the hyperbolic PDE are studied in next two lemmas, the proof of Theorem 1 is provided afterwards.

**Lemma 10.4.1.** There is a unique \(L^2(T)\) solution to the hyperbolic equation

\[
\begin{cases}
\frac{1}{r^m-1} \partial_r \left( r^{m-1} \partial_r K(r,s) \right) - \partial_s \left( s^{m-1} \partial_s \left( \frac{K(r,s)}{s^m} \right) \right) = -\frac{\sigma}{\epsilon} K(r,s), \\
K(r,r) = \frac{\sigma}{2\epsilon} (r-b), \\
\partial_r K(b,s) = 0.
\end{cases}
\]

(10.45)

**Proof.** A solution to hyperbolic system can be found following the procedure described in [52], for kernel equations required for stabilization of diffusion equations in spherical domain, or the procedure described in [122], for kernel equations required for stabilization of diffusion equations with spatially-variable diffusion coefficients.

**Lemma 10.4.2.** The system of differential algebraic equations (DAE), constituted by \(n-1\)
differential equations

\[
\begin{align*}
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_2(r) \right) &= \gamma_1(r) - \gamma_1(a), \\
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_3(r) \right) &= \gamma_2(r) - \gamma_2(a), \\
&\vdots \quad \vdots \quad \vdots \\
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_n(r) \right) &= \gamma_{n-1}(r) - \gamma_{n-1}(a),
\end{align*}
\]

(10.46)

with boundary conditions

\[
\begin{align*}
\gamma_i'(a) &= d_i, \\
\gamma_i'(b) &= 0,
\end{align*}
\]

(10.47)

(10.48)

for all \( i \in \{2,\ldots,n\} \), and by the algebraic equation

\[
\epsilon \partial_s K(r,a) + \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b-a) - \frac{m-1}{a} \right) K(r,a) + \sum_{i=1}^{n} (\gamma_i(r) - \gamma_i(a)) b_i = 0,
\]

(10.49)

has a unique solution \( \gamma_i(r) \in L^2(0,1), \ i \in \{1,\ldots,n\} \).

Proof. Define

\[
\tilde{\gamma}_i(r) = \gamma_i(r) - \gamma_i(a),
\]

(10.50)
for $i \in \{1, 2, \ldots, n\}$. By substitution

$$
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_2(r) \right) = \gamma_1(r),
$$

$$
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_3(r) \right) = \gamma_2(r),
$$

$$
\vdots \quad \vdots \quad \vdots
$$

$$
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_n(r) \right) = \gamma_{n-1}(r),
$$

with boundary conditions

$$
\gamma'_i(a) = d_i, \quad (10.52)
$$

$$
\gamma'_i(b) = 0, \quad (10.53)
$$

for all $i \in \{2, \ldots, n\}$, and by the algebraic equation

$$
\epsilon \partial_s K(r,a) - \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b - a) - \frac{m-1}{a} \right) K(r,a) + \sum_{i=1}^{n} \gamma_i(r)b_i = 0. \quad (10.54)
$$

Consider the regular Sturm-Liouville [123] problem

$$
\left\{ \frac{\epsilon}{r} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \phi_k(r) \right) = -\lambda_k \phi_k(r)r^{m-1}, \right.
$$

for $r \in (a,b)$, with boundary conditions

$$
\phi'_k(a) = 0,
$$

$$
\phi'_k(b) = 0,
$$

for $r \in (a,b)$, with $k \in \mathbb{N}$. The solution to (10.55) is available as an analytic expression [91],

$$
\phi_k(r) = c_k \left( \frac{r^{-\nu} J_\nu(\nu_k r)}{J_{\nu+1}(\nu_k r)} - r^{-\nu} \frac{J_{\nu+1}(\nu_k a)}{Y_{\nu+1}(\nu_k a)} Y_{\nu}(\nu_k r) \right), \quad (10.56)
$$
with \( v = \frac{m}{2} - 1 \). The values \( \mu_k \in \mathbb{R}, k \in \mathbb{N} \) are the solutions to the equation

\[
P_{v+1}(\mu_k a, \mu_k b) = 0,
\]

where \( P_v \) is the difference of cross-products of first and second-kind Bessel functions [124],

\[
P_v(x, y) = J_v(x)Y_v(y) - J_v(y)Y_v(x).
\]

The eigenvalues \( \lambda_k, k \in \mathbb{N} \) of the Sturm-Liouville problem (10.55) are

\[
\lambda_k = \epsilon \mu_k^2.
\]

Coefficients \( c_k, k \in \mathbb{N} \) are chosen for normalization, that is

\[
c_k = \frac{1}{\left\| r^{-v}J_v(\mu_k r) - r^{-v}J_{v+1}(\mu_k a)Y_v(\mu_k r) \right\|_{L_m^2}}.
\]

The set of functions \( \phi_k, k \in \mathbb{N} \) form a basis in the Hilbert space \( L_m^2 = L^2([a,b], r^{m-1} dr) \).

Consider a series representation of the functions \( \gamma_i, i \in \{1, 2, \cdots, n\} \) in terms of the basis \( \phi_k \in C^\infty(a,b) \), that is

\[
\gamma_i(r) = \sum_{k=0}^{\infty} p_{i,k} \phi_k(r).
\]

Consider also a series representation for the functions \( \frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_i(r) \right), i \in \{2, 3, \cdots, n\} \), that is

\[
\frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_i(r) \right) = \sum_{k=0}^{\infty} q_{i,k} \phi_k(r).
\]
From orthogonality of the basis functions, for all $i \in \{2, 3, \cdots, n\}$, and for all $k \in \mathbb{N}$

$$
\int_{a}^{b} \left( \frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_{i}(t) \right) - \gamma_{i-1}(r) \right) \phi_{k}(r) r^{m-1} dr = q_{i,k} - p_{i-1,k}.
$$

(10.63)

The differential equations (10.51) are satisfied if and only if the left hand of equation (10.63) is zero for all $i \in \{2, 3, \cdots, n\}$ and for all $k \in \mathbb{N}$, therefore

$$
q_{i,k} = p_{i-1,k}.
$$

(10.64)

Similarly, for all $k \in \mathbb{N}$

$$
\int_{a}^{b} \left( \epsilon \partial_{s} K(r,a) + \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b-a) - \frac{m-1}{a} \right) K(r,a) + \sum_{i=1}^{n} \gamma_{i}(r) b_{i} \right) \times \phi_{k}(r) r^{m-1} dr = \sum_{i=1}^{n} p_{i,k} - z_{k}
$$

(10.65)

with

$$
z_{k} = - \int_{a}^{b} \left( \epsilon \partial_{s} K(r,a) + \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b-a) - \frac{m-1}{a} \right) K(r,a) \right) \phi_{k}(r) r^{m-1} dr.
$$

(10.66)

The algebraic equation (10.54) is satisfied if and only if the left-hand side of equation (10.65) is zero for all $k \in \mathbb{N}$, therefore

$$
\sum_{i=1}^{n} p_{i,k} = -z_{k}.
$$

(10.67)

Further, from (10.62), orthogonality of the basis functions $\phi_{k}, k \in \mathbb{N}$, and using integration
by parts

\[ q_{i,k} = \int_{a}^{b} \frac{\epsilon}{r^{m-1}} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_i(r) \right) \phi_k(r) r^{m-1} dr, \]  
\[ = \epsilon \int_{a}^{b} \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \gamma_i(r) \right) \phi_k(r) dr; \]  
\[ = \epsilon r^{m-1} \frac{d}{dr} \gamma_i(r) \phi_k(r) \bigg|_{a}^{b} - \epsilon \int_{a}^{b} r^{m-1} \frac{d}{dr} \gamma_i(r) \frac{d}{dr} \phi_k(r) dr, \]  
\[ (10.68) \]

using boundary conditions for \( \gamma_i(r) \)

\[ q_{i,k} = -\epsilon a^{m-1} d_i \phi_k(a) - \epsilon r^{m-1} \gamma_i(r) \frac{d}{dr} \phi_k(r) \bigg|_{a}^{b} + \epsilon \int_{a}^{b} \gamma_i(r) \frac{d}{dr} \left( r^{m-1} \frac{d}{dr} \phi_k(r) \right) dr, \]  
\[ (10.71) \]

the equation and boundary conditions for \( \phi_k(r) \) result in

\[ q_{i,k} = -\epsilon a^{m-1} d_i \phi_k(a) - \lambda_k \int_{a}^{b} \gamma_i(r) \phi_k(r) r^{m-1} dr, \]  
\[ (10.72) \]

from definition of \( p_{i,k} \)

\[ q_{i,k} = -\epsilon a^{m-1} d_i \phi_k(a) - \lambda_k p_{i,k}, \]  
\[ (10.73) \]

substitution of (10.73) in (10.64) implies

\[ \lambda_k p_m + p_{i-1,k} = -\epsilon a^{m-1} d_i \phi_k(a). \]  
\[ (10.74) \]

For each \( k \in \mathbb{N} \), the \( n - 1 \) algebraic equations (10.74) together with the equation (10.67) result in a \( n \)-dimensional algebraic system that one needs to solve in order to compute \( \{q_{1,k}, q_{2,k}, \ldots, q_{n,k}\} \). In other words, the coefficients in the series (10.61) should satisfy an
infinite sequence of \( n \)-dimensional linear systems

\[
\begin{bmatrix}
\lambda_k & 1 & \cdots & 0 & 0 \\
0 & \lambda_k & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \lambda_k & 1 \\
b_n & b_{n-1} & \cdots & b_2 & b_1
\end{bmatrix}
\begin{bmatrix}
p_{n,k} \\
p_{n-1,k} \\
p_{2,k} \\
p_{1,k}
\end{bmatrix}
= \begin{bmatrix}
\beta_k d_n \\
\beta_k d_{n-1} \\
\beta_k d_2 \\
z_k
\end{bmatrix},
\tag{10.75}
\]

where

\[
\beta_k = -\epsilon a^{m-1} \phi_k(a),
\tag{10.76}
\]

\[
z_k = -\int_a^b \left( \epsilon \partial_s K(r,a) + \epsilon \left( \beta - \frac{\sigma}{2\epsilon} (b-a) - \frac{m-1}{a} \right) K(r,a) \right) \phi_k(r) r^{m-1} dr.
\tag{10.77}
\]

Note that the generalized Fourier coefficients define a function uniquely in the space of definition, that is \( L^2([a,b], r^{m-1} dr) \), for that reason, a unique solution of the algebraic system in the is a necessary and sufficient condition for the existence of a solution. Define

\[
D(\xi) = \det \begin{bmatrix}
\xi & 1 & 0 & \cdots & 0 & 0 \\
0 & \xi & 1 & \cdots & 0 & 0 \\
0 & 0 & \xi & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \xi & 1 \\
b_n & b_{n-1} & b_{n-2} & \cdots & b_2 & b_1
\end{bmatrix},
\tag{10.78}
\]

\[
= b_n + b_{n-1} \xi + b_{n-2} \xi^2 + \cdots + b_2 \xi^{n-2} + b_1 \xi^{n-1}.
\tag{10.79}
\]

The sequence of linear systems (10.75) has a unique solution \( q_{i,k} \), with \( i \in \{1,2,\ldots,n\} \),
for all $k \in \mathbb{N}$. This condition is related to the observability of the coupled system, since it defines a cancellation between the spectral values of the PDE and zeros of the ODE. This condition appears in Assumption 10.3.2. \qed

### 10.4.3 Proof of Theorem 1

**Proof.** The stability is then verified with Lyapunov-like functions

\begin{align*}
V_1(t) &= \frac{1}{2} \int_a^b w^2(r,t) r^{m-1} dr, \\
V_2(t) &= \frac{\epsilon \theta}{2} w(a,t)^2 a^{m-1} + \frac{1}{2} \int_a^b w_r^2(r,t) r^{m-1} dr,
\end{align*}

with

\[ \theta = \beta - \frac{\sigma}{2\epsilon} (b - a), \]

which satisfies $\theta > 0$, according to the condition (10.30). The time derivatives of $V_1(t)$ and $V_2(t)$ along the trajectories of the $w$-system are

\[ \frac{dV_1}{dt}(t) = \epsilon w(r,t) \partial_r w(r,t) r^{m-1} \bigg|_a^b - \epsilon \int_a^b (\partial_r w(r,t))^2 r^{m-1} dr - \sigma \int_a^b w(r,t)^2 r^{m-1} dr, \]

then,

\[ \frac{dV_1}{dt}(t) \leq -2V_1(t). \]
The time derivate of $V_2(t)$ is

$$\frac{dV_2}{dt}(t) \leq -\epsilon \theta w(a,t)^2 a^{m-1} - \epsilon \int_a^b \left( \frac{1}{r^{m-1}} \partial_r \left( r^{m-1} \partial_r w(r,t) \right) \right)^2 r^{m-1} dr - \sigma \int_a^b (\partial_r w(r,t))^2 r^{m-1} dr,$$

$$\leq -\epsilon \theta \sigma w(a,t)^2 a^{m-1} - \sigma \int_a^b (\partial_r w(r,t))^2 r^{m-1} dr.$$  \hspace{1cm} (10.86)

Therefore,

$$\frac{dV_2}{dt}(t) \leq -2\sigma V_2(t).$$  \hspace{1cm} (10.88)

From comparison principle

$$V_1(t) \leq \exp[-2\sigma t] V_1(0),$$  \hspace{1cm} (10.89)
$$V_2(t) \leq \exp[-2\sigma t] V_2(0),$$  \hspace{1cm} (10.90)

and consequently,

$$\|w(\cdot,t)\|_{L^2} \leq \exp[-\sigma t] \|w_0\|_{L^2},$$  \hspace{1cm} (10.91)
$$|w(a,t)| \leq \exp[-\sigma t] (|w_0(a)| + k_1 \|\partial_r w_0\|_{L^2}),$$  \hspace{1cm} (10.92)

with

$$k_1 = a^{-\frac{(m-1)}{2}} \sqrt{\epsilon \theta}. \hspace{1cm} (10.93)$$

From Lemma 10.7.1 in the Appendix,

$$|w(a,t)| \leq k_2 \exp[-\sigma t] \|w_0\|_{H^1}.$$  \hspace{1cm} (10.94)
with $k_2 = \max\{1, k_1\}$. The observer gain $L = [l_1, l_2, \ldots, l_n]^T$ is chosen via pole placement. That is, given a set of $n$ complex-valued numbers $\{\mu_1, \mu_2, \ldots, \mu_n\}$ with negative real parts, it is always possible to find $L$ such that the eigenvalues of $F = A - LC$, are exactly $\{\mu_1, \mu_2, \ldots, \mu_n\}$. From the variation of constants formula

$$
\tilde{z}(t) = \exp[Fl_1]z_0 + \int_0^t \exp[F(t-\tau)]Bw(a, \tau)d\tau.
$$  \hfill (10.95)

Then, there exits $k_3 > 0$, such that the norm of the state $\tilde{x}(t)$ is bounded as follows

$$
\|\tilde{z}(t)\|_2 \leq k_3 \exp[-\mu t]\|z_0\|_2 + k_3 \int_0^t \exp[-\mu(t-\tau)]\|w(a, \tau)\|d\tau,
$$  \hfill (10.96)

with $\mu = \min_{i \in \{1,2,\ldots,n\}} \{|\mu_i|\}$. From (10.30), it follows that $\sigma > \mu > 0$, and therefore

$$
\|\tilde{z}(t)\|_2 \leq k_3 \exp[-\mu t]\|z_0\|_2 + \frac{k_3 k_3}{\sigma - \mu} \exp[-\mu t] \|B\|_2 \|w_0\|_{H_1}.
$$  \hfill (10.97)

The inequalities imply that the zero solution of the target system is stable, with exponential bounds

$$
\|w(\cdot, t)\|_{L^2} \leq \exp[-\sigma t] \|w_0\|_{L^2},
$$  \hfill (10.98)

$$
\|\tilde{z}(t)\|_2 \leq k_3 \exp[-\mu t]\|z_0\|_2 + k_4 \exp[-\mu t] \|w_0\|_{H_1}.
$$  \hfill (10.99)

with

$$
k_4 = \frac{k_3 k_3}{\sigma - \mu} \|B\|_2.
$$  \hfill (10.100)
Since the pair of transformation $T_O$ and $T_u$ defined in (10.18), (10.28) and (10.29) are invertible and bounded, there exists positive $\kappa_1, \kappa_2$, such that

$$\|\tilde{x}(t)\|_2 \leq \kappa_1 \exp(-\mu t) (\|\tilde{x}_0\|_2 + \|\tilde{u}_0\|_{H^1}),$$

$$\|\tilde{u}(\cdot, t)\|_{L^2} \leq \kappa_2 \exp(-\mu t) (\|\tilde{x}_0\|_2 + \|\tilde{u}_0\|_{H^1}).$$

\[ \Box \]

### 10.5 Wellbore and Reservoir Model

The process of oil well drilling consists in creating a borehole several kilometres into the ground. Throughout the process, a drilling fluid (typically oil- or water-based mud) is circulated to lubricate and cool the drilling tools, evacuate mud cuttings and pressurize the well. The mud is pumped through the drillstring, flows through the drillbit and travels up the annular region, as schematically depicted on Figure ??.

When the pressure at the bottom of the well is lower than the pressure of the reservoir surrounding it, an influx of liquid, and potentially gas, will enter the annulus. We apply the observer design of the previous sections to estimate, from surface measurements only, the flow rate of a liquid influx as well as the near-wellbore reservoir pressure profile.

#### 10.5.1 Model

The finite-dimensional part of the following model is an adaptation from [125] to account for the liquid influx while the reservoir PDE is described in [111]. The model derives from first principles and the states $\mathbf{x}(t) = [p_c(t), p_p(t), q_d(t)]'$ and $u(r, t), r \in [r_w, r_e]$ denote, respectively, the pressure upstream the outlet choke, the pump pressure, the total influx into the annulus and the reservoir pressure profile. The model takes the following
form

\[
\frac{dx(t)}{dt} = Ax(t) + Bu(r_w,t), \quad (10.101)
\]

\[
y(t) = Cx(t), \quad (10.102)
\]

\[
\partial_t u(r,t) = \frac{\epsilon}{r} \partial_r (r \partial_r u(r,t)), \quad (10.103)
\]

\[
\partial_r u(r_w,t) = \beta u(r_w,t) + Dx(t), \quad (10.104)
\]

\[
\partial_r u(r_e,t) = 0, \quad (10.105)
\]

where

\[
A = \begin{bmatrix}
a_0 & 0 & 0 \\
0 & 0 & a_1 \\
0 & a_2 & a_3 \\
\end{bmatrix}, \quad B = \begin{bmatrix}
b_0 \\
0 \\
b_1 \\
\end{bmatrix}, \quad D = \begin{bmatrix}
d_0 & 0 & d_1 \\
\end{bmatrix}. \quad (10.106)
\]

Definition of the matrix elements are given in Table 10.1 and the physical parameters are given in Table 10.2. Two measurements are typically available on drilling facilities, namely pump and choke pressure, which yields

\[
C = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
\end{bmatrix}. \quad (10.107)
\]

These two measurements are required to make the pair \((A, C)\) observable. Thus, the design of Section 10.3 has to be slightly adapted to account for multiple outputs. We omit the details here for the sake of brevity, however, they pose no difficulty using a block observer canonical form, since the presence of multiple outputs only adds degrees of freedom to estimate the state of the scalar PDE.
Figure 10.1: Schematic of fluid flow-path in a wellbore.

Table 10.1: Definition of elements in the model matrices

<table>
<thead>
<tr>
<th>Element</th>
<th>Definition</th>
<th>Element</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_0 )</td>
<td>( \frac{\beta_a}{V_a} (\frac{A_a D_a^2}{32 \mu H} + \frac{K_c Z_c}{\sqrt{2 \rho_0 (p_c - p_0)}}) )</td>
<td>( a_1 )</td>
<td>( \frac{-\beta_d}{V_d} )</td>
</tr>
<tr>
<td>( a_3 )</td>
<td>( \frac{-32 \mu H}{M_d A_d D_d^2} + \frac{\rho_0 q_d}{M_d C_d^2 A_d^2} )</td>
<td>( a_2 )</td>
<td>( \frac{1}{M_d} )</td>
</tr>
<tr>
<td>( b_0 )</td>
<td>( \frac{\beta_a}{V_a} (\frac{A_a D_a^2}{32 \mu H}) )</td>
<td>( b_1 )</td>
<td>( \frac{-1}{M_d} )</td>
</tr>
<tr>
<td>( d_0 )</td>
<td>( \frac{-A_a D_a^2}{32 \mu \xi H} )</td>
<td>( d_1 )</td>
<td>( \frac{-1}{\xi} )</td>
</tr>
<tr>
<td>Parameter</td>
<td>Definition</td>
<td>Value</td>
<td>Unit</td>
</tr>
<tr>
<td>------------</td>
<td>-------------------------------------------</td>
<td>---------</td>
<td>-------</td>
</tr>
<tr>
<td>$\beta_{a,d}$</td>
<td>Bulk modulus</td>
<td>6.896e8</td>
<td>Pa</td>
</tr>
<tr>
<td>$D_a$</td>
<td>Annulus diameter</td>
<td>0.1809</td>
<td>m</td>
</tr>
<tr>
<td>$D_d$</td>
<td>Drillstring diameter</td>
<td>0.1143</td>
<td>m</td>
</tr>
<tr>
<td>$H$</td>
<td>Depth of the well</td>
<td>2000</td>
<td>m</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Mud viscosity</td>
<td>40e-2</td>
<td>Pa.s</td>
</tr>
<tr>
<td>$K_c$</td>
<td>Choke constant</td>
<td>0.0029</td>
<td>[-]</td>
</tr>
<tr>
<td>$Z_c$</td>
<td>Steady state choke opening</td>
<td>0.8</td>
<td>[-]</td>
</tr>
<tr>
<td>$\bar{p}_c$</td>
<td>Steady state choke pressure</td>
<td>1.675e5</td>
<td>Pa</td>
</tr>
<tr>
<td>$C_d$</td>
<td>Bit nozzle constant</td>
<td>0.8</td>
<td>[-]</td>
</tr>
<tr>
<td>$A_n$</td>
<td>Bit nozzle area</td>
<td>7.459e-4</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$p_o$</td>
<td>Reference pressure</td>
<td>1e5</td>
<td>Pa</td>
</tr>
<tr>
<td>$\rho_o$</td>
<td>Reference density</td>
<td>780</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Permeability</td>
<td>5e-12</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Porosity</td>
<td>0.2</td>
<td>[-]</td>
</tr>
<tr>
<td>$c_t$</td>
<td>Total compressibility (reservoir)</td>
<td>2.32e-9</td>
<td>Pa$^{-1}$</td>
</tr>
</tbody>
</table>

Table 10.2: Definition and values of wellbore and fluid parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{a,d}$</td>
<td>Area</td>
</tr>
<tr>
<td>$V_{a,d}$</td>
<td>Volume</td>
</tr>
<tr>
<td>$r_w$</td>
<td>Radius of annulus</td>
</tr>
<tr>
<td>$\xi$</td>
<td>$2\pi\kappa r_w H/\mu$</td>
</tr>
<tr>
<td>$M_d$</td>
<td>Integrated density per cross section, $\int_0^L (\rho(x)/A_d(x))dx$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$-d_0/\xi$</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Diffusivity constant, $\epsilon = \kappa/(\mu c_t \phi)$</td>
</tr>
</tbody>
</table>

Subscripts $a,d$  | annulus, drillstring
10.5.2 Numerical Simulations

A test case, where the opening of the choke valve (see Figure 10.2) is increased suddenly, is considered here to illustrate the results. This leads to reduction of the pressure at the bottom of the wellbore and thus result in an influx from the reservoir. Figure 10.2 shows the comparison between the influx from the plant, the influx estimated by the observer and an open-loop estimation. Since the dynamics are stable, one could expect the latter to provide an asymptotic estimate of the influx. This is not the case, however, due to the slow time-scale of the reservoir dynamics. A similar result is seen in estimating the near-wellbore reservoir profile as depicted in Figure 10.3 which is a snapshot of the reservoir pressure profile at 60s.

10.6 Conclusion

We have derived an observer for coupled ODE-PDE system with bidirectional coupling. The observer is derived following the backstepping method for PDE, i.e. defining
an integral transformation that maps the estimation error system to a stable target system. Interestingly, the well-posedness conditions for the kernel equations are exactly the conditions of observability of the coupled system. The design is applied to a model of wellbore-reservoir dynamics, used in the managed pressured drilling application. This allows us to estimate the influx from the reservoir by only using the measurements of the finite dimensional states that are typically available at the surface of drilling rigs.

The main shortcoming of the current design is the inability to modify the coefficient of the Robin boundary condition at the PDE-ODE interface. Future works include the modification of the transformation to compensate for this. Besides, the design of spatially-varying source terms in the PDE target system and a proper choice of closed-loop eigenvalues could be used to decrease the overshoot in the transient state estimation dynamics.
Lemma 10.7.1. For any function \( f \in C([a,b]) \),

\[
f(a) \leq \kappa_a \|f\|_{H^1},
\]

with \( \kappa_a = \frac{(b-a)^2 + 1}{b-a} \).

Proof. From the fundamental theorem of calculus and triangle inequality

\[
|f(a)| \leq |f(r)| + \int_a^b |\partial_\xi f(\xi)| d\xi
\]

for any \( r \in [a,b] \). Using Cauchy-Swartz inequality

\[
|f(a)| \leq |f(r)| + \sqrt{b-a} \sqrt{\int_a^b |\partial_r f(r)|^2 dr},
\]

using Young's inequality

\[
|f(a)|^2 \leq \left( \frac{\Xi + 1}{\Xi} \right) |f(r)|^2 + 2(b-a)(1+\Xi) \int_a^b |\partial_r f(r)|^2 dr.
\]

Since the last inequality holds for all \( r \in [a,b] \), it follows that

\[
(b-a)|f(a)|^2 \leq \frac{\Xi + 1}{\Xi} \int_a^b |f(r)|^2 dr + (1+\Xi)(b-a)^2 \int_a^b |\partial_r f(r)|^2 dr.
\]

for some \( \Xi > 0 \). Dividing both side by \( b-a \),

\[
|f(a)|^2 \leq \frac{\Xi + 1}{\Xi} \frac{1}{b-a} \int_a^b |f(r)|^2 dr + (1+\Xi)(b-a) \int_a^b |\partial_r f(r)|^2 dr,
\]
Choosing $\Xi = (b - a)^{-2}$, one obtains

$$|f(a)| \leq \kappa_a \|f\|_{H^1},$$

(10.114)

with $\kappa_a = \frac{(b - a)^2 + 1}{b - a}$.

\[\square\]

### 10.8 Acknowledgment

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Bibliography


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