Mathematical aspects of catalyst positioning in Lithium/air batteries

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Abstract

Lithium-Luft-Akkumulatoren haben in den letzten Jahren das Interesse vieler Wissenschaftler auf sich gezogen. Das Problem der Katalysatorpositionierung, welches die poröse Kathode während des Entladungsprozesses beschreibt, ist Teil der Forschung zur Optimierung der Kapazität von Lithium-Luft-Akkumulatoren. Während des Entladungsprozesses kommt es zu einem schwerwiegenden Problem: Die Sauerstoffreduktionsprodukte der Entladung sind in den organischen Elektrolyten unlöslich. Dadurch wird der Zufluss von Sauerstoff für die Reaktion mit Lithiumionen in die Pore verstopft und die Kapazität der Batterien begrenzt, weil die aktive Oberfläche innerhalb der Pore verengt wird. Die Dynamik des Entladungsprozesses wird durch ein Anfangs- und inhomogenes Randwertproblem für zwei eindimensionale partielle Differenzialgleichungen beschrieben. Die zwei Variablen des Systems sind der Porenradius innerhalb der Kathode und die Sauerstoffkonzentration zu bestimmten Koordinaten und Zeitpunkten.

Gegenstand der Arbeit ist es, einige Katalysatorpositionierungsmodelle zu untersuchen und das freie Volumen der Pore nach dem Verstopfen der Poren durch die abgelagerten Entladungsprodukte zu maximieren. Die Arbeit konzentriert sich auf die folgenden Bereiche:

Erstens untersuchen wir analytisch das Vorwärtsmodell, das die stetige Positionierung der Katalysatoren von Lithium-Luft-Akkumulatoren beschreibt. die korrekte Problemstellung, die Fréchet-Differenzierbarkeit des Porenradius und der Sauerstoffkonzentration in Abhängigkeit zur Katalysatorfunktion in einigen Räumen.

Zweitens stellen wir Optimierungsprobleme vor und analysieren die Sensitivitäts- und Adjoint-Methode, um sie zu lösen.

Schließlich werden einige numerische Methoden zur Lösung der Vorwärtsprobleme durchgeführt, und einige numerische Ansätze zur Lösung des Optimierungsproblems werden ebenfalls untersucht, um die theoretischen Ergebnisse zu veranschaulichen.

Abstract

Lithium/air batteries has been taken interest by many scientists over the last years. *The catalyst positioning problem* describing the porous cathode during the discharge process is concerned in the research of optimizing the capacity of *Lithium/air batteries*. During discharge process, there is a critical issue: the discharge oxygen reduction products is insoluble in the organic electrolytes. This clogs the oxygen entrance to the pore to be reacted with Lithium ions and limits the capacity of the batteries by narrowing the active surface inside the pore. The dynamics of the discharge process is described by the initial mixed boundary value problem for two one-dimensional partial differentiable equations. The two variables of the system are the pore radius inside the cathode and the oxygen concentration at certain coordinate and time.

The subject of the thesis is to investigate some catalyst positioning models and to maximize the free volume of the pore after pore clogging by the deposited discharged products. We aim at the following fields:

First, we research analytically the forward model describing continuous catalyst positioning in *Li/air batteries*: well-posedness of the problems, the Fréchet differentiability of the pore radius and the oxygen concentration with respect to catalytic function in some spaces.

Second, we present optimization problems and analyze the sensitivity and adjoint method to solve them.

Finally, some numerical methods are carried out to solve the forward problems and some numerical approach for solving optimization problem are also examined to illustrate the theoretical results.

Contents

Contents	vii
List of Figures	xi
1 Introduction	1
Introduction	1
1.1 Motivation	1
Motivation	1
1.2 Mathematical settings	6
1.2.1 Mathematical setting of the diffusion-limited model for Li/air batteries	7
1.2.2 Optimization Problems on catalyst positioning models	14
1.2.2.1 The first optimization problem	14
1.2.2.2 The second optimization problems	15
1.3 The main results of the Thesis	16
2 Mathematical preliminaries	19
2.1 Elementary concepts for PDEs	19
2.1.1 Sobolev spaces	19
2.1.2 Spaces involving time	20
2.2 Mixed boundary value problem for one-dimensional linear parabolic equations . . .	23
2.3 Convex analysis	29
3 Mathematical models for continuous catalyst positioning in Li/air batteries	31

CONTENTS

3.1	Formulation and weak solution of Problem I_a	31
3.2	The local existence and uniqueness of the weak solution of problem I_a	34
3.2.1	$\mathcal{T}$ is well defined in $\mathbf{M}_T$ and maps $\mathbf{M}_T$ into $\mathbf{X}_T \times \mathbf{Y}_T$ for T small enough . .	35
3.2.2	The mapping $\mathcal{T}$ maps $\mathbf{M}_T$ to $\mathbf{M}_T$ for T small enough.	38
3.2.3	$\mathcal{T}$ is contractive in the $\mathbf{X}_T \times \mathbf{Y}_T$ norm with T small enough.	40
3.2.4	The continuous dependency on the data of the weak solution in $\mathbf{M}_T$	45
3.3	The continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to $cat(x)$ in $W^{1,\infty}(\Omega)$ for problem I_a with T small enough.	46
3.4	On the Frechet differentiability of r and c with respect to $cat(x)$ for problem I_a	49
3.4.1	The sensitivity system	50
3.5	Formulation and weak solution of problem I_b	65
3.6	Existence and uniqueness of the weak solution of problem I_b with $cat(t, x)$ model . .	67
3.7	Sensitivity system for the Problem I_b	68
3.8	Formulation and weak solution of the problem II_a	71
4	Optimization Problems	75
4.1	The first optimization problem	75
4.1.1	Frechet differentiability of the objective functional with respect to catalytic function	76
4.1.2	The existence of the solution of the first optimization problem	77
4.2	The second optimization problem	78
4.2.1	Calculation of the adjoint operator r_{cat}^* for Problem I_a	80
4.2.2	Calculation of the adjoint operator r_{cat}^* for Problem I_b	86
5	Numerical Implementation	91
5.1	Forward Problems	91
5.1.1	Piecewise basic functions of the spaces V_h	94
5.1.2	The θ scheme for numerical solving the problems I and II	96
5.1.3	Comparison between the implicit FDM and the FEM.	99
5.2	Some remarks on the Greedy algorithm in Problem II_b and I_b using FDM.	102
5.3	The continuous positioning	104
5.3.1	Transformation of discrete catalytic functions to smooth catalytic functions . .	107

5.3.2	cat(x) model (Problems I_a and II_a)	109
5.3.3	cat(t,x) model (Problems I_b and II_b)	109
5.3.4	Comparing the two catalyst positioning models: cat(x) and cat(t,x)	111
5.4	The optimization problems	111
5.4.1	The first optimization problem for Problem I_a	112
5.4.2	The second optimization problem	114
Conclusions		117
A Elementary Theorems, Lemmas and other concepts		119
Appendix		119
A.1	Elementary Lemmas and Theorems	119
A.2	Huber functions	120
A.2.1	Continuously differentiable Huber C^1 function	120
A.2.2	Continuously differentiable C^2 Huber function	122
A.3	The Gaussian distribution (Normal distribution)	123
APPENDICES		118
Bibliography		127

List of Figures

1.1	Characteristics of some metal/oxygen battery couples adapted from [32]	1
1.2	Oxygen solubility $C_{O_2,0}$ and diffusivity D_{O_2} of the four considered electrolytes. . . .	2
1.3	A simple sketch of lithium air batteries adopted from [32].	3
1.4	The radius of pore with different electrolytes before pore clogging (the radius reaches to 0.1). Li_2O_2 is deposited in here in the upper side.	5
1.5	The growth profile of Li_2O_2 with centered-catalyst positioning, refered from [8] . . .	5
1.6	(a) Evolution of the minimal free volume after pore clogging as a function of the number of placed catalysts along the pore axis in $DMSO^{Li+}$ for a threshold of 6%. The red line indicates the minimal free volume obtained with the continuous growth model. The numbers of catalysts corresponding to 90%, 99%, 100% of the final occupied volume are marked in red. (b) Optimal distributions of catalysts along the pore axis corresponding to the three different cases marked in (a). This Figure is refered from [8]	6
1.7	Schematic representation of the modeled cathode geometry with porosity ϵ and tortuosity τ adapted from [8]	8
1.8	The radius of pore at certain times before pore clogging.	11
5.1	The subdivision of $\Omega = [0, 1]$, $x_0 = 0, x_{J-1} = 1$	94
5.2	The piecewise linear finite element basis function $\Phi_i(x)$, $i \in [1, J - 3]$	95
5.3	The piecewise linear finite element basis function $\Phi_{J-2}(x)$	95
5.4	The pore radii and the concentration of oxygen inside pore before pore clogging with $J = N = 100$ solving with FDM and FEM	101
5.5	Free pore volume, relative deviation and runtime for the implicit and explicit FDM .	101
5.6	The pore radii and the concentration of oxygen inside pore before pore clogging with $J = 100$ and different N in Problem I	103
5.7	The optimal numbers of catalysts from 1 to 100 by Greedy algorithm in Problem II _b	104

LIST OF FIGURES

5.8	Comparison of radii and concentration inside the pore with two optimal numbers of catalyst before pore clogged by Greedy algorithm in Problem II_b	105
5.9	radii and concentration inside the pore with 47 optimal number catalyst by Greedy algorithm in Problem II_b	106
5.10	The distribution of optimal number of catalysts of 47 catalyst positions	107
5.11	radii and concentration inside the pore i line plotting with 41 optimal number catalyst by Greedy algorithm in Problem I_b	108
5.12	The distribution of optimal number of catalysts of 41 catalyst positions in Problem I_b	109
5.13	The transformation from the local optimal discrete catalytic functions by Greedy algorithm in Problem II_b before pore reaches to 0.1 and 0.86 to continuous ones, with $\sigma_{trans} = 0$ in (5.49)	110
5.14	The transformation from local optimal discrete catalytic functions by Greedy algorithm in Problem II_b before pore reaches to 0.1 and 0.86 to continuous ones, with $\sigma_{trans} = 7\Delta x$ in (5.49)	110
5.15	Comparing the two catalyst positioning models, experimenting with the center-catalyst positioning. The crosses show the catalytic function at the initial time. Blue lines present the growth profiles of discharged product Li_2O_2 deposited along the pore surface after pore clogging in Problem I_a . The red lines are the growth of Li_2O_2 according to Problem I_b	111
5.16	Initial $cat(x)$ and optimal $cat(x)$ for Problem I_a in grid of $J = N = 20$	112
5.17	Adjoint method and Greedy method with $J=100$, $N=80$, number of time steps $M=1000000$	115
5.18	Adjoint method and by Greedy method in Problem I_a with $J=100$, $N=60$, number of time steps $M=1000000$. The Li_2O_2 is deposited in the upper side in this plot	116
A.1	The graphic of Huber C^1 function $h_{1,\gamma}(x)$ with $g = 1$ and $\gamma = 2$	121
A.2	The graphic of C^1 Huber function $H_{1,\gamma,R_0}(x)$ with $g = 1/2$, $\gamma = 50$, and $R_0 = 0.94$	122
A.3	Graphic of C^2 Huber function with $\gamma = 2$	123
A.4	Graphic of C^2 function $H_{2,\gamma}(x)$ with $\gamma = 2$, $\epsilon = \frac{1}{\gamma}$, $c_0 = \frac{1}{\gamma}$	124
A.5	The normal density $f(x)$	125

Chapter 1

Introduction

1.1 Motivation

Portable electronic devices play important roles in our daily modern life. It is imperative to research the efficient and environmentally friendly way of storing and delivering energy. Lithium/air batteries recently attract great attention of many engineers and scientists because of many advantages. They have higher potential theoretical energy values in comparison with the other metal/air batteries as shown in 1.1. Besides, with a porous structure cathode, they also are the good candidate of the lighter power source for aerial vehicles, camping equipments compared with ion-Lithium battery [32]. There are basically two kinds of Lithium/ air batteries: aqueous and non-aqueous. The non-aqueous differs from the aqueous Lithium/air batteries in that the discharged products are insoluble in the aqueous electrolytes, [1], [29], [30], which leads to the pore's passivation. However, the aqueous Lithium/air batteries require an isolated protection layer between metallic Lithium and the electrolyte, that will significantly limits the Li^+ - conductivity. For this difficulty, most of literatures concerning on Lithium/air batteries studying on the non-aqueous electrolyte batteries. For a detail research on the capacities of aqueous, non-aqueous Li/air and Li-ion batteries we refer to the article of Christensen et al. [5].

The main reactions in non-aqueous electrolyte Li/air batteries is given by

Metal/O ₂ couple	Ideal cell reaction ^a	Calculated open-circuit voltage at 25 °C (V)	Theoretical specific energy ^b (Wh kg ⁻¹)	
			Including O ₂	Excluding O ₂
Li/O ₂	4Li + O ₂ ⇌ 2Li ₂ O	2.91	5200	11,140
Al/O ₂	4Al + 3O ₂ ⇌ 2Al ₂ O ₃	2.73	4300	8,130
Ca/O ₂	2Ca + O ₂ ⇌ 2CaO	3.12	2990	4,180
Zn/O ₂	2Zn + O ₂ ⇌ 2ZnO	1.65	1090	1,350

^a The reduction of O₂ to O₂²⁻ usually occurs only in the presence of a catalyst; often the product is the peroxide, O₂²⁻.

^b Includes only the active materials. Since O₂ does not have to be carried in the battery, values are given for the cases of including and excluding O₂. The battery weight will increase once the discharge begins.

Figure 1.1: Characteristics of some metal/oxygen battery couples adapted from [32]

Introduction

	$c_{O_2,0} [10^{-6} \frac{\text{mol}}{\text{cm}^3}]$	$D_{O_2} [10^{-6} \frac{\text{cm}^2}{\text{s}}]$
PC^{Li^+}	3.20	2.24
$\text{TEGDME}^{\text{Li}^+}$	4.43	2.17
$\text{DMSO}^{\text{Li}^+}$	2.10	16.70
DME^{Li^+}	9.56	12.20

Figure 1.2: Oxygen solubility $C_{O_2,0}$ and diffusivity D_{O_2} of the four considered electrolytes.

Laoire et al. in the articles [23] and [24] assume that the oxygen reduction reactions (ORR) at the cathode surface during the discharge process, oxygen is consumed by its reaction with Lithium ion and generating the insoluble lithium peroxide as

and the oxygen evolution reaction (OER) has been formulated to be a direct decomposition process of Li_2O_2 according to

However there are a number of fundamental and practical problems requiring careful investigation. In [32] and [8], these are mentioned as: the role of some specific catalysts in promoting the cathode electrode reaction, optimization of electrode porosity, the structure of the porous cathode, the composition of the cathode electrode, and the prevention of water or carbon dioxide from entering the cell when operated in air. According to [1], [29] and [30], a critical difficulty that we have to overcome is that the discharged oxygen reduction products is insoluble in the organic electrolytes. The low oxygen solubility causes the deposition of the discharged products to the oxygen transporting side as written in [32] and [8] via diffusion-limited model and in [30] via steady-state model.

This clogs the oxygen entrance to the pore to be reacted with Lithium ions and limits the capacity of the batteries by narrowing the active surface inside the pore. There are a number of works that attempt to study this limitation of the batteries' capacity like [41], [29], [3], [25]. They have shown that the specific capacity is enhanced when the current density is decreased. However, in order to support the battery performance and optimize the charging time, the current density should be kept high. Overall, we have to focus on investigating the thickness, porosity and the oxygen solubility

Figure 1.3: A simple sketch of lithium air batteries adopted from [32].

Introduction

and diffusivity in different electrolytes [30] and [36]. The study of [8] aims at optimizing the activity and catalytic distribution at the active surface of the cathode to maximize the free volume of the pore after pore clogging by the deposited discharged products. Besides, the suggested Greedy algorithm of [8] based on a discrete propagation model to express the Li_2O_2 growth profile inside the pore is quite advantaged for comparing the effect of the performance among different electrolytes: PC^{Li^+} , $TEGDME^{Li^+}$, DME^{Li^+} and $DMSO^{Li^+}$. Electrolytes are characterized by its oxygen solubility $c_{O_2,0}$ and oxygen diffusivity D_{O_2} of the four considered electrolytes are shown at 1.3. In conclusion, DME^{Li^+} and $DMSO^{Li^+}$ show up the highest specific capacity (actually DME^{Li^+} is higher in this term); however $DMSO^{Li^+}$'s advantage is the electrochemical stability especially toward the species being produced during the charging process (cf. [9]). For this reason, we choose $DMSO^{Li^+}$ as a good candidate electrolyte for our numerical experiments and our models for continuous catalytic model.

In this work, we aim at maximizing the capacity of the batteries by optimal catalyst positioning. We propose some reasonable distribution of catalyst along the porous cathode to optimize the utilization pore volume of the cathode of the batteries during oxygen reduction process. Our motivation is taken from the work of Dabrowski et al [8]. The authors focus on optimizing and positioning of catalytically active sites within the pores to maximize the volume of discharge products before pore clogging. The Figure 1.4 shows the radius of the pore before pore's passivation with different electrolytes. In order to optimize the pore volume utilization, they use a simple propagation scheme to describe the active deposition of the discharge product around its neighborhood. In that work, the authors propose a discrete catalyst model for the discharge process, where the catalytic function taking the value of 1 (switch on) if the radius of the deposited oxygen reduction products of the pore at the neighborhood points reach to a specific threshold, or the value of 0 (switch off) if the radius of discharged product below than that threshold. The diffusion-limited mathematical model demonstrating the dynamic of this oxygen reduction progress that they use for the discrete catalyst model is based on the paper from Sandhu et al. [32]. Lately, they optimize the number of the distributed catalyst positions by mean of the greedy method which is used widely in engineering.

In the left graph of 1.5, the authors in [8] simulate the discrete propagation's evolution of the posited amount of Li_2O_2 inside the pore with center-catalyst positioning with different thresholds. Those thresholds correspond to different kinetic growth, from the island forming for large threshold (Volmer-Weber growth) to a layer-by-layer growth for small thresholds (Frank-van-der-Merwe growth). Later in our time-dependent catalytic model, we also show those relative growth kinetics mechanisms. In the right hand side of Figure 1.5, it is the growth profile time evolution of Li_2O_2 with threshold of 4%-6%, the one that shows the more natural growth of oxygen reduce reaction product.

Then the maximal utilization of the cathode capacity is carried out using the greedy algorithm, denoting V_{free} free volume of a pore after clogging and consider it as the objective function. In this algorithm, a catalyst function is supposed to be a "switch on-off" function, that takes the values of either 0 or 1. This algorithm is implemented iteratively, whose every single step, an optimal catalyst position is sought and will be kept in the next step, with adding a new point with catalyst on. The new optimal catalyst position will be solved out in the next step, and the greedy algorithm will be stopped to be implemented until the next combination of catalyst show a greater the free volume V_{free} inside the pore. Figure 1.6 shows the optimal number and optimal distribution of catalyst along the pore axis in $DMSO^{Li^+}$ for a threshold of 6%.

Figure 1.4: The radius of pore with different electrolytes before pore clogging (the radius reaches to 0.1). Li_2O_2 is deposited in here in the upper side.

Figure 1.5: The growth profile of Li_2O_2 with centered-catalyst positioning, referred from [8]

Figure 1.6: (a) Evolution of the minimal free volume after pore clogging as a function of the number of placed catalysts along the pore axis in $DMSO^{Li+}$ for a threshold of 6%. The red line indicates the minimal free volume obtained with the continuous growth model. The numbers of catalysts corresponding to 90%, 99%, 100% of the final occupied volume are marked in red. (b) Optimal distributions of catalysts along the pore axis corresponding to the three different cases marked in (a). This Figure is referred from [8]

The numerical implementation in [8] is based on the Finite Difference Method (FDM). The greedy method stops when it reaches the first local solution of catalyst function. We would like to present a slightly better optimal solution, the more "global" one by checking the whole iterative steps. This result will be described in details in Chapter 5. Besides, we also suppose Finite Element Method (FEM) to approximate the system of partial differential equations with initial and mixed boundary conditions describing the charging process. All the related analysis and comparisons will be also handed out in this chapter.

Our main interest in this work is to approach to the catalyst positioning problem by proposing a smooth propagation process with a continuous catalytic model. For the optimization problem, we will deal with by two approaches: the sensitivity method and the adjoint method, which are presented in chapter 4. We refer the readers the next section of Mathematical setting for more understanding on the mathematical features of the problem.

1.2 Mathematical settings

The mathematical model for Lithium/ion batteries and its simulation we refer the readers to the series of papers [28], [27], [13] from Ohlberger M. et al. In this work, as mentioned above, we focus only on the mathematical setting for Lithium/air batteries. According to [8] and [32], during the oxygen reduction reaction process, the concentration of oxygen inside the pore drops fast from the oxygen entering side into the other side. As a result, the solid product Li_2O_2 is generated and as in the non-aqueous electrolyte environment, Lithium-dioxide is deposited in the surface of the cathode

pore, which is the reason of the decrease of free volume. With time the pore clogging takes place and limits the oxygen starvation along the pore, Li_2O_2 -generated reaction could not be occurred any more and the discharge process has to be stop. This circumstance happened due to the low oxygen solunility and diffusivity in non-aqueous electrolytes. Some of theoritical and experimental research had been carried out on this passivation of the cathode of Lithium/air batteries [30], [40]. The mathematical model of this process is presented firstly by Sandhu et al. [32] with the diffusion limited conditions, and later Dabrowski et al. in [8] propose a mathematical description that is based on the latter Sandhu's model and the finite-sized electrolyte phase of Andrei et al. in [3]. The numerical experiments in Chapter 5 will show that the two continuous (catalytic constant) models have the familiar behaviour. In this section, we would like to set up the non-constant continuous catalytic models, in order to have a more natural view in this catalyst positioning problem for Lithium-Air batteries. First, we present the two constant continuous catalytic model based on [32] and [8].

1.2.1 Mathematical setting of the diffusion-limited model for Li/air batteries

In [32] and [8] the authors have been considering the model of n cylindrical pores of radius r_p , the porous cathode of volume V_{cath} , length l , and porosity ϵ , and tortuosity τ . If $r_p \ll l$, we can assume that the oxygen concentration c_{O_2} is angularly symmetric about the diffusion direction or the radial direction along the pore. Thus, the mathematical model is described by dimensionless pore radius, oxygen concentrtrion and distance along the pore coordinate increasing toward to the interior side of the Cathode. Both of mathematical models ([32] and [8]) lead to systems of partial differential equations. The first equation is a reaction - diffusion equation based on Fickian diffusion in a pourous structure without convection [19].

$$\partial_{t_p}(\epsilon c_{O_2}) = \partial_{x_p}(D_{O_2}^{eff} \partial_{x_p} c_{O_2}) + v_R(C_{O_2}, \epsilon, r_p) \quad (1.4)$$

Here, $D_{O_2}^{eff}$ is the effective diffusion coefficient, which considers the impact of porosity ϵ and tortuosity τ on the oxygen mass diffusivity D_{O_2} via $D_{O_2}^{eff} = D_{O_2} \epsilon / \tau$ or the rate of Li_2O_2 along the active sites located at the pore surfaces per unit cathode.

$v_R(C_{O_2}, \epsilon, r_p)$ represents the rate of Li_2O_2 formation per unit of cathode volume (conversion rate, e.g. [8]). It is written by

$$v_R(C_{O_2}, \epsilon, r_p) = -\frac{2\epsilon}{r_p} k C_{O_2}, \quad (1.5)$$

where k is the reaction rate constant per unit pore.

The rate of decrease of pore volume per unit of porous cathode caused by the deposition of Li_2O_2 along the active site of pore surface is given by

$$\partial_{t_p} \epsilon = v_R(C_{O_2}, \epsilon, r_p) \frac{M_{Li_2O_2}}{\rho_{Li_2O_2}} \quad (1.6)$$

The mathematical model of Sandhu et al [32] assumes the constant tortuosity $\tau = \tau_0 = (\epsilon_0)^{\frac{1}{2}}$ with porosity $\epsilon = \epsilon_0$ independent of time. Meanwhile, Dabrowski et al. [8] use the Bruggeman relation

Figure 1.7: Schematic representation of the modeled cathode geometry with porosity ϵ and tortuosity τ adapted from [8]

between tortuosity τ and porosity ϵ by $\tau = \epsilon^{-\frac{1}{2}}$ [4]. From the Bruggman formula and the initial values of the pore radius, tortuosity and porosity, in conclusion, the porosity and the pore radius are related to each other by

$$\frac{\epsilon}{\epsilon_0} = \left(\frac{r_p}{r_p^0} \right)^2 \quad (1.7)$$

in the first mathematical model ([32]), and

$$\left(\frac{\epsilon}{\epsilon_0} \right)^{\frac{3}{2}} = \left(\frac{r_p}{r_p^0} \right)^2 \quad (1.8)$$

in the second formulation [8], that lead to the two final normalized reaction-diffusion equations as partial differential equations:

$$\frac{\partial}{\partial t}(r^{\frac{4}{3}}c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^{\frac{1}{3}}c, \quad (t, x) \in Q_T, \quad (1.9)$$

and

$$\frac{\partial}{\partial t}(r^2c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T. \quad (1.10)$$

The dimensionless quantities are introduced for the equation (1.9) and (1.10) as: $t = \frac{t_p D_{O_2}}{\tau l^2}$, $t = \frac{t_p D_{O_2} \sqrt{\epsilon_0}}{l^2}$, and $r = \frac{r_p}{r_p^0}$, $x = \frac{x_p}{l}$, $c = \frac{c_{O_2}}{c_{O_2,0}}$, $0 \leq r, c, x \leq 1$, $0 < t < T$.

Denoting $Q_T = [0, 1] \times [0, T]$ and $\Omega = [0, 1]$, each of equations (1.9), (1.10) accompanied with the equation of decreasing rate of pore volume

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)c, \quad (t, x) \in Q_T, \quad (1.11)$$

and the initial conditions:

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.12)$$

$$c(0, x) = h(x), \quad (1.13)$$

and mixed boundary conditions:

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.14)$$

$$c_x(t, 1) = 0, \quad (1.15)$$

where $r = r(t, x)$, $c = c(t, x)$ are the pore radius and oxygen concentration inside the pore, whose width is normalized by 1(cm).

Introduction

The parameter γ and β are given by

$$\begin{aligned}\beta &= \frac{2k\tau l^2}{D_{O_2} r_p^0}, \\ \gamma &= \frac{k c_{O_2} M_{Li_2O_2} / \rho_{Li_2O_2}}{D_{O_2} r_p^0 / \tau l^2},\end{aligned}\tag{1.16}$$

where

$$k = \frac{i_{\text{geom}} r_p^0}{4F C_{O_2} \epsilon_0 l \int_0^1 r c dx},\tag{1.17}$$

for the first case and

$$\begin{aligned}\beta &= \frac{2k\tau l^2}{D_{O_2} \sqrt{\epsilon_0} r_p^0}, \\ \gamma &= \frac{3 l_c^2 k_s c_{O_2} M_{Li_2O_2} / \rho_{Li_2O_2}}{2 D_{O_2} \sqrt{\epsilon_0} r_p^0},\end{aligned}\tag{1.18}$$

where the oxygen reduction rate k is calculated according to Faraday's laws for the current density change per unit of cathode length dx_p . For more detail we refer the readers to the references [32] and [8].

$$k = \frac{i_{\text{geom}} \bar{r}_p^0}{4F C_{O_2} \epsilon_0 l \int_0^1 r^{\frac{1}{3}} c dx}.\tag{1.19}$$

Now we summarize the above constant catalyst positioning models.

Definition 1.1 (Problems I and II) *Problem I: The first mathematical model of [32] as follows*

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T, \tag{1.20a}$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)c, \quad (t, x) \in Q_T \tag{1.20b}$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \tag{1.20c}$$

$$c(0, x) = h(x), \tag{1.20d}$$

$$c(t, 0) = 1, \quad t \in [0, T], \tag{1.20e}$$

$$c_x(t, 1) = 0, \tag{1.20f}$$

where β and γ are given by equations (1.16) and (1.17) problem I.

Problem II: The second mathematical model of [8]

$$\frac{\partial}{\partial t}(r^{\frac{4}{3}} c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^{\frac{1}{3}} c, \quad (t, x) \in Q_T, \tag{1.21a}$$

Figure 1.8: The radius of pore at certain times before pore clogging.

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c), \quad (t, x) \in Q_T \quad (1.21b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.21c)$$

$$c(0, x) = h(x), \quad (1.21d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.21e)$$

$$c_x(t, 1) = 0, \quad (1.21f)$$

with β and γ defined by equations (1.18) and (1.19).

For the parameters concerned are in the both Problems (Problem I and problems II) we refer to [32] and [8]:

Parameters	
$r_{p,0}[cm]$	$2.00 \cdot 10^{-7}$
$l_c[cm]$	0.07
ϵ_0	0.73
$M_{Li_2O_2}[\frac{g}{mol}]$	45.8765
$\rho_{Li_2O_2}[\frac{g}{cm^3}]$	2.3
$i_{geom}[\frac{mA}{cm^2}]$	0.1

In the next Chapters we mainly investigate Problem I. A short formulation of Problem II is considered in Section 3.8. The results can be obtained by similar techniques for Problem II as the analysis features of the two parabolic equations in the two problems has similarities. We refer the readers to the mathematical setting in Chapter 2 and Chapter 3 for details.

The volume of the discharged product Li_2O_2 increases during discharge process and the pore is clogged rapidly as demonstrated in the Figure 1.1. The idea of the Greedy algorithm for the discrete catalyst positioning model by Dabrowski et al. in [8] is based one the step-by-step choice of a consequent distribution that is determined on the minimizing progress of an objective functional (the

Introduction

free volume left in the pore after the clogging deposition of Li_2O_2 takes place). The main strategy of the Greedy algorithm is to restrict a global optimization to many local optimization problems. Although the Greedy algorithm is a very efficient approach for this optimization problem on the discrete catalyst positioning and for comparing the effect among different electrolyte, it has some following restrictions:

- (i) The Greedy method is a forward-optimized method that depends on choosing the local minimizations after every single nodal Greedy step, therefore the running time can take very long (several weeks with C++).
- (ii) The model that this method relies on is the discrete (catalytic function get number 0 where there is no catalyst, number 1 where catalyst is positioned), while positioning catalyst should be expressed more geometrically by a positive real function, with different positive values at the sites along the pore. The higher values of the catalytic function at the sites where catalyst amount is more, and the lower values for the less active sites along the pore.
- (iii) The fast-gradient-typed methods can be applied only for a more continuous catalyst positioning models.

Thus, our idea is to set some model of continuous catalyst positioning characterizing the active catalytic sites along the pore, to investigate the mathematical perspective of the forward problem as well as the related optimization problems and to implement them numerically. Hence, we can give some idea about the optimal geometrical positioning of catalyst to maximize the capacity of the batteries.

We will present the two ways of constructing a catalytic model on Problem I and II as follows

- (a) We firstly suppose that $cat(x)$ is catalyst positioning from the initial time. The value of $cat(x)$ shows us the active sites effected by catalyst sited along the pore. The growth profile of the discharged product during the ORR process inside the pore is expressed by the model in the problem I or II with slight adjustment by putting $cat(x)$ to the right hand side of the equation (1.20b) or (1.21b) (the equations considering the decrease of free pore volume with respect to the deposition of Li_2O_2 in the surface of the pore). This catalytic function does not change with time, it takes the values from 0 to 1.

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(x)c, \quad (t, x) \in Q_T \quad (1.22)$$

- (b) Learning from the growth kinetics in the nature like bacteria growth and the simple propagation from [8], we propose a time-dependent catalytic function, whose effect is that, once the growth of the solid Li_2O_2 reaches to a certain threshold value, this growing trend is propagated to the neighbourhood sites. The function $cat(x, t)$ is written by the following partial differential equation

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(t, x)c, \quad (t, x) \in Q_T \quad (1.23)$$

where $cat(t, x)$ satisfies

$$cat_t(t, x) = \alpha_0 \int_0^1 H_{R_0}(r(cat; y, t))G(x - y) dy, \quad (1.24)$$

and

$$cat(0, x) = cat_0(x), \quad (1.25)$$

where α_0 is some small positive constant, R_0 is a positive constant, $0 < R_0 < 1$. The Huber function $H_{R_0}(r)$ and Gaussian distribution $G(x - y)$:

$$G(x - y) = \frac{1}{2\pi} \exp(-\frac{1}{2}(x - y)^2) \quad (1.26)$$

are presented more in details in Appendix A.2 and A.3.

Definition 1.2 (Problems I_a , I_b and II_a , II_b)

Problem I_a : The first mathematical model of [32] in the $cat(x)$ catalyst positioning model as follows

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T, \quad (1.27a)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(x)c, \quad (t, x) \in Q_T, \quad (1.27b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.27c)$$

$$c(0, x) = h(x), \quad (1.27d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.27e)$$

$$c_x(t, 1) = 0, \quad (1.27f)$$

where β and γ are given by equations (1.16) and (1.17).

Problem I_b : The first mathematical model of [32] in the $cat(t, x)$ catalyst positioning model as follows

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T, \quad (1.28a)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(t, x)c, \quad (t, x) \in Q_T, \quad (1.28b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.28c)$$

$$c(0, x) = h(x), \quad (1.28d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.28e)$$

$$c_x(t, 1) = 0, \quad (1.28f)$$

$$cat_t(t, x) = \alpha_0 \int_0^1 H_{R_0}(r(cat; y, t))G(x - y) dy, \quad cat(0, x) = cat_0(x), \quad (1.28g)$$

Introduction

with β and γ defined by equations (1.18) and (1.19).

Problem II_a: The first mathematical model of [8] in the $cat(t, x)$ catalyst positioning model as follows

$$\frac{\partial}{\partial t}(r^{\frac{4}{3}}c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^{\frac{1}{3}}c, \quad (t, x) \in Q_T, \quad (1.29a)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(x)c, \quad (t, x) \in Q_T, \quad (1.29b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.29c)$$

$$c(0, x) = h(x), \quad (1.29d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.29e)$$

$$c_x(t, 1) = 0, \quad (1.29f)$$

where β and γ are given by equations (1.16) and (1.17).

Problem II_b: The first mathematical model of [8] in the $cat(t, x)$ catalyst positioning model as follows

$$\frac{\partial}{\partial t}(r^{\frac{4}{3}}c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^{\frac{1}{3}}c, \quad (t, x) \in Q_T, \quad (1.30a)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(t, x)c, \quad (t, x) \in Q_T, \quad (1.30b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (1.30c)$$

$$c(0, x) = h(x), \quad (1.30d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (1.30e)$$

$$c_x(t, 1) = 0, \quad (1.30f)$$

$$cat_t(t, x) = \alpha_0 \int_0^1 H_{R_0}(r(cat; y, t))G(x - y) dy, \quad cat(0, x) = cat_0(x), \quad (1.30g)$$

with β and γ defined by equations (1.18) and (1.19).

1.2.2 Optimization Problems on catalyst positioning models

We herein would like to formulate the optimization problem of this catalyst positioning model.

1.2.2.1 The first optimization problem

We now aim at setting the optimization problems in order to maximize the volume of discharged products deposited before pore clogging. The first approach, we consider the minimization problem

of remaining pore volume with $T, 0 < T < \infty$ is the some final time.

For Problem I_a and Problem II_a , the free volume $V(cat)$ of the pore after some time T is defined by:

$$V(cat) = \int_0^1 r^2(cat; T, x) dx, \quad (1.31)$$

For Problem I_b and Problem II_b , the free volume $V(cat_0)$ of the pore after some time T is defined by:

$$V(cat_0) = \int_0^1 r^2(cat_0; T, x) dx, \quad (1.32)$$

We give the definition of the first optimization problem as follows:

Definition 1.3 (i) *The first optimization problem is for Problem I_a (alternatively for Problem II_a)*

$$\min_{cat \in A} V(cat), \quad (1.33)$$

where A is some set of catalytic function $cat(x)$, subject to Problem I_a (or Problem II_a alternatively).

(ii) *The first optimization problem is for Problem I_b (alternatively for Problem II_b)*

$$\min_{cat \in A_{cat_0}} V(cat_0), \quad (1.34)$$

where A_{cat_0} is some set of catalytic function at the initial time $cat(0, x) = cat_0(x)$, subject to Problem I_b (or Problem II_b alternatively).

The two problem (1.33) and (1.34) will be solved by dealing with the sensitivity systems and adjoint systems in chapter 4.

1.2.2.2 The second optimization problems

For the convenience to apply the adjoint method that we will present also in the Chapter 4, the second optimization problem, that minimizes the mean value of free volume in the pore in a small interval of time $[T_1, T]$. Therefore,

for Problem I_a and Problem II_a , we wish to minimize

$$\mathcal{V}(cat) = \int_{T_1}^T \int_0^1 r^2(cat; t, x) dx dt, \quad (1.35)$$

for Problem I_b and Problem II_b , the objective functional is defined by

$$\mathcal{V}(cat_0) = \int_{T_1}^T \int_0^1 r^2(cat_0; t, x) dx dt, \quad (1.36)$$

We give the definition of the first optimization problem as follows.

Definition 1.4 (i) *The first optimization problem is for Problem I_a (alternatively for Problem II_a)*

$$\min_{cat \in A} \mathcal{V}(cat), \quad (1.37)$$

where A is some set of catalytic function $cat(x)$, subject to Problem I_a (or Problem II_a alternatively).

(ii) *The first optimization problem is for Problem I_b (alternatively for Problem II_b)*

$$\min_{cat \in A_{cat_0}} \mathcal{V}(cat_0), \quad (1.38)$$

where A_{cat_0} is some set of catalytic function at the initial time $cat(0, x) = cat_0(x)$, subject to Problem I_b (or Problem II_b alternatively).

1.3 The main results of the Thesis

In the Chapter Introduction we present an overview on the subject of the Thesis and then the mathematical form with two "soft" propagation models of the catalyst problem and formulate the optimization problems on those models.

In the Chapter 1, we summarize some basic notions and results needed to the next Chapters.

In the chapter 2, the well-posedness of the forward problem is proved with choosing the appropriate functional spaces of the related parameters and variables. The Fréchet differentiability of the pore radius and the oxygen concentration with respect to catalytic function is also established in the related functional spaces.

In the chapter 3, the existence of the solution of optimization problems is considered by mean of sensitivity method and adjoint method. The ways to solve those optimization problems are shown therein.

In chapter 4, we solve numerically the optimization problem. Some methods are carried out to calculate the Frechet gradient in order to minimize optimal functional. We also propose some potential local optimal solutions of catalytic functions to the optimization problem.

For the sake of clarity for readers we make the following tables to indicates the proofs for the PDEs models: The existence, uniqueness of the solutions, the differentiability of parameter-to-state map r_{cat} or r_{cat_0} , the solvability of the two optimization methods and the numerical implementations:

- (i) The table 1.1 illustrates the existence, uniqueness of the solutions and the differentiability of parameter-to-state map for Problem I_a and I_b . In the chapter 3, Sections 3.1-3.2, we prove the well-posedness of the Problem I_a and the Frechet differentiability of radius r with respect to catalytic function $cat(x)$ in Section 3.4. In the Sections 3.6-3.7, we state the proofs of the well-posedness and the Frechet differentiability of radius r with respect to catalytic function $cat(x)$ of the Problem I_b . The proofs for the Problem II , II_a , II_b are supposed to achieve analogously.

Table 1.1: The well-posedness of solution and the differentiability of the parameter-to-state r_{cat} or r_{cat_0} for Problem I_a and I_b .

	I_a	I_b
The well-posedness	Sections 3.1-3.2	Section 3.6
The differentiability of r_{cat}	Section 3.4	Section 3.7

- (ii) The two optimization problems for the Problem I_a and I_b are considered in Chapter 4 and demonstrated in the table 1.2. We apply the sensitivity method for the first optimization problem and the adjoint method for the second optimization problem.

Table 1.2: The two optimization problems I_a and I_b

	I_a	I_b
The first optimization problem using sensitivity method	Section 4.2	Section 4.2
The second optimization problem using adjoint method	Subsection 4.2.1	Subsection 4.2.2

- (iii) In the Chapter 5 we consider the implementation for two optimization problems for the Problem I_a , that is expressed in the table 1.3.

Table 1.3: Numerical implementation for optimization problems

	I_a
The first optimization problem	Subsection 5.4.1
The second optimization problem	Subsection 5.4.2

Chapter 2

Mathematical preliminaries

This Chapter is devoted to provide some basic notions in Functional Analysis needed for linear parabolic equations in Hilbert spaces, and as well as some concepts of optimization theory. We start by giving definitions of Sobolev spaces and Sobolev-Bochner spaces and then parabolic PDEs with mixed boundary conditions, the regularity of its solution, delivery the solvability of the mixed boundary value problems.

2.1 Elementary concepts for PDEs

2.1.1 Sobolev spaces

Let Ω be an open, bounded subset of $\mathbb{R}^n$, $n = 1, 2, 3$.

Definition 2.1 (Weak partial derivative, p. 212, [12]) Let $L^1_{loc}(\Omega)$ be the set of locally integrable functions defined on the open set Ω . Suppose $u, v \in L^1_{loc}(\Omega)$, and α is multi-index. We say that v is the α^{th} -weak partial derivative of u , written

$$D^\alpha u = v, \quad (2.1)$$

provided

$$\int_{\Omega} u D^\alpha \varphi dx = (-1)^{|\alpha|} \int_{\Omega} v \varphi dx, \text{ for all } \varphi \in C_c^\infty(\Omega), \quad (2.2)$$

where $C_c^\infty(\Omega)$ denotes the space of infinitely differentiable functions $\varphi : \Omega \rightarrow \mathbb{R}$, with compact support in Ω . Here, $D^\alpha \varphi$ is defined as

$$D^\alpha \varphi = \frac{\partial^{|\alpha|} \varphi}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}$$

In this Thesis we need the following standard Sobolev spaces (See [20], [21], [12], [35])

Definition 2.2 (Space $H^1(\Omega)$) The Sobolev space $H^1(\Omega)$ is the set of all elements $u(x) \in L^2(\Omega)$ having weak (distributional) derivatives $\frac{\partial u}{\partial x_i} \in L^2(\Omega)$, $i = 1, \dots, n$, with scalar product

$$(u, v)_{H^1(\Omega)} := \int_{\Omega} u v + \sum_{i=1}^n \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_i} dx. \quad (2.3)$$

Definition 2.3 The Sobolev space H_0^1 is the completion of $C_0^1(\Omega)$ in the norm of $H^1(\Omega)$. In case Ω is piecewise Lipschitz boundary, we have

$$H_0^1(\Omega) = \{u \in H^1(\Omega), u|_{\partial\Omega} = 0\}.$$

Space $H^{-1}(\Omega)$ is dual space to space $H_0^1(\Omega)$. Space $(H^1(\Omega))'$ is dual space to space $H^1(\Omega)$.

Definition 2.4 For $f \in H^{-1}(\Omega)$ we define the norm

$$\|f\|_{H^{-1}(\Omega)} = \sup \left\{ \langle f, v \rangle \mid v \in H_0^1(\Omega), \|v\|_{H_0^1(\Omega)} \leq 1 \right\}$$

The functional space H^{-1} can be characterized as follows [12].

Theorem 2.5 1. Assume that $f \in H^{-1}(\Omega)$. Then there exist functions $f^0, f^1 \in L^2(\Omega)$ such that

$$\langle f, v \rangle = \int_{\Omega} (f^0 v + f^1 v_x) dx \quad (\forall v \in H_0^1(\Omega)) \quad (2.4)$$

2. Furthermore,

$$\|f\|_{H^{-1}(\Omega)} = \inf \left\{ \left(\int_{\Omega} \sum_{i=0}^1 |f^i|^2 dx \right)^{\frac{1}{2}} \mid f \text{ satisfies (2.4) for } f^0, f^1 \in L^2(\Omega) \right\}$$

2.1.2 Spaces involving time

To study the evolution equations, we need spaces involving time (section 23.5 in [38], Chapter 4 [37], [22] and chapter 5 in [12]).

Let X be a Banach space with norm $\|\cdot\|_X$.

Definition 2.6 P.285 [12] The space $L^p(0, T; X)$ consists of all measurable functions $u : [0, T] \rightarrow X$ with

1.

$$\|u\|_{L^p(0, T; X)} := \left(\int_0^T \|u(t)\|_X^p dt \right)^{\frac{1}{p}} < \infty$$

for $1 \leq p \leq \infty$, and

2. Mathematical preliminaries

2.

$$\|u\|_{L^\infty(0,T;X)} := \operatorname{esssup}_{0 \leq t \leq T} \|u(t)\|_X < \infty.$$

Definition 2.7 P.285 [12] The space $C(0, T; X)$ comprises all continuous functions $u : [0, T] \rightarrow X$ with

$$\|u\|_{C(0,T;X)} := \max_{0 \leq t \leq T} \|u\| \leq \infty.$$

A basic definition of studying evolution equations is the definition of generalized (weak) derivatives in time.

Definition 2.8 (Weak time derivative, P.285 [12]) Let $u \in L^1(0, T; X)$. we say $v \in L^1(0, T; X)$ is the weak derivative of order n of u , written

$$u^{(n)} = v,$$

provided

$$\int_0^T \phi^{(n)}(t) u(t) dt = (-1)^n \int_0^T \phi(t) v(t) dt \quad (2.5)$$

for all scalar test functions $\phi : (0, T) \rightarrow \mathbb{R}, \phi \in C_c^\infty(0, T)$.

This is a direct generalization of the notion of the weak derivative of real-valued functions. The integrals in (2.5) are vector-valued Lebesgue integrals (or Bochner integrals), which are defined by the Lebesgue integral of an integrable real-valued function as the L^1 -limit of integrals of simple functions. See [Wloka] for further understanding such integrals and the weak derivative of vector-valued functions.

Proposition 2.9 (Existence of $u^{(n)}$) P.120 [38] Assume that $V \subset H \subset V^*$ is an evolution triple, and let $1 \leq p, q \leq \infty, 0 < T < \infty$. Then the following statements are valid

- (i) *Uniqueness.* For $u \in L_p(0, T; V)$, the weak derivative $u^{(n)}$ is unique as an element of $L_q(0, T; V^*)$.
- (ii) *Existence.* Let $u \in L_p(0, T; V)$. Then there exists the weak derivative $u^{(n)} \in L_q(0, T; V^*)$ if there is a function $w \in L_q(0, T; V^*)$ such that

$$\int_0^T (u(t)|v)_H \varphi^{(n)}(t) dt = (-1)^n \int_0^T \langle w(t), v \rangle_{V^*} \varphi(t) dt.$$

Then $u^{(n)} = w$ and

$$\frac{d^n}{dt^n} (u(t)|v)_H = \langle u^{(n)}(t), v \rangle_{V^*}$$

holds for all $v \in V$ and almost all $t \in [0, T]$. Here, $\frac{d^n}{dt^n}$ denoted by the n -th weak derivative of real functions on $[0, T]$.

Proof. We refer Zeidler [38], proposition 23.20. ■

Proposition 2.10 (The space $W_p^1(0, T; V, H)$). Let $V \subset H \subset V^*$ is an evolution triple, and let $1 < p < \infty$, $p^{-1} + q^{-1} = 0$ and $0 < T < \infty$. Then the following statements hold

:

(i) The space $W_p^1(0, T; V, H)$. The set of all $u \in L^p(0, T; V)$ that have weak derivatives

$$u' \in L^q(0, T; V^*)$$

forms a real Banach space with the norm

$$\|u\|_{W_p^1} := \|u\|_{L^p(0, T; V)} + \|u'\|_{L^q(0, T; V^*)}$$

We will denote this space by $W_p^1(0, T; V, H)$

(ii) Regularization. The embedding

$$W_p^1(0, T; V, H) \hookrightarrow C([0, T]; H)$$

is continuous.

(iii) Integral by parts. For all $u, v \in W_p^1(0, T; V, H)$ and arbitrary t, s with $0 \leq s \leq t \leq T$, the following generalized formula of integration by parts holds:

$$(u(t)|v(t))_H - (u(s)|v(s))_H = \int_s^t \langle u'(\tau), v(\tau) \rangle_V d\tau + \langle u(\tau), v'(\tau) \rangle_V d\tau.$$

Here, the values $u(t), v(t), u(s), v(s)$ are the values of the continuous functions $u, v : [0, T] \rightarrow H$ in sense of (ii).

Proof. We refer Zeidler [38], proposition 23.23 and problem 23.10. ■

Lemma 2.11 [35] For all $y, p \in W(0, T; H^1(\Omega))$ the formula of integration by part holds

$$\int_0^T (y'(t), p(t))_{H_0^{-1}(\Omega), H_0^1(\Omega)} dt = (y(T), p(T))_{L^2(\Omega)} - (y(0), p(0))_{L^2(\Omega)} - \int_0^T (p'(t), y(t))_{H_0^{-1}(\Omega), H_0^1(\Omega)} dt.$$

Taking $p = y$ in the formula of integration by parts, we find that any $y \in W(0, T; H^1(\Omega))$ satisfies the useful identity

$$\int_0^T (y'(t), y(t))_{H_0^{-1}(\Omega), H_0^1(\Omega)} dt := \frac{1}{2} \|y(T)\|_{L^2(\Omega)}^2 - \frac{1}{2} \|y(0)\|_{L^2(\Omega)}^2.$$

Definition 2.12 We also define

$$W(0, T; H^1(\Omega)) = \{u : u \in L^2(0, T; H_0^1(\Omega)), u' \in L^2(0, T; H^{-1}(\Omega))\},$$

and

$$W(0, T; H^1(\Omega)) = \{u : u \in L^2(0, T; H^1(\Omega)), u' \in L^2(0, T; (H^1(\Omega))')\}$$

Lemma 2.13 (Variational lemma). *Let V be Banach space. Then it follows from $u \in L^1(0, T; X)$ and*

$$\int_0^T \varphi(t)u(t) dt = 0 \text{ for all } \varphi \in C_c^\infty(0, T)$$

that $u = 0$ in $L^1(0, T, X)$, i.e.,

$$u(t) = 0 \text{ for almost all } t \in [0, T]$$

Proof. We refer Zeidler [38], proposition 23.10. ■

Definition 2.14 Taking $\Omega = (0, 1)$, denote $Q_T = (0, T] \times \Omega$, we define space:

$$W^{1,\infty}(Q_T) = \{r \in L^\infty(Q_T), r_t \in L^\infty(Q_T), r_x \in L^\infty(Q_T)\},$$

2.2 Mixed boundary value problem for one-dimensional linear parabolic equations

We will use Fixed-point theory to approach our system of PDEs (problem *I* and *II* with different continuous catalyst models for Lithium/air batteries: Problems I_a, II_a, I_b, II_b). Every system consists of a diffusion equation and a decreasing radius equation. By mean of the Fixed-point method, we can consider only the diffusion equation in term of the equation of oxygen concentration c (the radius r is fixed). This diffusion equation leads us to considering an one-dimensional mixed boundary value parabolic equation, which is described as follows:

We assume Ω, Q_T are defined in Definition 2.14 for some fixed time $T > 0$. Consider the initial/boundary-value problem

$$\begin{cases} u_t + \mathcal{L}u = f, & \text{in } Q_T \\ u(t, 0) = 0, u_x(1) = 0, & t \in [0, T], \\ u(0, x) = u_0, & x \in \Omega, \end{cases} \quad (2.6)$$

where $f : Q \rightarrow \mathbb{R}$ and $u_0 : \Omega \rightarrow \mathbb{R}$ are given, and $u = u(t, x)$ is unknown, the operator $\mathcal{L}$ denotes for each $t \in [0, T]$ the second-order non-divergence partial differential operator

$$\mathcal{L}u = -a(t, x)u_{xx} + b(t, x)u_x + c(t, x)u, \quad (2.7)$$

for given coefficients $a(t, x), b(t, x), c(t, x)$ and

$$a(t, x) > \theta > 0, \text{ for a.e. } (x, t) \in Q_T. \quad (2.8)$$

Denote by $V = \{v \in H^1(\Omega), v(0) = 0\}$, and endow it with the scalar product:

$$\|v\|_V = \int_0^1 u_x v_x dx.$$

Define the bilinear formula:

$$B[u, v; t] := \int_{\Omega} a(\cdot, t) u_x v_x + (b(\cdot, t) + a_x(\cdot, t)) u_x v + c(\cdot, t) u v dx \quad (2.9)$$

for $u, v \in V$ a.e. $0 \leq t \leq T$.

To formulate a definition of a weak solution of the problem (2.6), we formally multiply (2.6) by a test function $v \in V$, integrate the result over Ω , and apply the formula of integration by part, we get

$$\langle u'(t), v \rangle_{V, V'} + B[u(t), v; t] = (f(t), v)_{L^2(\Omega)}, \text{ for a.e } 0 \leq t \leq T, \quad (2.10)$$

where B is defined by (2.9). In the equation (2.10), we have used the “vector-valued” notion $u(t) = u(\cdot, t)$. Further, in order to ensure that the definition of weak solution makes sense, we need the following assumptions.

Assumption 2.15 Assume that

(i) the coefficients of B in the formula (2.9) satisfy

$$a(x, t), a_x(x, t), b(x, t), c(x, t) \in L^\infty(Q_T). \quad (2.11)$$

(ii) Operator $\frac{\partial}{\partial t} + \mathcal{L}$ is the parabolic operator.

(iii) $f \in L^2(0, T; (H^1(\Omega))')$ and $u_0 \in L^2(\Omega)$.

We denote the duality pairing between $H^1(\Omega)$ and $(H^1(\Omega))'$ by

$$\langle \cdot, \cdot \rangle_{H^1(\Omega), (H^1(\Omega))'} : H^1(\Omega) \times (H^1(\Omega))' \rightarrow \mathbb{R}.$$

Now we introduce the definition of the weak solution as follows

Definition 2.16 (Weak solution of the problem (2.6)) We say that a function $u \in W(0, T; V)$ is a weak solution of the parabolic initial/boundary-value problem (2.6) if

1.

$$\langle u', v \rangle + B[u, v; t] = \langle f, v \rangle \quad (2.12)$$

for each $v \in V$ and for a.e. $t \in [0, T]$,

2. $u(0) = u_0$.

The initial condition $u(0) = u_0$ has meaning since $W(0, T; V) \hookrightarrow C(0, T; L^2(\Omega))$ (Proposition 2.10, item (ii)).

Since the coefficients of B are uniformly bounded in time, it repeating the proof of Theorem 2, p. 300 [12]. We have the following result:

Lemma 2.17 (*Energy estimate*). *There exist constants $\alpha, \beta > 0$ and $\gamma \geq 0$ such that*

(i)

$$|B[u, v]| \leq \alpha \|u\|_V \|v\|_V$$

and

(ii)

$$\beta \|u\|_V^2 \leq B[u, u] + \gamma \|u\|_{L^2(\Omega)}^2,$$

for all $u, v \in V$.

For further proof, we need also the following Theorem

Theorem 2.18 *There exist functions $\omega_k = \omega_k(x)$, $k = 1, 2, \dots$, that are*

(i) $\{\omega_k\}_{k=1}^\infty$ is an orthogonal basic of V .

(ii) $\{\omega_k\}_{k=1}^\infty$ is an orthonormal basic of $L^2(\Omega)$.

Proof. Following the proof from Theorem 1 (Eigenvalues of symmetric elliptic operators), p.335 [12] with replacing the Dirichlet boundary problem for elliptic equation by the mixed boundary problem for elliptic equations. Finally we choose $\{\omega_k\}_{k=1}^\infty$ the eigenfunctions of $L = -\Delta$ in V . ■

The first section of Chapter 7, Evans [12] is devoted to studying the weak solution of parabolic equations of the Dirichlet problem. The existence and regularity of weak solutions are established by the use of L^2 -energy estimates via the Galerkin method. For the regularity results, it is assumed that the coefficients of L are smooth on Ω and independent of t , which are not suitable for Problem I_a , I_b , II_a and II_b . We will then rely basically on the results from Evans [12] to prove the basic results on solving the mixed boundary condition (2.6) such as the existence, uniqueness and regularity of the weak solution.

We shall use the Galerkin method in chapter 7, [12] for studying the system (2.6) by approximating u by

$$u_m(t) := \sum_{k=1}^m d_m^k(t) \omega_k, \quad (2.13)$$

where

$$d_m^k(0) = (u_0, \omega_k), k = 1, \dots, m \quad (2.14)$$

To seek the function u_m , we project the equation (2.6) onto V_m , that leads to a systems of ordinary differential equations (ODEs) for u_m

$$(u_m', \omega_k) + B[u_m, \omega_k; t] = (f, \omega_k), \quad (2.15)$$

with $k = 1, \dots, m$ and $t \in [0, T]$. which by mean of the standard existence theory for ODEs has unique absolutely continuous solution. We recall the Theorem 1 (Construction of approximate solution) in p. 354 [12]:

Theorem 2.19 *For each integer $m = 1, 2, \dots$ there exists a unique function u_m of the form (2.13), satisfying (2.14) and (2.15).*

Theorem 2.20 *There exist a constant C , depending on Ω, T and the coefficient of B , such that*

$$\begin{aligned} \max_{0 \leq t \leq T} \|u_m(t)\|_{L^2(\Omega)} + \|u_m\|_{L^2(0, T; V)} + \|u_m'\|_{L^2(0, T; V')} &\leq \\ &\leq C \left(\|f\|_{L^2(0, T; L^2(\Omega))} + \|u_0\|_{L^2(\Omega)} \right), \end{aligned} \quad (2.16)$$

for $m = 1, 2, \dots$

Next, we let $m \rightarrow \infty$ to build a weak solution. According to the uniform estimates in (2.16), we see that the uniform bounds of the sequence $\{u_m\}$ in $W(0, T; V)$ is weakly compact in $W(0, T; V)$. We get the result about the existence of the weak solution:

Theorem 2.21 *Suppose that the assumptions 2.15 are satisfied. Then there exists a weak solution $u \in W(0, T; V)$ of the equation (2.6), and in fact*

$$u \in L^2(0, T; V) \cap L^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^2(\Omega)).$$

Reminding that the norm of V and $H^1(\Omega)$ are equivalent, we have estimate

$$\begin{aligned} \text{ess sup}_{[0, T]} \|u(t)\|_{L^2(\Omega)} + \|u\|_{L^2(0, T; H^1(\Omega))} + \|u'\|_{L^2(0, T; V')} &\leq \\ &\leq C \left(\|f\|_{L^2(0, T; L^2(\Omega))} + \|u_0\|_{H_0^1(\Omega)} \right). \end{aligned} \quad (2.17)$$

Theorem 2.22 *Suppose that the assumptions 2.15 are satisfied. Then the weak solution of the equation (2.6) is unique.*

Theorem 2.23 (Improved regularity)

Suppose $u \in W(0, T; V)$ is the weak solution of (2.6), where $\mathcal{L}$ is defined in 2.7. Suppose that the coefficients of $\mathcal{L}$ satisfies Assumptions 2.15 and

$$a_i(t, x) \in L^\infty(Q_T), \quad (2.18)$$

Assume also

$$u_0 \in V, f \in L^2(0, T; L^2(\Omega)).$$

Then

$$u \in L^2(0, T, H^2(\Omega)) \cap L^\infty(0, T; V), u' \in L^2(0, T; L^2(\Omega)),$$

and we have the estimate

$$\begin{aligned} \operatorname{ess\,sup}_{[0, T]} \|u(t)\|_V + \|u\|_{L^2(0, T; H^2(\Omega))} + \|u'\|_{L^2(0, T; L^2(\Omega))} &\leq \\ &\leq C \left(\|f\|_{L^2(0, T; L^2(\Omega))} + \|u_0\|_V \right). \end{aligned} \quad (2.19)$$

Proof. (Following the proof of Theorem 5, p. 360, [12].)

Multiplying the equation (2.15) by $d_m^k(t)$, and summing up all $k = 1, \dots, m$ we get

$$(u'_m, u'_m) + B[u_m, u'_m] = (f, u'_m), \text{ for a. e. } 0 \leq t \leq T. \quad (2.20)$$

We have

$$\begin{aligned} B[u_m, u'_m] &= \int_0^1 a(x, t) u_{m,x} u'_{m,x} + (b(x, t) + a_x(x, t)) u_{m,x} u'_m + c(x, t) u_m u'_m dx = \\ &= \frac{d}{dt} \left(\frac{1}{2} A[u_m, u_m] \right) - \frac{1}{2} \int_0^1 a_t u_{m,x} u_{m,x} dx + \int_0^1 (b(x, t) + a_x(x, t)) u_{m,x} u'_m + c(x, t) u_m u'_m dx =: \mathbf{A} + \mathbf{B}, \end{aligned} \quad (2.21)$$

where $\mathbf{A} = \frac{d}{dt} \left(\frac{1}{2} A[u_m, u_m] \right)$ with the symmetric bilinear form

$$A[u, v] := \int_0^1 a(x, t) u_{m,x} v_{m,x} dx, \quad u, v \in V$$

We have

$$|\mathbf{B}| \leq \left(C + \frac{C}{\epsilon} \right) \|u_m\|_V^2 + \epsilon \|u'_m\|_{L^2(\Omega)}^2, \text{ and } |(f, u'_m)| \leq \frac{C}{\epsilon} \|f\|_{L^2(\Omega)}^2 + \epsilon \|u'_m\|_{L^2(\Omega)}^2 \quad (2.22)$$

for $\epsilon > 0$.

Combining the above inequalities and the equation (2.20), we obtain

$$\begin{aligned} \|u'_m\|_{L^2(\Omega)}^2 + \frac{d}{dt} \left(\frac{1}{2} A[u_m, u_m] \right) &\leq \\ &\leq \left(\frac{C}{\epsilon} + C \right) \|u_m\|_V^2 + \frac{C}{\epsilon} \|f\|_{L^2(\Omega)}^2 + 2\epsilon \|u'_m\|_{L^2(\Omega)}^2 \end{aligned} \quad (2.23)$$

Choosing $\epsilon = \frac{1}{4}$ and integrating with respect to t over $[0, T]$, we get

$$\begin{aligned}
 & \int_0^T \|u'_m\|_{L^2(\Omega)}^2 dt + \sup_{0 \leq t \leq T} A[u_m(t), u_m(t)] \leq \\
 & \leq C \left(A[u_m(0), u_m(0)] + \int_0^T \|u_m\|_V^2 + \|f\|_{L^2(\Omega)}^2 dt \right) \leq \\
 & \leq C \left(\|u_0\|_V^2 + \|f\|_{L^2(0,T;L^2(\Omega))}^2 \right),
 \end{aligned} \tag{2.24}$$

according to equation (2.13) and (2.14), we can estimate $\|u_m(0)\|_V \leq \|u_0\|_V$. Furthermore as $A[u, u] \geq \theta \int_0^1 |Du|^2 dx$ for all $u \in V$, we have that

$$\sup_{0 \leq t \leq T} \|u(t)\|_V^2 \leq C \left(\|u_0\|_V^2 + \|f\|_{L^2(0,T;L^2(\Omega))}^2 \right). \tag{2.25}$$

Passing to limits as $m \rightarrow \infty$, we deduce $u \in L^\infty(0, T; V)$, $u' \in L^2(0, T, L^2(\Omega))$:

$$\|u\|_{L^\infty(0,T;V)} + \|u'\|_{L^2(0,T,L^2(\Omega))} \leq C \left(\|u_0\|_V^2 + \|f\|_{L^2(0,T;L^2(\Omega))}^2 \right). \tag{2.26}$$

In order to prove that $u \in L^2(0, T; H^2(\Omega))$ we recall the equation

$$(u', v) + B[u, v] = (f, v), \text{ for each } v \in V$$

We rewrite as

$$B[u, v] = (h, v),$$

where $h := f - u'$. As $h(t) \in L^2(\Omega)$, for a.e. $0 \leq t \leq T$.

We have for a.e. $0 \leq t \leq T$

$$u_{xx} = \frac{1}{a(t, x)} (b(t, x)u_x + c(t, x)u - h),$$

then we deduce the estimate

$$\|u\|_{H^2(\Omega)}^2 \leq C \left(\|h\|_{L^2(\Omega)}^2 + \|u_x\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\Omega)}^2 \right) \leq C \left(\|f\|_{L^2(\Omega)}^2 + \|u'\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\Omega)}^2 \right) \tag{2.27}$$

Integrating the above estimate and using the estimates from (2.26), we complete the proof for this theorem. ■

2.3 Convex analysis

The aim of this subsection is to provide an overview about convex analysis that are needed in the following. Some notations and basic facts will be introduced, for more details we refer to [7]. For minimizing the functionals in the following, we need to introduce the concept of derivatives of functionals and the optimization methods. They can be regarded as an analogous case to directional or total derivatives of real functions: Gateaux derivative or Fréchet derivative.

Let X and Y Banach spaces and a given map $f : U \rightarrow Y$, where $U \subset X$ is an open subset.

Definition 2.24 (*G-derivative at a point*). The map f is called *Gâteaux-differentiable* (*G-differentiable*) at $x \in U$ if there exists a map $T : X \rightarrow Y$ such that

$$f(x + th) - f(x) - tT(h) = o(t), \quad t \rightarrow 0,$$

for all $h \in X$, with $\|h\|_X = 1$. The map $T =: f'(x)$ is the *Gâteaux derivative* of f at x and is defined by $\partial G f(x, h) = f'(x)h$.

Definition 2.25 (*F-derivative at a point*). The map f is called *Fréchet-differentiable* (*F-differentiable*) at $x \in U$ if there exists a linear map $T \in L(X, Y)$ such that

$$f(x + h) - f(x) - Th = R(x, h), \quad \lim_{\|h\|_X \rightarrow 0} \frac{\|R(x, h)\|_Y}{\|h\|_X} = 0.$$

for all $h \in X$ is some neighborhood of zero. If T exists, The map $f'(x) := T$ is called *Fréchet derivative* of f at x and is defined by $df(x; h) = f'(x)h$.

Definition 2.26 (*F-derivative or G-derivative on domain U*). If the Fréchet-derivative (or Gâteaux-derivative) exists for all $x \in U$, then the mapping

$$f' : U \subset X \rightarrow L(X, Y), \quad x \mapsto f'(x)$$

is called *Fréchet-derivative* (or *Gâteaux-derivative*) of f on U .

Chapter 3

Mathematical models for continuous catalyst positioning in Li/air batteries

In this Chapter we study the well-posedness of the two models of continuous catalyst positioning in Li/air batteries (see Subsection 1.2, equations (1.22) and (1.23)). These forward models are well-posed in a certain set of some functional spaces.

3.1 Formulation and weak solution of Problem I_a

We recall problem I_a from (1.20a)-(1.20f) with slight reformulation on β and γ as follows:

Let $c = c(t, x) : Q_T \rightarrow \mathbb{R}$ be the oxygen concentration inside the pore and $r = r(t, x) : Q_T \rightarrow \mathbb{R}$ the pore radius. Then c and r satisfy the system of partial differential equations

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T, \quad (3.1)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)cat(x) c, \quad (t, x) \in Q_T \quad (3.2)$$

With initial conditions:

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$c(0, x) = h(x), \quad (3.4)$$

and mixed boundary conditions:

$$c(t, 0) = 1, \quad t \in [0, T], \quad (3.5)$$

$$c_x(t, 1) = 0, \quad t \in [0, T], \quad (3.6)$$

the functions $h(x)$ and $cat(x)$ are supposed to satisfy

$$\begin{aligned} h(0) &= 1, h(1) = 0, \\ h &\in W^{2,\infty}(\Omega), \\ cat &\in W^{1,\infty}(\Omega), \end{aligned} \tag{3.7}$$

where

$$\begin{aligned} \beta(t, r, c) &= \frac{D_1}{\int_0^1 r H_\epsilon(c) dx}, \\ \gamma(t, r, c) &= \frac{D_2}{\int_0^1 r H_\epsilon(c) dx}, \end{aligned} \tag{3.8}$$

with ϵ being a small positive number. The constants D_1, D_2 are some given positive numbers. The function H_ϵ has the following form

$$H_\epsilon(x) = \begin{cases} x, & \text{if } x \geq -\frac{a}{\gamma} + c_0, \\ 2\epsilon - \epsilon \left[\frac{2\gamma-1}{4\gamma} - \frac{\gamma x}{2} - \frac{\gamma}{2}(\gamma x - \gamma c_0 + a)(\gamma x - \gamma c_0 + b) + \frac{\gamma^3}{2}(\gamma x - \gamma c_0 + a)^2(\gamma x - \gamma c_0 + b)^2 \right], & \\ \text{if } -\frac{b}{\gamma} + c_0 < x \leq -\frac{a}{\gamma} + c_0, \\ \epsilon, & \text{otherwise,} \end{cases} \tag{3.9}$$

where

$$a := 1 - \frac{1}{2\gamma}, \quad b := 1 + \frac{1}{2\gamma}, \quad \gamma > 0. \tag{3.10}$$

$H_\epsilon(x) \geq \epsilon, \forall x \in \mathbb{R}$, H_ϵ is monotone, C^2 continuously differentiable (see Appendix A.2 and [10]). The graphic of $H_\epsilon(x)$ is plotted in Figure A.4.

Remark 3.1 $H_\epsilon(u)$ is bounded in $L^\infty(Q_T)$.

Supposing additionally that r and c are smooth enough and $0 < r_\alpha \leq r, \forall (t, x) \in Q_T$, after expanding the derivatives in the both sides of (3.1), and dividing the both sides by r^2 , we get

$$c_t - c_{xx} - \frac{2r_x c_x}{r} + \frac{(2r_t + \frac{D_1}{\int_0^1 r H_\epsilon(c) dx})c}{r} = 0, \quad (t, x) \in Q_T. \tag{3.11}$$

We will transform the non-homogeneous problem (3.11), (3.4)-(3.6) in a homogeneous one by setting

$$u(t, x) = c(t, x) - 1. \tag{3.12}$$

Then $u(t, 0) = u_x(t, 1) = 0$. Denoting $u_0(x) = h(x) - 1$, the equation (3.11) leads to

$$u_t - u_{xx} - \frac{2r_x u_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(u+1) dx} \right) u = - \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(u+1) dx} \right), \quad (t, x) \in Q_T. \quad (3.13)$$

Inserting r_t from (3.4) as $r_t = -\frac{D_2}{\int_0^1 r H_\epsilon(u+1) dx} \text{cat}(x)(u+1)$, $(t, x) \in Q_T$ into the right hand side of (3.13), then the problem (3.1) – (3.6) leads to the following problem

$$u_t - u_{xx} - \frac{2r_x u_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 \text{cat}(x)}{r \int_0^1 r H_\epsilon(u+1) dx} \right) u = \frac{2D_2 \text{cat}(x) - D_1}{r \int_0^1 r H_\epsilon(u+1) dx}, \quad (t, x) \in Q_T, \quad (3.14)$$

$$r_t = -\frac{D_2}{\int_0^1 r H_\epsilon(u+1) dx} \text{cat}(x)(u+1), \quad (t, x) \in Q_T, \quad (3.15)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$u(0, x) = u_0(x), \quad x \in \Omega, \quad (3.16)$$

$$u(t, 0) = u_x(t, 1) = 0, \quad t \in [0, T]. \quad (3.17)$$

We begin a study of this problem by defining a weak solution.

Definition 3.2 A pair $(r, u) \in W^{1,\infty}(Q_T) \times W(0, T; H^1(\Omega))$ is said to be a weak solution of (3.14), (3.15), (3.3), (3.16), and (3.17) if the following equalities are satisfied

$$\begin{aligned} (u_t, v)_{((H^1(\Omega))^*, H^1(\Omega))} + \int_0^1 u_x v_x dx - \int_0^1 \frac{2r_x u_x}{r} v dx + \int_0^1 \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 \text{cat}(x)}{r \int_0^1 r H_\epsilon(u+1) dx} \right) u v dx = \\ = \int_0^1 \frac{2D_2 \text{cat}(x) - D_1}{r \int_0^1 r H_\epsilon(u+1) dx} v dx, \quad (3.18) \\ \forall v \in V, \quad a.e. \, t \in [0, T], \end{aligned}$$

where V is defined in Chapter 2.

$$u(0, x) = u_0(x), \quad x \in [0, 1]. \quad (3.16)$$

$$r(t, x) = 1 - \int_0^t \frac{D_2}{\int_0^1 r H_\epsilon(u+1) dx} \text{cat}(x) (u(\tau, x) + 1) d\tau, \quad t \in [0, T]. \quad (3.19)$$

3.2 The local existence and uniqueness of the weak solution of problem I_a

To prove that there exists a solution to the system (3.14), (3.15), (3.3), (3.16), and (3.17), we will apply the Banach fixed point theorem. For this purpose, we define following spaces

$$\mathbf{X}_T = \left\{ r \in L^\infty(Q_T); r_x, r_t \in L^2(0, T, L^\infty(\Omega)) \right\},$$

with the norm

$$\|r\|_{\mathbf{X}_T} = \|r\|_{L^\infty(Q_T)} + \|r_t\|_{L^2(0, T, L^\infty(\Omega))} + \|r_x\|_{L^2(0, T, L^\infty(\Omega))},$$

and

$$\mathbf{Y}_T = \left\{ u \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)), u' \in L^2(0, T; L^2(\Omega)) \right\},$$

with the norm

$$\|u\|_{\mathbf{Y}_T} = \|u\|_{L^2(0, T; H^2(\Omega))} + \|u\|_{L^\infty(0, T; H^1(\Omega))} + \|u'\|_{L^2(0, T; L^2(\Omega))},$$

where u', u'' denoted by $\frac{du}{dt}, \frac{d^2u}{dt^2}$ respectively. With M, r_α, ϵ are some given positive constants we define the set

$$\mathbf{M}_T = \left\{ (r, u), r \in \mathbf{X}_T, u \in \mathbf{Y}_T, \|r - 1\|_{\mathbf{X}_T} + \|u - u_0\|_{\mathbf{Y}_T} \leq M; r_\alpha \leq r \leq R; \forall \text{a.e. } (t, x) \in Q_T \right\}, \quad (3.20)$$

where $0 < r_\alpha < 1 < R$.

Remark 3.3 $\mathbf{M}_T$ is closed, convex and bounded in $\mathbf{X}_T \times \mathbf{Y}_T$.

For $(\bar{r}, \bar{u}) \in \mathbf{M}_T$ define the operator $\mathcal{T}$

$$\mathcal{T} : \mathbf{M}_T \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T$$

by $(r, u) = \mathcal{T}(\bar{r}, \bar{u})$, where

$$r(t, x) = 1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x)(\bar{u} + 1) d\tau. \quad (3.21)$$

and u is the solution to the parabolic equation

$$u_t + \mathcal{L}u = f, \quad (3.22)$$

with the initial and boundary condition (3.16), (3.17). Here

$$\begin{aligned} \mathcal{L}u &= -u_{xx} - \frac{2r_x u_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 \text{cat}(x)}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx} \right) u, \\ \text{and } f &= \frac{2D_2 \text{cat}(x) - D_1}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx}. \end{aligned} \quad (3.23)$$

We will employ the Banach fixed point theorem to prove the existence of a fixed point of the system (3.21), (3.22) with the conditions (3.16), (3.17). We have the following result:

Theorem 3.4 *Under the conditions in (3.7), which are $cat \in W^{1,\infty}(\Omega)$ and $u_0 = h - 1 \in W^{2,\infty}(\Omega)$, there exist exactly one weak solution (u, r) on M_T of (3.14), (3.15), (3.3), (3.16), and (3.17), where T is small enough.*

The idea of using fixed point technique we take from the Master Thesis of Grutzner [17]

The scheme of the proof will proceed as below:

- 1) $\mathcal{T}$ is defined on M_T and maps M_T into $X_T \times Y_T$
- 2) There exists T small enough such that $\mathcal{T}$ maps M_T to M_T .
- 3) There exists T small enough such that $\mathcal{T}$ is s -contractive in $X_T \times Y_T$, i.e

$$\|\mathcal{T}(u_1, r_1) - \mathcal{T}(u_2, r_2)\|_{X_T \times Y_T} \leq s \|(u_1, r_1) - (u_2, r_2)\|_{X_T \times Y_T},$$

for all $(u_1, r_1), (u_2, r_2) \in M_T$, and for $0 \leq s < 1$.

3.2.1 $\mathcal{T}$ is well defined in M_T and maps M_T into $X_T \times Y_T$ for T small enough

Proposition 3.5 *With $(\bar{r}, \bar{u}) \in M_T$, $cat(x)$ fixed and satisfies (3.7), the followings hold*

(i)

$$\|r_t\|_{L^\infty} \leq C(M, T, \epsilon, r_\alpha, cat).$$

(ii)

$$\|r_x\|_{L^\infty(Q)} \leq C(M, T, \epsilon, r_\alpha, cat).$$

$C(M, T, \epsilon, r_\alpha, cat)$ in (i) and (ii) is a positive constant depending on $M, T, \epsilon, r_\alpha, cat$.

(iii) *There exists a positive constant T_1 such that*

$$r > r_\alpha, \forall (t, x) \in [0, T_1] \times [0, 1].$$

(iv) *The coefficients of the operator $\mathcal{L}$ in (3.23) are belong to $L^\infty(Q_{T_1})$.*

Proof.

- (i) From (3.21), with $(\bar{r}, \bar{u}) \in M_T$, using triangle inequality, Hölder's inequality and equation (3.21),

we get

$$\begin{aligned}
 \|r_x\|_{L^\infty(Q_T)} &= \left\| \left(1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x)(\bar{u} + 1) d\tau \right) \right\|_{L^\infty(Q_T)} = \\
 &= \sup_{t,x} \left| \int_0^t \left(\frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}_x(\bar{u} + 1) + \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x) \bar{u}_x \right) d\tau \right| \leq \\
 &\leq \frac{D_2}{r_\alpha \epsilon} \|\text{cat}\|_{L^\infty(\Omega)} \sup_x \int_0^T |\bar{u} + 1| dt + \frac{D_2}{r_\alpha \epsilon} \|\text{cat}_x\|_{L^\infty(\Omega)} \sup_x \int_0^T |\bar{u}_x| dt \leq \\
 &\leq C(\epsilon, r_\alpha, \text{cat}) \sup_x \left(\int_0^T |\bar{u}| dt + \int_0^T |\bar{u}_x| dt + T \right) \leq \\
 &\leq C(\epsilon, r_\alpha, \text{cat}) \sup_x \left(\int_0^T |\bar{u}| dt + \left(T \int_0^T |\bar{u}_x|^2 dt \right)^{\frac{1}{2}} + T \right) \leq \\
 &\leq C(M, T, \epsilon, r_\alpha, \text{cat}).
 \end{aligned}$$

In the last step in the above inequality we use result (2.26) in Theorem 2.23.

(ii) Further,

$$\|r_t\|_{L^\infty(Q_T)} = \left\| \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x)(\bar{u} + 1) \right\|_{L^\infty(Q)} \leq C(M, T, \epsilon, r_\alpha, \text{cat}).$$

(iii) Finally, due to (3.21), we see that $r \geq r_\alpha$, if

$$\int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x)(\bar{u} + 1) d\tau \leq 1 - r_\alpha. \quad (3.24)$$

Meanwhile, we have the following estimate

$$\int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} \text{cat}(x)(\bar{u} + 1) d\tau \leq tC(M, T, \epsilon, r_\alpha, \text{cat}).$$

Therefore by choosing $T_1 < \frac{1-r_\alpha}{2C(M, T, \epsilon, r_\alpha, \text{cat})}$, we arrive at (3.24), which is required to prove. ■

Remark 3.6 With $(\bar{r}, \bar{u}) \in \mathbf{M}_{T_1}$, f in (3.23) belongs to $L^2(Q_{T_1})$.

Remark 3.7 With h satisfying (3.7), the function $u_0 \in V$.

Theorems 2.21 and 2.22 follow the following results.

Theorem 3.8 Suppose that $(\bar{r}, \bar{u}) \in \mathbf{M}_{T_1}$. There exists a unique solution $u \in W(0, T_1)$ of (3.22), (3.16), (3.17).

Theorem 3.9 (Improved regularity) Suppose that $(\bar{r}, \bar{u}) \in \mathbf{M}_{T_1}$ and $u \in W(0, T_1; V)$, is the weak solution of (3.22), (3.16), (3.17). Then

$$u \in L^2(0, T_1, H^2(\Omega)) \cap L^\infty(0, T_1; H_0^1(\Omega)), u' \in L^2(0, T_1; L^2(\Omega)),$$

and we have estimate

$$\begin{aligned} \operatorname{ess\,sup}_{[0, T_1]} \|u(t)\|_{H^1(\Omega)} + \|u\|_{L^2(0, T_1; H^2(\Omega))} + \|u'\|_{L^2(0, T_1; L^2(\Omega))} &\leq \\ &\leq C(M, T_1, \epsilon, r_\alpha, cat) \left(\|f\|_{L^2(0, T_1; L^2(\Omega))} + \|u_0\|_V \right). \end{aligned} \quad (3.25)$$

For convenience for further proof, we suppose $T_1 \leq 1$.

The following lemmas are employed from the above theorems.

Lemma 3.10 Assume $(\bar{r}, \bar{u}) \in \mathbf{M}_{T_1}$, then the weak solution u of the equation (3.22), (3.16), (3.17) satisfies following estimate

$$\begin{aligned} \operatorname{ess\,sup}_{[0, T_1]} \|u - u_0\|_{H^1(\Omega)} + \|u - u_0\|_{L^2(0, T_1; H^2(\Omega))} + \|(u - u_0)'\|_{L^2(0, T_1; L^2(\Omega))} &\leq \\ &\leq C(M, T_1, \epsilon, r_\alpha, u_0, cat) \sqrt{T_1} \end{aligned} \quad (3.26)$$

Proof.

We see that $(u - u_0)$ is the solution of the equation

$$w_t - \mathcal{L}w = f_w, \quad (3.27)$$

with homogeneous initial and mixed-boundary conditions. The function

$$\begin{aligned} f_w &= f - \mathcal{L}u_0 = \\ &= \frac{2D_2 cat(x) - D_1}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx} + (u_0)_{xx} + \frac{2r_x(u_0)_x}{r} - \left(2r_t + \frac{D_1}{\int_0^1 r H_\epsilon(\bar{u} + 1) dx} - \frac{2D_2 cat(x)}{\int_0^1 r H_\epsilon(\bar{u} + 1) dx} \right) u_0. \end{aligned} \quad (3.28)$$

Applying Theorem 3.9 to the equation (3.27), we deduce the two estimates

$$\operatorname{ess\,sup}_{[0, T_1]} \|u - u_0\|_{H^1(\Omega)} + \|u - u_0\|_{L^2(0, T_1; H^2(\Omega))} + \|(u - u_0)'\|_{L^2(0, T_1; L^2(\Omega))} \leq C(M, T_1, \epsilon, r_\alpha, cat) \|f_w\|_{L^2(0, T_1; L^2(\Omega))}, \quad (3.29)$$

Using Proposition 3.5, we estimate

$$\begin{aligned} \|f_w\|_{L^2(0,T_1;L^2(\Omega))} &\leq \left\| \frac{2D_2 cat(x) - D_1}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx} \right\|_{L^2(0,T_1;L^2(\Omega))} + \\ &+ \left\| (u_0)_{xx} + \frac{2r_x(u_0)_x}{r} - \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx} - \frac{2D_2 cat(x)}{r \int_0^1 r H_\epsilon(\bar{u} + 1) dx} \right) u_0 \right\|_{L^2(0,T_1;L^2(\Omega))} \leq \\ &\leq C(M, T_1, \epsilon, r_\alpha, u_0, cat) \sqrt{T_1}. \end{aligned}$$

Thus we arrive at (3.26). ■

It follows from this lemma and the continuous embedding $H^1(\Omega) \subset L^\infty(\Omega)$ the following statement.

Corollary 3.11 *The weak solution u of problem (3.22), (3.16), (3.17) satisfies following estimates*

$$(i) \quad \|u\|_{L^\infty(Q_{T_1})} = \text{ess sup}_{t,x} |u| \leq C(M, T_1, \epsilon, r_\alpha, u_0, cat). \quad (3.30)$$

$$(ii) \quad \|u_x\|_{L^2(0,T;L^\infty(\Omega))} \leq C(M, T_1, \epsilon, r_\alpha, u_0, cat). \quad (3.31)$$

$$(iii) \quad \|u_x\|_{L^\infty(0,T;L^2(\Omega))} \leq C(M, T_1, \epsilon, r_\alpha, u_0, cat). \quad (3.32)$$

3.2.2 The mapping $\mathcal{T}$ maps M_T to M_T for T small enough.

Lemma 3.12 *With small enough T , $\mathcal{T}$ maps M_T to M_T .*

Proof. The scheme of the proof is as follows

1. The condition $(\bar{r}, \bar{u})$

$$\|\bar{r} - 1\|_{\mathbf{X}_T} + \|\bar{u} - u_0\|_{\mathbf{Y}_T} \leq M$$

follows that (r, u) also satisfies

$$\|r - 1\|_{\mathbf{X}_T} + \|u - u_0\|_{\mathbf{Y}_T} \leq M.$$

2. The condition $r_\alpha \leq \bar{r} \leq R$ implies that $r_\alpha \leq r \leq R, \forall (t, x) \in Q_T$, where $Q_T = [0, T] \times [0, 1]$, with T small enough.

Now we prove these statements.

1. We will estimate each term of the norm

$$\begin{aligned} \|(r-1, u-u_0)\|_{\mathbf{X}_T \times \mathbf{Y}_T} &= \|r-1\|_{\mathbf{X}_T} + \|u-u_0\|_{\mathbf{Y}_T} = \|r-1\|_{L^\infty(Q_T)} + \|r_t\|_{L^2(0,T;L^\infty(\Omega))} + \|r_x\|_{L^2(0,T;L^\infty(\Omega))} + \\ &+ \operatorname{ess\,sup}_{[0,T]} \|u-u_0\|_{H^1(\Omega)} + \|u-u_0\|_{L^2(0,T;H^2(\Omega))} + \|(u-u_0)'\|_{L^2(0,T;L^2(\Omega))}. \end{aligned} \quad (3.33)$$

From (3.167) and Proposition 3.5, we have

(i) The condition $(\bar{r}, \bar{u}) \in \mathbf{M}_T$ implies that $\|\bar{u}\|_{L^\infty(Q_T)} \leq C(M, u_0)$. Therefore,

$$\begin{aligned} \|r-1\|_{L^\infty(Q_T)} &= \operatorname{ess\,sup}_{t,x} \left| \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u}+1) dx} \operatorname{cat}(x)(\bar{u}+1) d\tau \right| \leq \\ &\leq T C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}) \operatorname{ess\,sup}_{x,t} (|\bar{u}|+1) \leq \\ &\leq T C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}). \end{aligned} \quad (3.34)$$

(ii) Similarly,

$$\|r_t\|_{L^2(0,T;L^\infty(\Omega))} \leq \sup_x \left(\int_0^T \left(\frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u}+1) dx} \operatorname{cat}(x)(\bar{u}+1) \right)^2 dt \right)^{\frac{1}{2}} \leq \sqrt{T} C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}). \quad (3.35)$$

(iii) The condition $(\bar{r}, \bar{u}) \in \mathbf{M}_T$ implies that $\|\bar{u}_x\|_{L^2(0,T;L^\infty(\Omega))} \leq C(M, u_0)$. Hence applying the Hölder inequality, we obtain

$$\begin{aligned} \|r_x\|_{L^2(0,T;L^\infty(\Omega))}^2 &\leq \int_0^T \sup_x \left(1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u}+1) dx} \operatorname{cat}(x)(\bar{u}+1) d\tau \right)_x^2 dt \leq \\ &\leq \int_0^T \sup_x \left(\int_0^t \left(\frac{C_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u}+1) dx} \operatorname{cat}_x(\bar{u}+1) + \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u}+1) dx} \operatorname{cat}(x) \bar{u}_x \right) d\tau \right)^2 dt \leq \\ &\leq C(r_\alpha, \epsilon, \operatorname{cat}) \int_0^T \sup_{x,t} \int_0^T (1 + |\bar{u}|^2 + |\bar{u}_x|^2) dt dt \leq \\ &\leq T C(r_\alpha, \epsilon, \operatorname{cat}) (1 + \|\bar{u}\|_{L^\infty(Q_T)}^2 + \|\bar{u}_x\|_{L^2(0,T;L^\infty(\Omega))}^2) \leq T C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}). \end{aligned} \quad (3.36)$$

Therefore

$$\|r_x\|_{L^2(0,T;L^\infty(\Omega))} \leq \sqrt{T} C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}). \quad (3.37)$$

Combining (3.25), (3.34), (3.37), (3.37) we obtain

$$\|r-1\|_{\mathbf{X}_T} + \|u\|_{\mathbf{Y}_T} \leq \sqrt{T} C(M, T, u_0, r_\alpha, \epsilon, \operatorname{cat}). \quad (3.38)$$

Then

$$\|r-1\| + \|u\| \leq M, \forall t < T_2,$$

where $T_2 = \frac{1}{2} \frac{1}{\sqrt{T} C(M, T, u_0, r_\alpha, \epsilon, cat)}$.

2. We have proven in the Proposition 3.5 that $r \geq r_\alpha$ for T small enough. From (3.167) it follows that

$$\begin{aligned} r &\leq 1 + \left| \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{u} + 1) dx} cat(x) (\bar{u}(\tau, x) + 1) d\tau \right| \leq \\ &\leq tC(M, T, u_0, r_\alpha, \epsilon, cat) + 1 \end{aligned} \quad (3.39)$$

Thus $r \leq R$ for $t \in [0, T_3]$, where $T_3 = \frac{R-1}{2C(M, T, u_0, r_\alpha, \epsilon, cat)}$. Hence for T satisfying:

$$T \leq T^* = \min \{T_1, T_2, T_3\} \quad (3.40)$$

the $\mathcal{T}$ maps $\mathbf{M}_T$ into $\mathbf{M}_T$.

■

3.2.3 $\mathcal{T}$ is contractive in the $\mathbf{X}_T \times \mathbf{Y}_T$ norm with T small enough.

Let $(\bar{u}_1, \bar{r}_1), (\bar{u}_2, \bar{r}_2) \in \mathbf{M}_{T^*}$, where T^* is defined in (3.40). Suppose that

$$\begin{aligned} \mathcal{T}(\bar{u}_1, \bar{r}_1) &= (u_1, r_1), \\ \mathcal{T}(\bar{u}_2, \bar{r}_2) &= (u_2, r_2). \end{aligned} \quad (3.41)$$

Then $\bar{u}_1, \bar{r}_1, u_1, r_1$ and $\bar{u}_2, \bar{r}_2, u_2, r_2$ satisfy the equations (3.14), (3.15), (3.15), (3.16), (3.17) and (3.3). Denoting $\tilde{u} = u_1 - u_2, \tilde{r} = r_1 - r_2$. Subtracting the two parabolic equations and the two differential equations, we have the following system.

$$\begin{aligned} \tilde{u}_t - \tilde{u}_{xx} - \frac{r_{1x}}{r_1} \tilde{u}_x + \left(\frac{2r_{1t}}{r_1} + \frac{D_1 - 2D_2 cat(x)}{r_1 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} \right) \tilde{u} &= \left(\frac{2r_{1x}}{r_1} - \frac{2r_{2x}}{r_2} \right) u_{2x} - \left(\frac{2r_{1t}}{r_1} - \frac{2r_{2t}}{r_2} \right) u_2 + \\ &+ (2D_2 cat(x) - D_1) \left(\frac{1}{r_1 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{r_2 \int_0^1 r_2 H_\epsilon(\bar{u}_2 + 1) dx} \right) (u_2 + 1) \end{aligned} \quad (3.42)$$

with the initial and boundary conditions

$$\tilde{u}(0, x) = 0, \quad (3.43)$$

$$\tilde{u}(t, 0) = \tilde{u}_x(t, 1) = 0, t \in [0, T^*], \quad (3.44)$$

coupled with the equation

$$\tilde{r} = -D_2 \text{cat}(x) \left[\int_0^t \frac{\bar{u}_1 - \bar{u}_2}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1) dx} d\tau + \int_0^t (\bar{u}_2 + 1) \left(\frac{1}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{\int_0^1 \bar{r}_2 H_\epsilon(\bar{u}_2 + 1) dx} \right) d\tau \right]. \quad (3.45)$$

We have the following result.

Lemma 3.13 *Suppose that the functions $h, \text{cat}, H_\epsilon$ satisfy (3.7), (A.12), (3.9). The following estimate for the problem (3.42), (3.43), (3.44) on $Q_{T^*} = [0, T^*] \times [0, 1]$ holds*

$$\begin{aligned} & \text{ess sup}_{[0, T^*]} \|\tilde{u}(t)\|_{H^1(\Omega)} + \|\tilde{u}\|_{L^2(0, T^*; H^2(\Omega))} + \|\tilde{u}'\|_{L^2(0, T^*; L^2(\Omega))} \leq \\ & \leq C(M, T^*, \epsilon, r_\alpha, u_0, \text{cat}) \sqrt{T^*} \left(\|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} + \|\bar{u}_1 - \bar{u}_2\|_{L^2(0, T^*; H^2(\Omega))} + \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(0, T^*; H^1(\Omega))} \right). \end{aligned} \quad (3.46)$$

Proof. Applying Theorem 3.9 to the parabolic equation (3.42), and denoting by f_{12} its left hand side, we estimate f_{12} in the $L^2(Q_{T^*})$ norm as follows

$$\begin{aligned} \|f_{12}\|_{L^2(Q_{T^*})} & \leq \left\| \left(\frac{2r_{1x}}{r_1} - \frac{2r_{2x}}{r_2} \right) u_{2x} \right\|_{L^2(Q_{T^*})} + \left\| \left(\frac{2r_{1t}}{r_1} - \frac{2r_{2t}}{r_2} \right) u_2 \right\|_{L^2(Q_{T^*})} + \\ & + \left\| \left(2D_2 \text{cat}(x) - D_1 \right) \left(\frac{1}{r_1 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{r_2 \int_0^1 r_2 H_\epsilon(\bar{u}_2 + 1) dx} \right) (u_2 + 1) \right\|_{L^2(Q_{T^*})} \end{aligned} \quad (3.47)$$

Due to (3.30)

$$\begin{aligned} \|f_{12}\|_{L^2(Q_{T^*})} & \leq C(M, \text{cat}) \left(\underbrace{\left\| \left(\frac{r_{1x}}{r_1} - \frac{r_{2x}}{r_1} \right) u_{2x} \right\|_{L^2(Q_{T^*})}}_{A_1} + \underbrace{\left\| \left(\frac{r_{2x}}{r_1} - \frac{r_{2x}}{r_2} \right) u_{2x} \right\|_{L^2(Q_{T^*})}}_{A_2} + \underbrace{\left\| \left(\frac{r_{1t}}{r_1} - \frac{r_{2t}}{r_1} \right) u_2 \right\|_{L^2(Q_{T^*})}}_{A_3} + \right. \\ & + \underbrace{\left\| \left(\frac{r_{2t}}{r_1} - \frac{r_{2t}}{r_2} \right) u_2 \right\|_{L^2(Q_{T^*})}}_{A_4} + \underbrace{\left\| \left(\frac{1}{r_1 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{r_2 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} \right) \right\|_{L^2(Q_{T^*})}}_{A_5} + \\ & + \underbrace{\left\| \left(\frac{1}{r_2 \int_0^1 r_1 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{r_2 \int_0^1 r_2 H_\epsilon(\bar{u}_1 + 1) dx} \right) \right\|_{L^2(Q_{T^*})}}_{A_6} + \\ & \left. + \underbrace{\left\| \left(\frac{1}{r_2 \int_0^1 r_2 H_\epsilon(\bar{u}_1 + 1) dx} - \frac{1}{r_2 \int_0^1 r_2 H_\epsilon(\bar{u}_2 + 1) dx} \right) \right\|_{L^2(Q_{T^*})}}_{A_7} \right). \end{aligned} \quad (3.48)$$

1. Since $r_1 \geq r_\alpha$, $r_2 \geq r_\alpha$ and

$$\begin{aligned} r_1(t, x) &= 1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1) dx} cat(x)(\bar{u}_1 + 1) d\tau, \\ r_2(t, x) &= 1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r}_2 H_\epsilon(\bar{u}_2 + 1) dx} cat(x)(\bar{u}_2 + 1) d\tau, \end{aligned} \quad (3.49)$$

we have

$$\begin{aligned} A_1 &\leq \frac{1}{r_\alpha} \|(r_{1x} - r_{2x})u_{1x}\|_{L^2(Q_{T^*})} \leq \\ &= \frac{1}{r_\alpha} D_2 \|cat\|_{W^{1,\infty}(\Omega)} \left(\left\| u_{1x} \int_0^t \left(\frac{\bar{u}_{1x}}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1)} - \frac{\bar{u}_{2x}}{\int_0^1 \bar{r}_2 H_\epsilon(\bar{u}_2 + 1)} \right) d\tau \right\|_{L^2(Q_{T^*})} + \right. \\ &\quad \left. + \left\| u_{1x} \int_0^t \left(\frac{\bar{u}_1 + 1}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1)} - \frac{\bar{u}_2 + 1}{\int_0^1 \bar{r}_2 H_\epsilon(\bar{u}_2 + 1)} \right) d\tau \right\|_{L^2(Q_{T^*})} \right) \leq \\ &\leq C(r_\alpha, \epsilon, cat) \left(\underbrace{\left\| u_{1x} \int_0^t (\bar{u}_{1x} - \bar{u}_{2x}) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{11}} + \underbrace{\left\| u_{1x} \int_0^t (\bar{u}_{2x} + 1) \int_0^1 (\bar{r}_1 - \bar{r}_2) H_\epsilon(\bar{u}_1 + 1) dx d\tau \right\|_{L^2(Q_{T^*})}}_{A_{12}} + \right. \\ &\quad \left. + \underbrace{\left\| u_{1x} \int_0^t (\bar{u}_{2x} + 1) \int_0^1 \bar{r}_2 (H_\epsilon(\bar{u}_2 + 1) - H_\epsilon(\bar{u}_1 + 1)) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{13}} + \underbrace{\left\| u_{1x} \int_0^t (\bar{u}_1 - \bar{u}_2) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{12}} + \right. \\ &\quad \left. + \underbrace{\left\| u_{1x} \int_0^t (\bar{u}_2 + 1) \int_0^1 (\bar{r}_1 - \bar{r}_2) H_\epsilon(\bar{u}_1 + 1) dx d\tau \right\|_{L^2(Q_{T^*})}}_{A_{15}} + \right. \\ &\quad \left. + \underbrace{\left\| u_{1x} \int_0^t (\bar{u}_2 + g) \int_0^1 \bar{r}_2 (H_\epsilon(\bar{u}_2 + 1) - H_\epsilon(\bar{u}_1 + 1)) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{16}} \right). \end{aligned} \quad (3.50)$$

Applying the Hölder inequality, taking into account that u_{2x} satisfies (3.38), and $H^2(\Omega)$ continuous embedded in $L^\infty(\Omega)$, we get

$$\begin{aligned} (A_{11})^2 &= \int_0^{T^*} \int_0^1 u_{1x} \left(\int_0^t (\bar{u}_{1x} - \bar{u}_{2x}) d\tau \right)^2 dx dt \leq \int_0^T \int_0^1 \left(|u_{1x}|^2 T \int_0^{T^*} (\bar{u}_{1x} - \bar{u}_{2x})^2 dt \right) dx dt = \\ &= T \int_0^{T^*} \operatorname{ess\,sup}_x |u_{1x}|^2 dt \operatorname{ess\,sup}_x \int_0^{T^*} (\bar{u}_{1x} - \bar{u}_{2x})^2 dt \int_0^1 \operatorname{ess\,sup}_{t \in [0, T^*]} |u_{1x}|^2 dx \leq \end{aligned}$$

$$\begin{aligned}
 &\leq^{(3.38)} C(M, T^*, \epsilon, r_\alpha, u_0, cat) T \|\bar{u}_{1x} - \bar{u}_{2x}\|_{L^2(0, T^*; L^\infty(\Omega))}^2 \leq \\
 &\leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) T^* \|\bar{u}_1 - \bar{u}_2\|_{L^2(0, T^*; H^2(\Omega))}^2.
 \end{aligned} \tag{3.51}$$

Similarly, as $H_\epsilon(\bar{u}_1 + 1)$ is bounded in $L^\infty(Q_{T^*})$, we have

$$\begin{aligned}
 (A_{12})^2 &\leq C \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} \int_0^T \int_0^1 u_{1x} \left(\int_0^t (\bar{u}_{2x} + 1) d\tau \right)^2 dx dt \leq \\
 &\leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) T^* \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}^2.
 \end{aligned} \tag{3.52}$$

Since H_ϵ is Lipschitz continuous with respect to u , we get

$$\begin{aligned}
 (A_{13})^2 &\leq C \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} \int_0^{T^*} \int_0^1 u_{1x} \left(\int_0^t (\bar{u}_{2x} + g) d\tau \right)^2 dx dt \leq \\
 &\leq C(M, T, \epsilon, r_\alpha, u_0, cat) T \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})}^2.
 \end{aligned} \tag{3.53}$$

Similarly, for the three remain terms A_{12}, A_{15}, A_{16} in (3.60), we have:

$$(A_{12})^2 \leq C(M, T, \epsilon, r_\alpha, u_0, cat) T^* \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})}^2, \tag{3.54}$$

$$(A_{15})^2 \leq C(M, T, \epsilon, r_\alpha, u_0, cat) T \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}^2, \tag{3.55}$$

and

$$(A_{15})^2 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) T^* \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})}^2, \tag{3.56}$$

From (3.51) – (3.55), we conclude that

$$A_1 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} \left(\|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} + \|\bar{u}_1 - \bar{u}_2\|_{L^2(0, T^*; H^2(\Omega))} \right). \tag{3.57}$$

2. By the same technique as above, we get:

$$A_2 \leq C(M, T, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}. \tag{3.58}$$

3. Now we get estimate A_3 as follows

$$\begin{aligned}
 A_3 &\leq \frac{1}{r_\alpha} \|(r_{1t} - r_{2t})u_2\|_{L^2(Q_{T^*})} \leq \\
 &= \frac{1}{r_\alpha} D_2 \|cat\|_{W^{1,\infty}(\Omega)} \left\| u_2 \int_0^t \left(\frac{\bar{u}_1 + 1}{\int_0^1 \bar{r}_1 H_\epsilon(\bar{u}_1 + 1)} - \frac{\bar{u}_2 + 1}{\int_0^1 \bar{r}_2 H_\epsilon(\bar{u}_2 + 1)} \right) d\tau \right\|_{L^2(Q_{T^*})} \leq
 \end{aligned}$$

$$\begin{aligned}
 &\leq \frac{1}{r_\alpha} D_2 \|cat\|_{W^{1,\infty}(\Omega)} \left(\underbrace{\left\| u_2 \int_0^t (\bar{u}_1 - \bar{u}_2) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{31}} + \underbrace{\left\| u_2 \int_0^t (\bar{u}_2 + 1) \int_0^1 (\bar{r}_1 - \bar{r}_2) H_\epsilon(\bar{u}_1 + 1) dx d\tau \right\|_{L^2(Q_{T^*})}}_{A_{32}} + \right. \\
 &\quad \left. + \underbrace{\left\| u_2 \int_0^t (\bar{u}_2 + g) \int_0^1 \bar{r}_2 (H_\epsilon(\bar{u}_2 + 1) - H_\epsilon(\bar{u}_1 + 1)) d\tau \right\|_{L^2(Q_{T^*})}}_{A_{33}} \right). \tag{3.59}
 \end{aligned}$$

By the same technique as above, we conclude:

$$A_3 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} (\|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} + \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}). \tag{3.60}$$

Similarly, we have:

4.

$$A_4 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} (\|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} + \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}), \tag{3.61}$$

5.

$$A_5 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} (\|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} + \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}), \tag{3.62}$$

6.

$$A_6 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} (\|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} + \|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})}), \tag{3.63}$$

7.

$$A_7 \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})}. \tag{3.64}$$

Finally,

$$\begin{aligned}
 &\|f_{12}\|_{L^2(Q_{T^*})} \leq \\
 &\leq C(M, T, \epsilon, r_\alpha, u_0, cat) \sqrt{T} (\|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} + \|\bar{u}_1 - \bar{u}_2\|_{L^2(0,T;H^2(\Omega))} + \|\bar{u}_1 - \bar{u}_2\|_{L^2(0,T;H^2(\Omega))}), \tag{3.65}
 \end{aligned}$$

which implies (3.46). ■

From (3.45), we also obtain the following result:

Lemma 3.14 *The functions r_1, r_2 defined in (3.41) satisfy the estimate:*

$$\|r_1 - r_2\|_{\mathbf{X}} \leq T^* C(M, \epsilon, cat) \left(\|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} + \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(Q_{T^*})} \right). \quad (3.66)$$

Proof. It is easily to get the proof from considering the equation (3.45). ■

Theorem 3.15 *There exists a positive number T^{**} such that $\mathcal{T}$ is s -contractive in $\mathbf{X}_T \times \mathbf{Y}_T$ if $T \leq T^{**}$, where s is a positive constant less than 1.*

Proof. From the Lemmas 3.13 and 3.13, we get the estimate

$$\begin{aligned} & \|r_1 - r_2\|_{\mathbf{X}_{T^*}} + \|u_1 - u_2\|_{\mathbf{Y}_{T^*}} \leq \\ & \leq C(M, T^*, \epsilon, r_\alpha, u_0, cat) \sqrt{T^*} \left(\|\bar{r}_1 - \bar{r}_2\|_{L^\infty(Q_{T^*})} + \|\bar{u}_1 - \bar{u}_2\|_{L^2(0, T^*; H^2(\Omega))} + \|\bar{u}_1 - \bar{u}_2\|_{L^\infty(0, T^*; H^1(\Omega))} \right). \end{aligned} \quad (3.67)$$

Then $\mathcal{T}$ is s -contractive in $\mathbf{X}_{T^*} \times \mathbf{Y}_{T^*}$ norm with $s \leq \frac{1}{2}$, if $T \leq T^{**} = \min\{\frac{1}{2C^2(M, T^*, \epsilon, r_\alpha, u_0, cat)}, T^*\}$. ■

Finally, the theorem 3.4 is as a result of applying Banach fixed point Theorem, Lemma 2.7 and Theorem 2.10.

3.2.4 The continuous dependency on the data of the weak solution in M_T

Theorem 3.16 *Let (r, u) be the weak solution of the system (3.14), (3.15), (3.3), (3.16), and (3.17) on Q_T . Then it continuously depends on the the data*

$$\|u\|_{\mathbf{Y}_T} + \|r\|_{\mathbf{X}} \leq C(M, T, \epsilon, r_\alpha, cat) \sqrt{T} \|u_0\|_{H^2(\Omega)}. \quad (3.68)$$

Proof.

In one hand, according to Lemma 3.10,

$$\begin{aligned} & \text{ess sup}_{[0, T]} \|u\|_{H^1(\Omega)} + \|u\|_{L^2(0, T; H^2(\Omega))} + \|u'\|_{L^2(0, T; L^2(\Omega))} \leq \\ & \leq C(M, T, r_\alpha, cat) \sqrt{T} \|u_0\|_{H^2(\Omega)}. \end{aligned} \quad (3.69)$$

In another hand, from (3.167) and $(r, u) \in M_T$, we can obtain the following estimate

$$\|r - 1\|_{\mathbf{X}_T} \leq C_1(M, T, \epsilon, r_\alpha, cat) \sqrt{T} \left(\|u\|_{L^\infty(Q)} + \|u_x\|_{L^2(0, T; L^\infty(\Omega))} \right). \quad (3.70)$$

Combine (3.69) and (3.70) we get (3.68) ■

3.3. The continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to $cat(x)$ in $W^{1,\infty}(\Omega)$ for problem I_a with T small enough.

3.3 The continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to $cat(x)$ in $W^{1,\infty}(\Omega)$ for problem I_a with T small enough.

Let $cat_1(x), cat_2(x) \in W^{1,\infty}(\Omega)$, and assume that there exists a positive constant C_{cat} such that

$$\begin{aligned} \|cat_1(x)\|_{W^{1,\infty}(\Omega)} &\leq C_{cat}, \\ \|cat_2(x)\|_{W^{1,\infty}(\Omega)} &\leq C_{cat}. \end{aligned} \quad (3.71)$$

Suppose that $(u_1, r_1), (u_2, r_2) \in \mathbf{M}_T$, where $T \leq T^{**}$, satisfy problem (3.14), (3.15), (3.3), (3.16), and (3.17). Then we have:

$$u_{1t} - u_{1xx} - \frac{2r_{1x}u_{1x}}{r_1} + \left(\frac{2r_{1t}}{r_1} + \frac{D_1 - 2D_2cat_1(x)}{r_1 \int_0^1 r_1 H_\epsilon(u_1 + 1)dx} \right) u_1 = \frac{2D_2cat_1(x) - D_1}{r_1 \int_0^1 r_1 H_\epsilon(u_1 + 1)dx}, \quad (t, x) \in Q_T, \quad (3.72)$$

$$r_{1t} = -\frac{D_2}{\int_0^1 r_1 H_\epsilon(u_1 + 1)dx} cat_1(x)(u_1 + 1), \quad (t, x) \in Q_T, \quad (3.73)$$

$$r_1(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$u_1(0, x) = u_0(x), \quad x \in \Omega, \quad (3.74)$$

$$u_{1x}(t, 1) = 0, \quad t \in [0, T], \quad (3.75)$$

and

$$u_{2t} - u_{2xx} - \frac{2r_{2x}u_{2x}}{r_2} + \left(\frac{2r_{2t}}{r_2} + \frac{D_1 - 2D_2cat_2(x)}{r_2 \int_0^1 r_2 H_\epsilon(u_2 + 1)dx} \right) u_2 = \frac{2D_2cat_2(x) - D_1}{r_2 \int_0^1 r_2 H_\epsilon(u_2 + 1)dx}, \quad (t, x) \in Q_T, \quad (3.76)$$

$$r_{2t} = -\frac{D_2}{\int_0^1 r_2 H_\epsilon(u_2 + 1)dx} cat_1(x)(u_2 + 1), \quad (t, x) \in Q_T, \quad (3.77)$$

$$r_2(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$u_2(0, x) = u_0(x), \quad x \in \Omega, \quad (3.78)$$

$$u_{2x}(t, 1) = 0, \quad t \in [0, T]. \quad (3.79)$$

Denote $\mathcal{U} = u_1 - u_2$, $\mathcal{R} = r_1 - r_2$, we have the following Theorem.

Theorem 3.17 *There exist T small enough and positive constant $C(M, T, \epsilon, r_\alpha, u_0, C_{cat})$ such that*

$$\|\mathcal{U}\|_{Y_T} + \|\mathcal{R}\|_{W^{1,\infty}(Q_T)} \leq C(M, T, \epsilon, r_\alpha, u_0, C_{cat}) \|cat_1 - cat_2\|_{W^{1,\infty}(\Omega)}, \quad (3.80)$$

where

$$\begin{aligned} \|\mathcal{R}\|_{W^{1,\infty}(Q_T)} &= \|\mathcal{R}\|_{L^\infty(Q_T)} + \|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)}, \\ \|cat_1 - cat_2\|_{W^{1,\infty}(\Omega)} &= \|cat_1 - cat_2\|_{L^\infty(\Omega)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)}. \end{aligned}$$

Proof. Subtracting (3.76) by (3.72), denoting $\mathcal{U} = u_1 - u_2$, $\mathcal{R} = r_1 - r_2$ we get:

$$\begin{aligned} \mathcal{U}_t - \mathcal{U}_{xx} - \frac{2r_{1x}}{r_1} \mathcal{U}_x + \left(\frac{r_{1t}}{r_1} + \frac{D_1 - 2D_2 cat_2}{r_1 \int_0^1 r_2 H_\epsilon(u_2 + 1) dx} \right) \mathcal{U} = \\ = \frac{\mathcal{R}_t u_2}{r_1} + \frac{2u_{2x} \mathcal{R}_x}{r_1} - \left(\frac{r_{2t} u_2 + 2u_{2x} r_{2x}}{r_1 r_2} + \frac{2D_2 cat_2 u_2 + 2D_2 cat_2 - D_1 u_2 - D_1}{r_1 r_2 \int_0^1 r_2 H_\epsilon(u_2 + 1) dx} \right) \mathcal{R} + \\ + \frac{D_1 u_2 + D_1 + 2D_2 cat_2 u_2 + 2D_2 cat_2}{r_2 \int_0^1 r_1 H_\epsilon(u_1 + 1) dx \int_0^1 r_2 H_\epsilon(u_1 + 1) dx} \int_0^1 \mathcal{R} H_\epsilon(u_1 + 1) dx + \frac{(cat_1 - cat_2)(2D_2 u_1 + 2D_2)}{r_1 \int_0^1 r_1 H_\epsilon(u_1 + 1) dx} + \\ + \frac{D_1 u_2 + D_1 - 2D_2 cat_2 u_2 - 2D_2}{r_2 \int_0^1 r_2 H_\epsilon(u_1 + 1) dx \int_0^1 r_2 H_\epsilon(u_2 + 1) dx} \int_0^1 r_2 (H_\epsilon(u_1 + 1) dx - H_\epsilon(u_2 + 1) dx). \end{aligned} \quad (3.81)$$

Subtracting (3.77) by (3.73), we have:

$$\begin{aligned} \mathcal{R}_t = -D_2 \left(\frac{(cat_1 - cat_2)(u_1 + 1)}{\int_0^1 r_1 H_\epsilon(u_1 + 1) dx} + \frac{cat_2 \mathcal{U}}{\int_0^1 r_1 H_\epsilon(u_1 + 1) dx} - \right. \\ \left. \frac{cat_2(u_2 + 1) \int_0^1 \mathcal{R} H_\epsilon(u_1 + 1) dx}{\int_0^1 r_1 H_\epsilon(u_1 + 1) dx \int_0^1 r_2 H_\epsilon(u_1 + 1) dx} - \frac{cat_2(u_2 + 1) \int_0^1 r_2 (H_\epsilon(u_1 + 1) - H_\epsilon(u_2 + 1)) dx}{\int_0^1 r_2 H_\epsilon(u_1 + 1) dx \int_0^1 r_2 H_\epsilon(u_2 + 1) dx} \right). \end{aligned} \quad (3.82)$$

In one hand, applying Theorem 2.23 to the equation (3.81) with homogeneous initial and mixed boundary conditions, we have

$$\begin{aligned} \|\mathcal{U}\|_{Y_T} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \left(\|\mathcal{R}_t\|_{L^2(Q_T)} + \|u_{2x} \mathcal{R}_x\|_{L^2(Q_T)} + \|r_{2t} \mathcal{R}\|_{L^2(Q_T)} + \|u_{2x} \mathcal{R}\|_{L^2(Q_T)} + \right. \\ \left. + \|\mathcal{R}\|_{L^2(Q_T)} + \|cat_1 - cat_2\|_{L^2(\Omega)} + \|\mathcal{U}\|_{L^2(Q_T)} \right). \end{aligned} \quad (3.83)$$

From Proposition 3.5, we know that $\mathcal{R} \in W^{1,\infty}(Q_T)$, we estimate:

$$\|u_{2x} \mathcal{R}_x\|_{L^2(Q_T)} \leq \|\mathcal{R}_x\|_{L^2(0,T;L^\infty(\Omega))} \|u_{2x}\|_{L^\infty(0,T;L^2(\Omega))} \leq M \|\mathcal{R}_x\|_{L^2(0,T;L^\infty(\Omega))} \leq M \sqrt{T} \|\mathcal{R}_x\|_{L^\infty(Q_T)}. \quad (3.84)$$

3.3. The continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to $cat(x)$ in $W^{1,\infty}(\Omega)$ for problem I_a with T small enough.

Similarly,

$$\|r_{2t}\mathcal{R}\|_{L^2(Q_T)} \leq M \sqrt{T} \|\mathcal{R}\|_{L^\infty(Q_T)}, \quad (3.85)$$

and

$$\|u_{2x}\mathcal{R}\|_{L^2(Q_T)} \leq M \sqrt{T} \|\mathcal{R}\|_{L^\infty(Q_T)}. \quad (3.86)$$

Putting the estimates (3.84) – (3.86) into (3.83), we obtain:

$$\|\mathcal{U}\|_{Y_T} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \sqrt{T} (\|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)} + \|\mathcal{U}\|_{L^\infty(Q_T)}). \quad (3.87)$$

Thus, for $T < T_4 = \frac{1}{2C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat})}$, we deduce:

$$\|\mathcal{U}\|_{Y_T} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \sqrt{T} (\|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}). \quad (3.88)$$

In another hand, from the equation (3.82) and the homogeneous initial condition, we have the followings estimates:

$$\|\mathcal{R}\|_{L^\infty(Q_T)} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) T (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}). \quad (3.89)$$

$$\|\mathcal{R}_t\|_{L^\infty(Q_T)} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}). \quad (3.90)$$

$$\begin{aligned} \|\mathcal{R}_x\|_{L^\infty(Q_T)} &\leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) T (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)}) + \\ &+ C(R, r_\alpha, \epsilon, M) (\|\mathcal{U}_x\|_{L^2(0,T;L^\infty(\Omega))} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|\mathcal{U}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(Q_T)}). \end{aligned} \quad (3.91)$$

Hence,

$$\begin{aligned} &\|\mathcal{R}\|_{L^\infty(Q_T)} + \|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)} \leq \\ &\leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) T (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)} + \|cat_1 - cat_2\|_{L^\infty(Q_T)}) + \\ &+ C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) (\|\mathcal{U}_x\|_{L^2(0,T;L^\infty(\Omega))} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|\mathcal{U}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)}). \end{aligned} \quad (3.92)$$

Moreover, from (3.89), for $T < T_5 = \frac{1}{2C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat})}$, we have the following estimate:

$$\|\mathcal{R}\|_{L^\infty(Q_T)} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) T (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}). \quad (3.93)$$

Without loss of generality, we assume that $T < 1$. Continuing the estimate (3.92) with using (3.93), we obtain:

$$\begin{aligned} & \|\mathcal{R}\|_{L^\infty(Q_T)} + \|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)} \leq \\ & \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) T (\|\mathcal{U}\|_{L^\infty(Q_T)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}) + \\ & + C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) (\|\mathcal{U}_x\|_{L^2(0,T;L^\infty(\Omega))} + \|\mathcal{U}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)} + \|cat_{1x} - cat_{2x}\|_{L^\infty(\Omega)}). \end{aligned} \quad (3.94)$$

From (3.87), we also see that,

$$\begin{aligned} & \|\mathcal{U}\|_{L^\infty(Q_T)} + \|\mathcal{U}_x\|_{L^2(0,T;L^\infty(\Omega))} \leq \|\mathcal{U}\|_{Y_T} \leq \\ & \leq C(R, r_\alpha, \epsilon, M) C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \sqrt{T} (\|\mathcal{R}_t\|_{L^\infty(Q_T)} + \|\mathcal{R}_x\|_{L^\infty(Q_T)} + \|\mathcal{R}\|_{L^\infty(Q_T)} + \|cat_1 - cat_2\|_{L^\infty(\Omega)}). \end{aligned} \quad (3.95)$$

As $T < 1$, hence $T < \sqrt{T}$, continuing the estimate (3.94) with using (3.95), we obtain:

$$\begin{aligned} \|\mathcal{R}\|_{W^{1,\infty}(Q_T)} & \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \sqrt{T} (\|\mathcal{R}\|_{W^{1,\infty}(Q_T)} + \|cat_1 - cat_2\|_{W^\infty(\Omega)}) + \\ & + C(R, r_\alpha, \epsilon, M) \|cat_1 - cat_2\|_{W^{1,\infty}(\Omega)}. \end{aligned} \quad (3.96)$$

From (3.96), for $T < T_6 = (\frac{1}{2C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat})})^2$, we have:

$$\|\mathcal{R}\|_{W^{1,\infty}(Q_T)} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \|cat_1 - cat_2\|_{W^{1,\infty}(\Omega)}. \quad (3.97)$$

Putting (3.97) into (3.88), we get:

$$\|\mathcal{U}\|_{Y_T} \leq C(M, T^{**}, \epsilon, r_\alpha, u_0, C_{cat}) \|cat_1 - cat_2\|_{W^{1,\infty}(\Omega)}. \quad (3.98)$$

Finally, from (3.97), (3.98), with $T < T^{***} = \min\{T_4, T_5, T_6, T^{**}\}$ we get (3.80). ■ Due to the continuous embedding of $W^{1,\infty}(Q_T)$ in $\mathbf{X}_T$, from Theorem 3.17, we have the following remark:

Corollary 3.18 (r, c) is continuous in $\mathbf{X}_T \times \mathbf{Y}_T$ with respect to $cat(x)$ in $W^{1,\infty}(\Omega)$ for problem I_a with T small enough.

3.4 On the Frechet differentiability of r and c with respect to $cat(x)$ for problem I_a

Definition 3.19 Under the assumptions of Theorem 3.4 we define the state mapping $\mathcal{P}$ as following

$$\begin{aligned} \mathcal{P} : W^{1,\infty}(\Omega) & \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T \\ cat & \longmapsto \mathcal{P}(cat) = (r(cat), c(cat)) \end{aligned} \quad (3.99)$$

From the above section 3.1 and 3.2, we know that $\mathcal{P}$ is defined. In this section we will consider the differentiability of the state mapping.

3.4.1 The sensitivity system

We want to present a sensitivity system of equations to calculate $r_{cat}\delta$, for this we refer [11].

Let μ a positive number, we have

$$r_t(cat) = -\frac{D_2 cat c}{\int_0^1 r H_\epsilon(c) dx}, \quad (3.100)$$

$$r_t(cat + \mu\delta) = -\frac{D_2(cat + \mu\delta)c(cat + \mu\delta)}{\int_0^1 r(cat + \mu\delta) H_\epsilon(c(cat + \mu\delta)) dx}, \quad (3.101)$$

where c, r satisfy (3.11), (3.15), (3.3), (3.16), (3.17) and $c(cat + \delta), r(cat + \delta)$ satisfy (3.11), (3.15), (3.3), (3.16), (3.17) with replacing cat by $cat + \mu\delta$.

Substracting (3.101) to (3.100), we get

$$r_t(cat + \delta) - r_t = \frac{-D_2(cat + \mu\delta)c(cat + \mu\delta) \int_0^1 r H_\epsilon(c) dx + D_2 D_2 cat c \int_0^1 r(cat + \mu\delta) H_\epsilon(c(cat + \mu\delta)) dx}{\int_0^1 r(cat + \mu\delta) H_\epsilon(c(cat + \mu\delta)) dx \int_0^1 r H_\epsilon(c) dx}. \quad (3.102)$$

Dividing two sides of (3.102) by μ , we obtain

$$\begin{aligned} \left(\frac{r(cat + \delta) - r}{\mu} \right)_t &= \frac{-D_2 \left(\frac{cat + \mu\delta - cat}{\mu} \right) c(cat + \mu\delta) + D_2 cat \frac{c(cat + \mu\delta) - c}{\mu}}{\int_0^1 r(cat + \mu\delta) H_\epsilon(c(cat + \mu\delta)) dx \int_0^1 r H_\epsilon(c) dx} + \\ &+ D_2 cat c \int_0^1 \left(\frac{r - r(cat + \mu\delta)}{\epsilon} H_\epsilon(c) dx + \int_0^1 r(cat + \mu\delta) \frac{H_\epsilon(c) - H_\epsilon(c(cat + \mu\delta))}{\mu} dx \right). \end{aligned} \quad (3.103)$$

Denote

$$\eta(t, x) := \frac{\partial r}{\partial cat}(cat)\delta, \quad \frac{\partial r}{\partial \varphi}(t, x) := \frac{\partial c}{\partial cat}(cat)\delta, \quad (3.104)$$

letting $\mu \rightarrow 0$ in (3.103), we deduce

$$\eta_t = -\frac{D_2 cat \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \varphi + H_\epsilon(c) \eta dx - \frac{D_2 \delta c}{\int_0^1 r H_\epsilon(c) dx}, \quad (3.105)$$

η satisfies the homogeneous initial condition .

Now we consider the parabolic equation (3.11), for $c = c(cat)$ and $c(cat + \mu\delta)$, subtracting the two equations

$$c_t - c_{xx} - \frac{2r_x c_x}{r} + \frac{(2r_t + \frac{D_1}{\int_0^1 r H_\epsilon(c) dx})c}{r} = 0, \quad (t, x) \in Q_T. \quad (3.106)$$

$$\frac{c_t(cat + \mu\delta) - c_{xx}(cat + \mu\delta) - \frac{2r_x(cat + \mu\delta)c_x(cat + \mu\delta)}{r(cat + \mu\delta)} + (2r_t(cat + \mu\delta) + \frac{D_1}{\int_0^1 r(cat + \mu\delta)H_\epsilon(c(cat + \mu\delta))dx})c(cat + \mu\delta)}{r(cat + \mu\delta)} = 0, \quad (t, x) \in Q_T, \quad (3.107)$$

we get

$$\begin{aligned} c_t(cat + \mu\delta)c_t - (c_{xx}(cat + \mu\delta) - c_{xx}) - \left(\frac{2r_x(cat + \mu\delta)c_x(cat + \mu\delta)}{r(cat + \mu\delta)} - \frac{2r_x c_x}{r} \right) + \\ + \left(\frac{(2r_t(cat + \mu\delta)c(cat + \mu\delta))}{r(cat + \mu\delta)} - \frac{(2r_t c)}{r} \right) + \left(\frac{D_1 c(cat + \mu\delta)}{r(cat + \mu\delta) \int_0^1 r(cat + \mu\delta)H_\epsilon(c(cat + \mu\delta))dx} - \frac{D_1 c}{r \int_0^1 rH_\epsilon(c)dx} \right) = 0 \end{aligned} \quad (3.108)$$

Dividing two sides of (3.108) by μ , we obtain

letting $\mu \rightarrow 0$ in (3.108), we obtain

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{2r_x\varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 rH_\epsilon(c)dx} \right) \varphi - \frac{D_1 c}{r(\int_0^1 rH_\epsilon(c)dx)^2} \int_0^1 H_\epsilon(c)\eta + rH'_\epsilon(c)\varphi dx - \\ - \frac{2c_x\eta_x}{r} + \frac{2c\eta_t}{r} + \left(\frac{2r_x c_x}{r^2} - \frac{2r_t c}{r^2} - \frac{D_1 c}{r^2 \int_0^1 rH_\epsilon(c)dx} \right) \eta = 0 \end{aligned} \quad (3.109)$$

Putting (3.105) into (3.109), we deduce

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{2r_x\varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 rH_\epsilon(c)dx} - \frac{2cD_2 cat}{\int_0^1 rH_\epsilon(c)dx} \right) \varphi = \\ = \left(\frac{2D_2 catc^2}{r(\int_0^1 rH_\epsilon(c))^2} - \frac{D_1 c}{r(\int_0^1 rH_\epsilon(c)dx)^2} \right) \int_0^1 H_\epsilon(c)\eta + rH'_\epsilon(c)\varphi dx + \\ + \frac{2c_x\eta_x}{r} - \left(\frac{2r_x c_x}{r^2} - \frac{2r_t c}{r^2} - \frac{D_1 c}{r^2 \int_0^1 rH_\epsilon(c)dx} \right) \eta + \frac{2D_2 \delta c^2}{r \int_0^1 rH_\epsilon(c)dx}, \end{aligned} \quad (3.110)$$

φ satisfies the homogeneous initial and mixed boundary conditions.

Definition 3.20 (*The sensitivity system*)

The system (3.105), (3.110) with the homogeneous initial and mixed boundary conditions:

$$\eta(0, x) = 0, \quad x \in [0, 1], \quad (3.111a)$$

$$\varphi(0, x) = 0, \quad x \in [0, 1], \quad (3.111b)$$

$$\varphi(t, 0) = 0, \quad t \in [0, T], \quad (3.111c)$$

$$\varphi_x(t, 1) = 0, \quad t \in [0, T], \quad (3.111d)$$

$$(3.111e)$$

is called sensitivity system.

We define a weak solution.

Definition 3.21 A pair $(\eta, \varphi) \in W^{1,\infty}(Q_T) \times W(0, T; H^1(\Omega))$ is said to be a weak solution of the sensitivity system that is defined in Definition 3.20 if the following equalities are satisfied

$$\begin{aligned} (\varphi_t, v)_{((H^1(\Omega))^*, H^1(\Omega))} + \int_0^1 \varphi_x v_x dx - \int_0^1 \frac{2r_x \varphi_x}{r} v dx + \int_0^1 \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(c) dx} - \frac{2c D_2 cat}{\int_0^1 r H_\epsilon(c) dx} \right) \varphi v dx = \\ = \int_0^1 H_\epsilon(c) \eta + r H'_\epsilon(c) \varphi dx \int_0^1 \left(\frac{2D_2 cat c^2}{r (\int_0^1 r H_\epsilon(c))^2} - \frac{D_1 c}{r (\int_0^1 r H_\epsilon(c) dx)^2} \right) v dx + \int_0^1 \frac{2c_x \eta_x}{r} v dx - \\ - \int_0^1 \left(\frac{2r_x c_x}{r^2} - \frac{2r_t c}{r^2} - \frac{D_1 c}{r^2 \int_0^1 r H_\epsilon(c) dx} \right) \eta v dx + \int_0^1 \frac{2D_2 \delta c^2 v}{r \int_0^1 r H_\epsilon(c) dx} dx \forall v \in V, \quad a.e. \quad t \in [0, T]. \end{aligned} \quad (3.112)$$

$$\varphi(0, x) = 0, \quad x \in [0, 1]. \quad (3.113)$$

$$\eta(t, x) = \int_0^t \left(-\frac{D_2 cat \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \varphi + H_\epsilon(c) \eta - \frac{\delta c}{\int_0^1 r H_\epsilon(c) dx} \right) d\tau, \quad t \in [0, T]. \quad (3.114)$$

Similarly to Sections 3.1 and 3.2, for some given positive constant N , we define the set

$$N_T = \{(\eta, \varphi), \eta \in \mathbf{X}_T, \varphi \in \mathbf{Y}_T, \|\eta\|_{\mathbf{X}_T} + \|\varphi\|_{\mathbf{Y}_T} \leq N\}. \quad (3.115)$$

We present the following theorem:

Theorem 3.22 There exist T small enough such that $r(cat) \in \mathbf{X}_T$ and $c(cat) \in \mathbf{Y}_T$ are Fréchet differentiable with respect to $cat \in W^{1,\infty}(\Omega)$.

In order to show that $r(cat), c(cat)$ are Fréchet differentiable, we will prove the following items:

1. There exist unique weak solution $(\eta, \varphi) \in N_T$ of the sensitivity system and they are linear, bounded with respect to $\delta \in W^{1,\infty}(\Omega)$ with T small enough.

$$2. \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|r(cat+\delta)-r(cat)-\eta\|_{\mathbf{X}_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0 \text{ and } \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|c(cat+\delta)-c(cat)-\varphi\|_{\mathbf{Y}_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0$$

We have the following results.

Lemma 3.23 *There exist solution $(\eta, \varphi) \in N_T$ of sensitivity system that is defined in Definition 3.20 and they are linear, bounded with respect to $\delta \in W^{1,\infty}(\Omega)$ with T small enough.*

Proof. We define operator

$$\mathcal{F} : N_T \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T$$

as follows:

For $(\bar{\eta}, \bar{\varphi}) \in N_T$ define $(\eta, \varphi) = \mathcal{F}(\bar{\eta}, \bar{\varphi})$ as the solution of the system

$$\eta(t, x) = \int_0^t \left(-\frac{D_2 cat \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \bar{\varphi} + H_\epsilon(c) \bar{\eta} - \frac{\delta c}{\int_0^1 r H_\epsilon(c) dx} \right) d\tau, \quad (3.116)$$

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{r_x \varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(c) dx} + \frac{2c D_2 cat}{\int_0^1 r H_\epsilon(c) dx} \right) \varphi = \\ = \left(\frac{2D_2 cat c^2}{r(\int_0^1 r H_\epsilon(c))^2} - \frac{D_1 c}{r(\int_0^1 r H_\epsilon(c) dx)^2} \right) \int_0^1 H_\epsilon(c) \bar{\eta} + r H'_\epsilon(c) \bar{\varphi} dx + \\ + \frac{2c_x \eta_x}{r} - \left(\frac{2r_x c_x}{r^2} + \frac{2r_t c}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r H_\epsilon(c) dx} \right) \eta + \frac{2 D_2 \delta c^2}{r \int_0^1 r H_\epsilon(c) dx}, \end{aligned} \quad (3.117)$$

with homogeneous initial and mixed boundary condition for φ as written in (3.111b) – (3.111d). Similarly to Section 3.1 and Section 3.2, by applying Banach fixed point theorem, there exist unique weak solution $(\eta, \varphi) \in N_T$ of the sensitivity system with T small enough. Besides, as the sensitivity system is linear with respect to cat , η and φ , then η and φ are linear with respect to δ . Finally, we will show that $\|\eta\|_{\mathbf{X}_T}$ and $\|\varphi\|_{\mathbf{Y}_T}$ are bounded with respect to $\|\delta\|_{W^{1,\infty}(\Omega)}$.

In one hand, apply Theorem 3.9 to the equation (3.110), we obtain

$$\|\varphi\|_{\mathbf{Y}_T} \leq C(M, T, \epsilon, r_\alpha, cat, H_\epsilon) \left(\sqrt{T} (\|\varphi\|_{\mathbf{Y}_T} + \|\eta\|_{\mathbf{X}_T}) + \|\delta\|_{L^2(Q_T)} \right). \quad (3.118)$$

For $T < T_7 = \frac{1}{2C^2(M, T, \epsilon, r_\alpha, cat)}$, continuing (3.116)

$$\|\varphi\|_{\mathbf{Y}_T} \leq C_1(M, T, \epsilon, r_\alpha, cat) \left(\sqrt{T} \|\eta\|_{\mathbf{X}_T} + \|\delta\|_{L^2(Q_T)} \right). \quad (3.119)$$

In the other hand, from (3.105), we get

$$\|\eta\|_{\mathbf{X}_T} \leq C(M, T, \epsilon, r_\alpha, cat) \sqrt{T} (\|\eta\|_{\mathbf{X}_T} + \|\varphi\|_{\mathbf{Y}_T} + \|\delta\|_{L^\infty(Q_T)}) \quad (3.120)$$

Putting (3.119) into (3.120),

$$\|\eta\|_{\mathbf{X}_T} \leq C_2(M, T, \epsilon, r_\alpha, cat) \sqrt{T} (\|\eta\|_{\mathbf{X}_T} + \|\delta\|_{L^\infty(Q_T)}) \quad (3.121)$$

We have, for $T < T_8 = \frac{1}{2C_2^2(M, T, \epsilon, r_\alpha, cat)}$, the estimate

$$\|\eta\|_{\mathbf{X}_T} \leq C(M, T, \epsilon, r_\alpha, cat) \sqrt{T} \|\delta\|_{L^\infty(Q_T)}. \quad (3.122)$$

Combining (3.122) and (3.119), for $T < T^{****} = \min\{T^{***}, T_7, T_8\}$ we have

$$\|\varphi\|_{\mathbf{Y}_T} \leq C(M, T, \epsilon, r_\alpha, cat) \sqrt{T} \|\delta\|_{L^\infty(Q_T)}, \quad (3.123)$$

which is required to prove. ■

We have following Lemma:

Lemma 3.24 *Denote*

$$\xi = r(cat + \delta) - r(cat) - \eta,$$

and

$$\psi = c(cat + \delta) - c(cat) - \varphi.$$

Then ξ and ψ satisfy the following system

$$\psi_t - \psi_{xx} - \frac{2r_x\psi_x}{r(cat + \delta)} + F_1(\xi, \psi) = F_2(\eta, \varphi) + \omega_\delta, \quad (t, x) \in Q_T, \quad (3.124a)$$

$$\xi_t = F_3(\xi, \psi) + F_4(\eta, \varphi) + \omega_\delta \quad (t, x) \in Q_T, \quad (3.124b)$$

$$\xi(0, x) = 0, \quad x \in \Omega, \quad (3.124c)$$

$$\psi(0, x) = 0, \quad (3.124d)$$

$$\psi(t, 0) = 0, \quad t \in [0, T], \quad (3.124e)$$

$$\psi_x(t, 0) = 0, \quad (3.124f)$$

where $F_2(\eta, \varphi)$, $F_4(\eta, \varphi)$ contain only the functions in two variables η and φ , in which the lowest-degree term is of the second degree and $F_1(\xi, \psi)$, $F_3(\xi, \psi)$ are linear with respect to ξ and ψ .

$$\|\omega_\delta\|_{L^\infty(Q_T)} = o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (3.125)$$

Proof.

Now we aim to get a system of equations of ξ and ψ . We see that, (ξ, ψ) satisfy homogeneous initial and mix-boundary conditions:

$$\begin{aligned} \xi(0, x) &= 0 \\ \psi(0, x) &= 0 \\ \psi(t, 0) &= 0 \\ \psi_x(t, 0) &= 0 \end{aligned} \quad (3.126)$$

Using Taylor expansion

$$H_\epsilon(c(cat + \delta)) - H_\epsilon(c) = H'_\epsilon(c)(c(cat + \delta) - c) + \frac{1}{2}H''_\epsilon(c^*)(c(cat + \delta) - c) + o((c(cat + \delta) - c)^2), \quad (3.127)$$

From the Fréchet differentiability of $c \in \mathbf{Y}_T$ with respect to $cat \in W^{1,\infty}(\Omega)$, we rewrite (3.127) as follows

$$H_\epsilon(c(cat + \delta)) - H_\epsilon(c) = H'_\epsilon(c)(c(cat + \delta) - c) + \frac{1}{2}H''_\epsilon(c^*)(c(cat + \delta) - c) + \omega_\delta, \quad (3.128)$$

where

$$\|\omega_\delta\|_{L^\infty(Q_T)} = o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (3.129)$$

We calculate some expressions, which we will need later for obtaining a system of equations of ξ and ψ .

$$\begin{aligned} I_1 &= \frac{1}{\int_0^1 r H_\epsilon(c) dx} - \frac{1}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx} = \\ &= \frac{1}{\int_0^1 r H_\epsilon(c) dx} - \frac{1}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \frac{1}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \frac{1}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx} = \\ &= \frac{\int_0^1 (r(cat + \delta) - r) H_\epsilon(c(cat + \delta)) dx}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \frac{\int_0^1 r (H_\epsilon(c(cat + \delta)) - H_\epsilon(c)) dx}{\int_0^1 r H_\epsilon(c) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} = \\ &= \frac{\int_0^1 \xi H_\epsilon(c(cat + \delta)) dx}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \frac{\int_0^1 r H'_\epsilon(c) \psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} \\ &+ \frac{1}{2} \frac{\int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} + \frac{\int_0^1 \eta H_\epsilon(c(cat + \delta)) dx}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\ &+ \frac{\int_0^1 r H'_\epsilon(c) \varphi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} + \frac{1}{2} \frac{\int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \omega_\delta = I_1(\xi, \psi) + I_1(\eta, \varphi) + \omega_\delta \end{aligned} \quad (3.130)$$

where

$$\begin{aligned} I_1(\xi, \psi) &= \frac{\int_0^1 \xi H_\epsilon(c(cat + \delta)) dx}{\int_0^1 r (cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \frac{\int_0^1 r H'_\epsilon(c) \psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} \\ &+ \frac{1}{2} \frac{\int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} \end{aligned} \quad (3.131)$$

and

$$I_1(\eta, \varphi) = \frac{\int_0^1 \eta H_\epsilon(c(cat + \delta))dx}{\int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c(cat + \delta))dx} + \frac{\int_0^1 r H'(c)\varphi dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c)dx} + \frac{1}{2} \frac{\int_0^1 r H''(c*)\varphi^2 dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx}. \quad (3.132)$$

We see that $I_1(\xi, \psi)$ is linear with respect to ξ or ψ , and $I_1(\eta, \varphi)$ contains only the expressions of second degree in two variable η and φ .

We also note that

$$\begin{aligned} I_2 &= \frac{1}{\int_0^1 r H_\epsilon(c)dx} - \frac{1}{\int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \frac{\int_0^1 r H'_\epsilon(c)\varphi + H_\epsilon(c)\eta dx}{(\int_0^1 r H_\epsilon(c)dx)^2} = \\ &= I_1 - \frac{\int_0^1 r H'_\epsilon(c)\varphi + H_\epsilon(c)\eta dx}{(\int_0^1 r H_\epsilon(c)dx)^2} = I_1(\xi, \psi) + I_1(\eta, \varphi) - \frac{\int_0^1 r H'_\epsilon(c)\varphi + H_\epsilon(c)\eta dx}{(\int_0^1 r H_\epsilon(c)dx)^2} + \omega_\delta = \\ &= I_1(\xi, \psi) + \left(\frac{\int_0^1 \eta H_\epsilon(c(cat + \delta))dx}{\int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c(cat + \delta))dx} + \frac{\int_0^1 r H'(c)\varphi dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c)dx} + \frac{1}{2} \frac{\int_0^1 r H''(c*)\varphi^2 dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx} \right) - \frac{\int_0^1 r H'_\epsilon(c)\varphi + H_\epsilon(c)\eta dx}{(\int_0^1 r H_\epsilon(c)dx)^2} + \omega_\delta = \\ &= I_1(\xi, \psi) + \underbrace{\left(\frac{\int_0^1 \eta H_\epsilon(c(cat + \delta))dx}{\int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c(cat + \delta))dx} - \frac{\int_0^1 H_\epsilon(c)\eta dx}{(\int_0^1 r H_\epsilon(c)dx)^2} \right)}_{I_{21}} + \\ &+ \underbrace{\left(\frac{\int_0^1 r H'(c)\varphi dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c)dx} - \frac{\int_0^1 r H'(c)\varphi dx}{(\int_0^1 r H_\epsilon(c)dx)^2} \right)}_{I_{22}} + \underbrace{\frac{1}{2} \frac{\int_0^1 r H''(c*)\varphi^2 dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx}}_{I_{23}(\varphi)} + \omega_\delta, \end{aligned} \quad (3.133)$$

where ω_δ is defined in (3.129).

Meanwhile,

$$I_{21} = I_{21}(\xi, \psi) + I_{21}(\eta, \varphi), \quad (3.134)$$

where

$$I_{21}(\xi, \psi) = \frac{\int_0^1 r H'_\epsilon(c)\psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c(cat + \delta))dx} + \frac{1}{2} \frac{\int_0^1 \eta H''_\epsilon(c*)(c(cat + \delta) - c + \varphi)\psi dx}{\int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c(cat + \delta))dx} -$$

$$\begin{aligned}
 & - \frac{\int_0^1 \eta H_\epsilon(c) dx \int_0^1 H_\epsilon(c(cat + \delta)) \xi dx}{(\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^2 \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{\int_0^1 \eta H_\epsilon(c) dx \int_0^1 H_\epsilon(c(cat + \delta)) \xi dx}{(\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^2 \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + \\
 & + \left(\frac{\int_0^1 \eta H_\epsilon(c) dx}{(\int_0^1 r H_\epsilon(c) dx)^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \frac{\int_0^1 \eta H_\epsilon(c) dx}{(\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^3 (\int_0^1 r H_\epsilon(c) dx)^2} \right) \\
 & \left(\int_0^1 r H'_\epsilon(c) \psi dx + \frac{1}{2} \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx \right) + \\
 & + \frac{1}{2} \frac{\int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{(\int_0^1 r H_\epsilon(c) dx)^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \omega_\delta, \tag{3.135}
 \end{aligned}$$

$$\begin{aligned}
 I_{21}(\eta, \varphi) = & \frac{\int_0^1 \eta H'_\epsilon(c) \varphi dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \frac{\int_0^1 \eta H''_\epsilon(c^*) \varphi^2 dx}{\int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{\int_0^1 \eta H_\epsilon(c) dx}{(\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^3 (\int_0^1 r H_\epsilon(c) dx)^2} \left(\int_0^1 r H'_\epsilon(c) \varphi dx + \frac{1}{2} \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx \right) + \\
 & + \frac{\int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H'_\epsilon(c) \varphi dx}{(\int_0^1 r H_\epsilon(c) dx)^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \omega_\delta. \tag{3.136}
 \end{aligned}$$

Besides,

$$I_{22} = I_{22}(\psi) + I_{22}(\varphi), \tag{3.137}$$

where

$$I_{22}(\psi) = - \frac{\int_0^1 r H'_\epsilon(c) \varphi dx}{(\int_0^1 r H_\epsilon(c) dx)^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx} \left(\int_0^1 r H'_\epsilon(c) \psi dx + \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx \right), \tag{3.138}$$

$$I_{22}(\varphi) = - \frac{\int_0^1 r H'_\epsilon(c) \varphi dx}{(\int_0^1 r H_\epsilon(c) dx)^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx} \left(\int_0^1 r H'_\epsilon(c) \varphi^2 dx + \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx \right) + \omega_\delta. \tag{3.139}$$

Denoting that

$$I_2(\xi, \psi) = I_1(\xi, \psi) + I_{21}(\xi, \psi) + I_{22}(\psi),$$

$$I_2(\eta, \varphi) = I_{21}(\eta, \varphi) + I_{22}(\varphi),$$

then $I_2 = I_2(\xi, \psi) + I_2(\eta, \varphi) + \omega_\delta$. Note that $I_2(\xi, \psi)$ is linear with respect to ξ or ψ , and $I_2(\eta, \varphi)$ contains the functions in two variables η and φ , in which the lowest-degree term is of the second degree. From (3.100), (3.101) and (3.105), we have

$$\begin{aligned} r_t(cat + \delta) - r_t - \eta_t = & -\frac{D_2 cat \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \frac{D_2 \delta \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + \\ & + (D_2 cat \varphi - D_2 \delta c) \underbrace{\left(\frac{1}{\int_0^1 r H_\epsilon(c) dx} - \frac{1}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} \right)}_{I_1} + \\ & + D_2 cat c \underbrace{\left(\frac{1}{\int_0^1 r H_\epsilon(c) dx} - \frac{1}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \frac{\int_0^1 r H'_\epsilon(c) \varphi + H_\epsilon(c) \eta dx}{(\int_0^1 r H_\epsilon(c) dx)^2} \right)}_{I_2} + \omega_\delta. \end{aligned} \quad (3.140)$$

Combining (3.122) with the above equalities

$$\begin{aligned} \xi_t = & -\frac{D_2 cat \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + \frac{D_2 \delta \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + (D_2 cat \varphi - D_2 \delta c) I_1(\xi, \psi) + \\ & + D_2 cat c (I_1(\xi, \psi) + I_{21}(\xi, \psi) + I_{22}(\xi, \psi)) + (D_2 cat \varphi - D_2 \delta c) I_1(\eta, \varphi) + D_2 cat c (I_{21}(\eta, \varphi) + I_{22}(\eta, \varphi) + I_3(\varphi)) + \omega_\delta. \end{aligned} \quad (3.141)$$

Denote

$$\begin{aligned} F_3(\xi, \psi) = & -\frac{D_2 cat \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + \frac{D_2 \delta \psi}{\int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} + (D_2 cat \varphi - D_2 \delta c) I_1(\xi, \psi) + \\ & + D_2 cat c (I_1(\xi, \psi) + I_{21}(\xi, \psi) + I_{22}(\xi, \psi)), \end{aligned} \quad (3.142)$$

$$F_4(\eta, \varphi) = (D_2 cat \varphi - D_2 \delta c) I_1(\eta, \varphi) + D_2 cat c (I_{21}(\eta, \varphi) + I_{22}(\eta, \varphi) + I_3(\varphi)), \quad (3.143)$$

we get (3.124b). We notice that $F_3(\xi, \psi)$ is linear with respect to ξ and ψ , $F_4(\eta, \varphi)$ contains only the functions in two variables η and φ , in which the lowest-degree term is of the second degree. Due to Lemma 3.23, $\eta \in \mathbf{X}_T$ and $\varphi \in \mathbf{Y}_T$ are linear bounded with respect to $\delta \in W^{1,\infty}(\Omega)$ with some T small enough. Therefore,

$$\frac{\|F_4(\eta, \varphi)\|_{L^2(\mathcal{Q})}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (3.144)$$

Subtracting (3.106) by (3.107)

$$\begin{aligned}
 & (c_t(cat + \delta) - c_t) - (c_{xx}(cat + \delta) - c_{xx}) - \left(\frac{2r_x(cat + \delta)c_x(cat + \delta)}{r(cat + \delta)} - \frac{2r_t c}{r} \right) + \\
 & + \left(\frac{2r_t(cat + \delta)c(cat + \delta)}{r(cat + \delta)} - \frac{2r_t c}{r} \right) + \left(\frac{D_1 c(cat + \delta)}{r(cat + \delta) \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \frac{D_1 c}{r \int_0^1 r H_\epsilon(c)dx} \right) = 0
 \end{aligned} \tag{3.145}$$

which is equivalent to

$$\begin{aligned}
 & (c_t(cat + \delta) - c_t) - (c_{xx}(cat + \delta) - c_{xx}) - \frac{2(r_x(cat + \delta) - r_x)c_x(cat + \delta)}{r(cat + \delta)} - \frac{2r_x(c_x(cat + \delta) - c_x)}{r(cat + \delta)} + \\
 & + \frac{2r_x c_x(r(cat + \delta) - r)}{r r(cat + \delta)} + \frac{2r_t(cat + \delta)(c(cat + \delta) - c)}{r(cat + \delta)} + \frac{2(r_t(cat + \delta) - r_t)c}{r(cat + \delta)} - \frac{2r_t c(r(cat + \delta) - r)}{r r(cat + \delta)} + \\
 & + \frac{D_1 c(c(cat + \delta) - c)}{r(cat + \delta) \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \frac{D_1 c(r(cat + \delta) - r)}{r r(cat + \delta) \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \\
 & - \frac{D_1 c \int_0^1 (r(cat + \delta) - r)H_\epsilon(c(cat + \delta))dx}{r \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c)dx} - \frac{D_1 c \int_0^1 r(H_\epsilon(c(cat + \delta)) - H_\epsilon(c))dx}{r \int_0^1 r H_\epsilon(c)dx \int_0^1 r H_\epsilon(c)dx} = 0.
 \end{aligned} \tag{3.146}$$

Now subtracting (3.109) by (3.146)

$$\begin{aligned}
 & (c_t(cat + \delta) - c_t - \varphi_t) - (c_{xx}(cat + \delta) - c_{xx} - \varphi_{xx}) - \underbrace{\left(\frac{2(r_x(cat + \delta) - r_x)c_x(cat + \delta)}{r(cat + \delta)} - \frac{2c_x \eta_x}{r} \right)}_{G_1} - \\
 & - \underbrace{\left(\frac{2r_x(c_x(cat + \delta) - c_x)}{r(cat + \delta)} - \frac{2r_x \varphi_x}{r} \right)}_{G_2} + \underbrace{\left(\frac{2r_x c_x(r(cat + \delta) - r)}{r r(cat + \delta)} - \frac{2r_x c_x \eta}{r^2} \right)}_{G_3} + \\
 & + \underbrace{\left(\frac{2r_t(cat + \delta)(c(cat + \delta) - c)}{r(cat + \delta)} - \frac{2r_t \varphi}{r} \right)}_{G_4} + \underbrace{\left(\frac{2(r_t(cat + \delta) - r_t)c}{r(cat + \delta)} - \frac{2c \eta_t}{r} \right)}_{G_5} - \\
 & - \underbrace{\left(\frac{2r_t c(r(cat + \delta) - r)}{r r(cat + \delta)} - \frac{2r_t c \eta}{r^2} \right)}_{G_6} + \underbrace{\left(\frac{D_1(c(cat + \delta) - c)}{r(cat + \delta) \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \frac{D_1 \varphi}{r \int_0^1 r H_\epsilon(c)dx} \right)}_{G_7} - \\
 & - \underbrace{\left(\frac{D_1 c(r(cat + \delta) - r)}{r r(cat + \delta) \int_0^1 r(cat + \delta)H_\epsilon(c(cat + \delta))dx} - \frac{D_1 c \eta}{r^2 \int_0^1 r H_\epsilon(c)dx} \right)}_{G_8} - \\
 & - \underbrace{\left(\frac{D_1 c \int_0^1 r H'_\epsilon(c)(c(cat + \delta) - c)dx}{r \int_0^1 r H_\epsilon(c(cat + \delta))dx \int_0^1 r H_\epsilon(c)dx} - \frac{D_1 c \int_0^1 r H'_\epsilon(c)\varphi dx}{r (\int_0^1 r H_\epsilon(c)dx)^2} \right)}_{G_9}
 \end{aligned}$$

$$\begin{aligned}
 & - \frac{1}{2} \frac{D_1 c \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c)^2 dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 & - \left(\frac{D_1 c \int_0^1 (r(cat + \delta) - r) H'_\epsilon(c)(c(cat + \delta) - c) dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 c \int_0^1 r H_\epsilon(c) \eta dx}{r (\int_0^1 r H_\epsilon(c) dx)^2} \right) - \\
 & - \frac{D_1 c \int_0^1 (r(cat + \delta) - r) H'_\epsilon(c)(c(cat + \delta) - c) dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\
 & - \frac{D_1 c \int_0^1 (r(cat + \delta) - r) H''_\epsilon(c^*)(c(cat + \delta) - c)^2 dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \omega_\delta = 0. \tag{3.147}
 \end{aligned}$$

Now we analyze $G_1 - G_{13}$:

$$G_1 = \frac{2\xi c_x(cat + \delta)}{r(cat + \delta)} + \frac{2\eta_x \psi}{r(cat + \delta)} - \frac{2\eta_x c_x \xi}{r r(cat + \delta)} + \frac{2\eta_x \varphi}{r(cat + \delta)} - \frac{2\eta_x c_x \eta}{r r(cat + \delta)} = G_1(\xi, \psi) + G_1(\eta, \varphi). \tag{3.148}$$

$$G_2 = \frac{2r_x \psi_x}{r(cat + \delta)} - \frac{2r_x \varphi_x \xi}{r r(cat + \delta)} - \frac{2r_x \varphi_x \eta}{r r(cat + \delta)} = G_2(\xi, \psi) + G_2(\eta, \varphi). \tag{3.149}$$

$$G_3 = \frac{2r_x c_x \psi}{r r(cat + \delta)} - \frac{2r_x \eta c_x \xi}{r^2 r(cat + \delta)} - \frac{2r_x c_x \eta^2}{r^2 r(cat + \delta)} = G_3(\xi, \psi) + G_3(\eta, \varphi). \tag{3.150}$$

$$G_4 = \frac{2r_t \psi}{r(cat + \delta)} + \frac{2\varphi \xi_t}{r(cat + \delta)} + \frac{2\varphi \eta_t}{r(cat + \delta)} - \frac{2r_t \varphi \xi}{r r(cat + \delta)} - \frac{2r_t \varphi \eta}{r r(cat + \delta)}. \tag{3.151}$$

Putting (3.124b) into (3.151), we get

$$G_4 = \frac{2r_t \psi}{r(cat + \delta)} + \frac{2\varphi(F_3(\xi, \psi) + F_4(\eta, \varphi) + \omega_\delta)}{r(cat + \delta)} + \frac{2\varphi \eta_t}{r(cat + \delta)} - \frac{2r_t \varphi \xi}{r r(cat + \delta)} - \frac{2r_t \varphi \eta}{r r(cat + \delta)} = G_2(\xi, \psi) + G_2(\eta, \varphi). \tag{3.152}$$

$$G_5 = \frac{2c \xi_t}{r(cat + \delta)} - \frac{2c \eta_t \xi}{r r(cat + \delta)} - \frac{2c \eta_t \eta}{r r(cat + \delta)} = G_5(\xi, \psi) + G_5(\eta, \varphi). \tag{3.153}$$

Putting (3.124b) into (3.153), we have

$$G_5 = \frac{2c(F_3(\xi, \psi) + F_4(\eta, \varphi) + \omega_\delta)}{r(cat + \delta)} - \frac{2c\eta_t\xi}{r r(cat + \delta)} - \frac{2c\eta_t\eta}{r r(cat + \delta)} = G_5(\xi, \psi) + G_5(\eta, \varphi). \quad (3.154)$$

$$G_6 = \frac{2r_t c \xi}{r r(cat + \delta)} - \frac{2r_t c \eta \xi}{r^2 r(cat + \delta)} - \frac{2r_t c \eta^2}{r^2 r(cat + \delta)} = G_6(\xi, \psi) + G_6(\eta, \varphi). \quad (3.155)$$

$$\begin{aligned} G_7 = & \frac{D_1 \psi}{r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 \varphi \xi}{r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 \varphi \int_0^1 \xi H_\epsilon(c(cat + \delta)) dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 \varphi \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{1}{2} \frac{D_1 \varphi \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 \varphi \eta}{r r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 \varphi \int_0^1 \eta H_\epsilon(c(cat + \delta)) dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 \varphi \int_0^1 r H'_\epsilon(c) \varphi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \frac{1}{2} \frac{D_1 \varphi \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} = G_7(\xi, \psi) + G_7(\eta, \varphi). \end{aligned} \quad (3.156)$$

$$\begin{aligned} G_8 = & \frac{D_1 c \xi}{r r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 c \eta \xi}{r^2 r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 c \eta \int_0^1 \xi H_\epsilon(c(cat + \delta)) dx}{r^2 \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 c \eta \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\ & - \frac{1}{2} \frac{D_1 c \eta \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \frac{D_1 c \eta^2}{r^2 r(cat + \delta) \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx} - \\ & - \frac{D_1 c \eta \int_0^1 \eta H_\epsilon(c(cat + \delta)) dx}{r^2 \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \frac{D_1 c \eta \int_0^1 r H'_\epsilon(c) \varphi dx}{r^2 \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\ & - \frac{1}{2} \frac{D_1 c \eta \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{r \int_0^1 r^2 H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} = G_8(\xi, \psi) + G_8(\eta, \varphi). \end{aligned} \quad (3.157)$$

$$\begin{aligned}
 G_9 &= \frac{D_1 c \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \frac{D_1 c \int_0^1 r H'_\epsilon(c) \varphi dx \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \\
 &- \frac{1}{2} \frac{D_1 c \int_0^1 r H'_\epsilon(c) \varphi dx \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \\
 &- \frac{D_1 c (\int_0^1 r H'_\epsilon(c) \varphi dx)^2}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \frac{1}{2} \frac{D_1 c \int_0^1 r H'_\epsilon(c) \varphi dx \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} = \\
 &= G_9(\xi, \psi) + G_9(\eta, \varphi).
 \end{aligned} \tag{3.158}$$

$$\begin{aligned}
 G_{10} &= -\frac{1}{2} \frac{D_1 c \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r (\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^2} - \frac{1}{2} \frac{D_1 c \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{r (\int_0^1 r H_\epsilon(c(cat + \delta)) dx)^2} = \\
 &= G_{10}(\xi, \psi) + G_{10}(\eta, \varphi).
 \end{aligned} \tag{3.159}$$

$$\begin{aligned}
 G_{11} &= \frac{D_1 c \int_0^1 H_\epsilon(c) \xi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} - \\
 &- \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 &- \frac{1}{2} \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 &- \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 H_\epsilon(c(cat + \delta)) \xi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 &- \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H'_\epsilon(c) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \frac{1}{2} \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H''_\epsilon(c^*)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \\
 &- \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H'_\epsilon(c) \varphi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 &- \frac{1}{2} \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H''_\epsilon(c^*) \varphi^2 dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} - \\
 &- \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 H_\epsilon(c(cat + \delta)) \varphi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c) dx} -
 \end{aligned}$$

$$\begin{aligned}
 & - \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H'_\epsilon(c) \varphi dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} - \frac{1}{2} \frac{D_1 c \int_0^1 \eta H_\epsilon(c) dx \int_0^1 r H''_\epsilon(c) \varphi^2 dx}{r \int_0^1 r H_\epsilon(c(cat + \delta)) dx (\int_0^1 r H_\epsilon(c) dx)^2} = \\
 & = G_{11}(\xi, \psi) + G_{11}(\eta, \varphi). \tag{3.160}
 \end{aligned}$$

$$\begin{aligned}
 G_{12} = & - \frac{D_1 c \int_0^1 \xi H'_\epsilon(c)(c(cat + \delta) - c) dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{D_1 c \int_0^1 \eta H'_\epsilon(c) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{D_1 c \int_0^1 \eta H'_\epsilon(c) \varphi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} = G_{12}(\xi, \psi) + G_{12}(\eta, \varphi). \tag{3.161}
 \end{aligned}$$

$$\begin{aligned}
 G_{13} = & \frac{1}{2} \frac{D_1 c \int_0^1 \xi H''_\epsilon(c)(c(cat + \delta) - c)^2 dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{1}{2} \frac{D_1 c \int_0^1 \eta H''_\epsilon(c)(c(cat + \delta) - c + \varphi) \psi dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} + \\
 & + \frac{1}{2} \frac{D_1 c \int_0^1 \eta H''_\epsilon(c) \varphi^2 dx}{r \int_0^1 r(cat + \delta) H_\epsilon(c(cat + \delta)) dx \int_0^1 r H_\epsilon(c(cat + \delta)) dx} = G_{13}(\xi, \psi) + G_{13}(\eta, \varphi). \tag{3.162}
 \end{aligned}$$

Combine (3.147) and the equalities from (3.148) - (3.159), we deduce

$$\psi_t - \psi_{xx} - \frac{2r_x \psi_x}{r(cat + \delta)} + \sum_{i=1}^{13} G_i(\xi, \psi) = - \sum_{i=1}^{13} G_i(\eta, \varphi) + \omega_\delta, \tag{3.163}$$

where $F_1(\xi, \psi) = \sum_{i=1}^{13} G_i(\xi, \psi)$ is linear with respect to ψ, ξ_x, ξ and the coefficients $F_2(\eta, \varphi) = \sum_{i=1}^{13} G_i(\eta, \varphi)$ contain only the functions in variables η, φ, η_x and φ_x in which the lowest-degree term is of the second degree. Moreover, for the sake of Lemma 3.23, $\eta \in \mathbf{X}_T$ and $\varphi \in \mathbf{Y}_T$ are linear bounded with respect to $\delta \in W^{1,\infty}(\Omega)$ with some T small enough. Hence, it satisfies that

$$\frac{\|F_2(\eta, \varphi)\|_{L^2(\mathcal{Q})}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = o(\|\delta\|_{W^{1,\infty}(\Omega)}). \tag{3.164}$$

The lemma now follows from (3.141), (3.143), (3.142), (3.163) and (3.126). ■

We define a weak solution of system (3.124a) – (3.124f) in the following sense.

Definition 3.25 A pair $(\xi, \psi) \in W^{1,\infty}(Q_T) \times W(0, T; H^1(\Omega))$ is said to be a weak solution of the system (3.124a) – (3.124f) if the following equalities are satisfied

$$\begin{aligned} (\psi_t, v)_{((H^1(\Omega))^*, H^1(\Omega))} + \int_0^1 \psi_x v_x dx - \int_0^1 \frac{2r_x \psi_x}{r(cat + \delta)} v dx + \int_0^1 F_1(\xi, \psi) v dx = \\ = \int_0^1 (F_2(\eta, \varphi) + \omega_\delta) v dx \forall v \in V, \text{ a.e. } t \in [0, T]. \end{aligned} \quad (3.165)$$

$$\psi(0, x) = 0, \quad x \in [0, 1]. \quad (3.166)$$

$$\xi(t, x) = \int_0^t F_3(\xi, \psi) + F_4(\eta, \varphi) + \omega_\delta d\tau, \quad t \in [0, T]. \quad (3.167)$$

Let $N^{\xi, \psi}$ be some positive constant, denote the set

$$N_T^{\xi, \psi} = \{(\xi, \psi), \xi \in \mathbf{X}_T, \psi \in \mathbf{Y}_T, \|\xi\|_{\mathbf{X}_T} + \|\psi\|_{\mathbf{Y}_T} \leq N^{\xi, \psi}\}. \quad (3.168)$$

We have the following result:

Theorem 3.26 There exist enough small positive number T such that the system (3.165) – (3.167) has unique solution on $N_T^{\xi, \psi}$ and

$$(i) \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|\xi\|_{\mathbf{X}_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0,$$

$$(ii) \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|\psi\|_{\mathbf{Y}_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0.$$

Proof. We define the operator

$$\mathcal{K} : N_T^{\xi, \psi} \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T$$

as follows.

For $(\tilde{\xi}, \tilde{\psi}) \in N_T^{\xi, \psi}$ define $(\xi, \psi) = \mathcal{K}(\tilde{\xi}, \tilde{\psi})$ as the solution of the system

$$\xi(t, x) = \int_0^t (F_3(\tilde{\xi}, \tilde{\psi}) + F_4(\eta, \varphi) + \omega_\delta) d\tau, \quad (3.169)$$

$$\psi_t - \psi_{xx} - \frac{2r_x \psi_x}{r(cat + \delta)} + F_1(\xi, \psi) = F_2(\eta, \varphi) + \omega_\delta, \quad (3.170)$$

with homogeneous initial and mixed boundary condition for ψ as written in (3.124d) – (3.124f). Similarly to Section 3.1 and Section 3.2, by applying Banach fixed point theorem, there exist unique weak solution $(\xi, \psi) \in N_T^{\xi, \psi}$ of the system (3.124a) – (3.124f) with T small enough. Using the similar

technique in Section 3.1 and Section 3.2 and using Gronwall's inequality, for T small enough, we have the following estimates:

$$\|\xi\|_{\mathbf{X}_T} + \|\psi\|_{\mathbf{Y}_T} \leq C = C(M, T, \epsilon, r_\alpha, cat) \left(\|F_2(\eta, \varphi) + \omega_\delta\|_{L^2(0,T;L^2(\Omega))} + \|F_4(\eta, \varphi) + \omega_\delta\|_{L^2(0,T;L^2(\Omega))} \right). \quad (3.171)$$

The Theorem now follows from (3.144), (3.164) and (3.171). $\blacksquare$

3.5 Formulation and weak solution of problem I_b

Now we consider the case of cat depending on the both variables x and t .

$$c_t = c_{xx} + \frac{2r_x c_x}{r} - \frac{(2r_t + \frac{D_1}{\int_0^1 r H_\epsilon(c) dx})c}{r}, \quad (t, x) \in Q_T. \quad (3.172)$$

$$r_t = -\frac{D_2}{\int_0^1 r H_\epsilon(u + g) dx} cat(x)c, \quad (t, x) \in Q_T, \quad (3.173)$$

$$cat_t = \alpha_0 \int_0^1 H_{R_0}(r(y, t)) G(x - y) dy, \quad (3.174)$$

where α_0 is some positive number. with the initial and mixed boundary conditions

$$r(0, x) = r_\alpha(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$c(0, x) = h(x), \quad (3.4)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (3.12)$$

$$c_x(t, 1) = 0, \quad t \in [0, T], \quad (3.6)$$

$$cat(0, x) = cat_0(x) \quad (3.175)$$

We suppose the conditions on h and cat_0 by

$$\begin{aligned} h(0) &= 0, h(1) = 0, \\ h &\in W^{1,\infty}(\Omega), \\ cat_0 &\in W^{1,\infty}(\Omega). \end{aligned} \quad (3.176)$$

The functions $\beta(t, r, c)$ and $\gamma(t, r, c)$ are kept as in (3.8), where $H_\epsilon(x)$ is from (A.12). Using the similar change of variables of $w(t, x) = c(t, x) - 1$ in Problem I (system of (3.172)-(3.174)) and conditions (3.3)-(3.6), we deduce the new equivalent system

$$w_t - w_{xx} - \frac{2r_x w_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 \text{cat}(t, x)}{r \int_0^1 r H_\epsilon(w+1) dx} \right) w = \frac{2D_2 \text{cat}(t, x) - D_1}{r \int_0^1 r H_\epsilon(w+1) dx}, \quad (t, x) \in Q_T, \quad (3.177)$$

$$r_t = -\frac{D_2}{\int_0^1 r H_\epsilon(w+g) dx} \text{cat}(t, x)(w+1), \quad (t, x) \in Q_T, \quad (3.178)$$

$$\text{cat}_t = \alpha_0 \int_0^1 H_{R_0}(r(y, t)) G(x-y) dy, \quad (3.174)$$

$$r(0, x) = r_\alpha(x) = 1, \quad x \in \Omega, \quad (3.3)$$

$$w(0, x) = w_0(x) = h(0) - 1, \quad x \in \Omega, \quad (3.179)$$

$$w_x(t, 1) = 0, \quad t \in [0, T], \quad (3.180)$$

$$\text{cat}(0, x) = \text{cat}_0(x). \quad (3.181)$$

The solution of this system is understood in the following sense:

Definition 3.27 *The pair $(r, w) \in W^{1,\infty}(Q_T) \times W(0, T; H^1(\Omega))$ is said to be a weak solution of (3.177)-(3.181), (3.3), if the following equalities are satisfied*

$$\begin{aligned} (w_t, v)_{((H^1(\Omega))^*, H^1(\Omega))} + \int_0^1 w_x v_x dx - \int_0^1 \frac{2r_x w_x}{r} v dx + \int_0^1 \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 \text{cat}(t, x)}{r \int_0^1 r H_\epsilon(w+1) dx} \right) u v dx = \\ = \int_0^1 \frac{2D_2 \text{cat}(t, x) - D_1}{r \int_0^1 r H_\epsilon(w+1) dx} v dx, \\ \forall v \in V, \text{ and with a.e. } t \in [0, T], \end{aligned} \quad (3.182)$$

where $V = \{v \in H^1(\Omega), v(0) = 0\}$,

$$w(0, x) = w_0(x) = h(0) - 1, \quad x \in \Omega, \quad (3.179)$$

$$r(t, x) = 1 - \int_0^t \frac{D_2}{\int_0^1 r H_\epsilon(u + g) dx} cat(t, x) (u(\tau, x) + 1) d\tau, \quad t \in [0, T], \quad (3.183)$$

where

$$cat(t, x) = cat_0(x) + \alpha_0 \int_0^t \int_0^1 H_{R_0}(r(y, t)) G(x - y) dy. \quad (3.184)$$

3.6 Existence and uniqueness of the weak solution of problem I_b with $cat(t, x)$ model

Recalling the spaces $\mathbf{X}_T$, $\mathbf{Y}_T$ and set $\mathbf{M}_T \in \mathbf{X}_T \times \mathbf{Y}_T$ in the page 34, we define an operator $\mathcal{S}$

$$\mathcal{S} : \mathbf{M}_T \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T$$

For $(\bar{r}, \bar{w}) \in \mathbf{M}_T$ define $(r, w) = \mathcal{S}(\bar{r}, \bar{w})$ as the solution of following system of the equations

$$cat(t, x) = cat_0(x) + \alpha_0 \int_0^t \int_0^1 H_{R_0}(\bar{r}(t, y)) G(x - y) dy, \quad (3.185)$$

$$r(t, x) = 1 - \int_0^t \frac{D_2}{\int_0^1 \bar{r} H_\epsilon(\bar{w} + 1) dx} cat(t, x) (\bar{w} + 1) d\tau, \quad (3.186)$$

$$w_t + \mathcal{L}w = f, \quad (3.187)$$

with the initial and boundary condition (3.16), (3.17), where

$$\begin{aligned} \mathcal{L}w = -w_{xx} - \frac{2r_x w_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1 - 2D_2 cat(x)}{r \int_0^1 r H_\epsilon(\bar{w} + 1) dx} \right) w, \\ f = \frac{2D_2 cat(x) - D_1}{r \int_0^1 r H_\epsilon(\bar{w} + 1) dx}. \end{aligned} \quad (3.188)$$

We follow the similar approach for proving problem I_a to deal with the problem I_b :

- 1) $\mathcal{S}$ is defined from $\mathbf{M}_T$ onto $\mathbf{X}_T \times \mathbf{Y}_T$.
- 2) For T small enough such that $\mathcal{S}$ maps $\mathbf{M}_T$ to $\mathbf{M}_T$.
- 3) For T small enough such that $\mathcal{S}$ is s -contractive in $\mathbf{X}_T \times \mathbf{Y}_T$, i.e

$$\|\mathcal{S}(w_1, r_1) - \mathcal{S}(w_2, r_2)\|_{\mathbf{X}_T \times \mathbf{Y}_T} \leq s^* \|(w_1, r_1) - (w_2, r_2)\|_{\mathbf{X}_T \times \mathbf{Y}_T},$$

for all $(w_1, r_1), (w_2, r_2) \in \mathbf{M}_T$, and for $0 \leq s^* < 1$.

We have

Remark 3.28 Under condition on $cat_0(x)$ in (3.176), $cat(t, x)$ from equation (3.174) belongs to space $W^{1,\infty}(\Omega)$.

Thanks to above remark, we can reply the whole steps of the proof in section 3.2 for the existence and uniqueness of the weak solution of the problem I_a .

3.7 Sensitivity system for the Problem I_b

Suppose that r, c, cat are the solution of Problem I_b with the initial condition on cat is $cat(0, x) = cat_0$, and $r(cat_0 + \mu\delta), c(cat_0 + \mu\delta), cat(cat_0 + \mu\delta)$ are the solution of I_b with $cat(cat_0 + \mu\delta, 0, x) = cat_0 + \mu\delta$. Here $\delta \in W^{1,\infty}(\Omega)$.

Denote

$$\begin{aligned}\eta(t, x) &:= \frac{\partial r}{\partial cat_0}(cat_0)\delta = \lim_{\mu \rightarrow 0} \frac{r(cat_0 + \mu\delta) - r}{\mu}, \\ \varphi(t, x) &:= \frac{\partial c}{\partial cat_0}(cat_0)\delta = \lim_{\mu \rightarrow 0} \frac{c(cat_0 + \mu\delta) - c}{\mu}, \\ \psi(t, x) &:= \frac{\partial cat}{\partial cat_0}(cat_0)\delta = \lim_{\mu \rightarrow 0} \frac{cat(cat_0 + \mu\delta) - cat(cat_0)}{\mu}.\end{aligned}\tag{3.189}$$

Using the same technique in section 3.4, the sensitivity system for problem I_b is given by

$$\eta_t(t, x) = -\frac{D_2 c \psi}{\int_0^1 r H_\epsilon(c) dx} - \frac{D_2 cat_0 \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat_0 c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \varphi + H_\epsilon(c) \eta - \frac{\delta c}{\int_0^1 r H_\epsilon(c) dx}, \tag{3.190}$$

$$\begin{aligned}\varphi_t - \varphi_{xx} - \frac{r_x \varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat}{\int_0^1 r H_\epsilon(c) dx} \right) \varphi = \\ = - \left(\frac{D_1 c}{r(\int_0^1 r H_\epsilon(c) dx)^2} - \frac{2D_2 cat c^2}{r(\int_0^1 r H_\epsilon(c))^2} \right) \int_0^1 H_\epsilon(c) \bar{\eta} + r H'_\epsilon(c) \bar{\varphi} dx + \\ + \frac{2c_x \eta_x}{r} - \left(\frac{2r_x c_x}{r^2} + \frac{2r_t c}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r H_\epsilon(c) dx} \right) \eta - \frac{2\delta c^2}{r \int_0^1 r H_\epsilon(c) dx},\end{aligned}\tag{3.191}$$

and

$$\psi_t(t, x) = \int_0^1 H'_{R_0}(cat_0; y, t) \eta(y, t) G(x - y) dy, \tag{3.192}$$

with the initial conditions and boundary conditions

$$\eta(0, x) = 0, \quad (3.193)$$

$$\varphi(0, x) = 0, \quad (3.194)$$

$$\varphi(t, 0) = 0, \quad (3.195)$$

$$\varphi_x(t, 1) = 0, \quad (3.196)$$

$$\psi(0, x) = \delta. \quad (3.197)$$

Denote $\zeta(t, x) = \psi(t, x) - \delta(x)$, (3.190), (3.192) and (3.197) become

$$\eta_t(t, x) = -\frac{D_2 c \zeta}{\int_0^1 r H_\epsilon(c) dx} - \frac{D_2 c \delta}{\int_0^1 r H_\epsilon(c) dx} - \frac{D_2 cat \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 cat c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \varphi + H_\epsilon(c) \eta - \frac{\delta c}{\int_0^1 r H_\epsilon(c) dx}, \quad (3.198)$$

$$\zeta_t(t, x) = \int_0^1 H'_{R_0}(cat_0; y, t) \eta(y, t) G(x - y) dy, \quad (3.199)$$

$$\zeta(0, x) = 0. \quad (3.200)$$

Remark 3.29 For clarity, we use notation $H_{R_0}(cat_0; y, t)$ for the function $H_{R_0}(r(t, y))$ to note that $r(y, t) = r(cat_0; y, t)$.

In order to show that $r(cat_0)$, $c(cat_0)$ are Fréchet differentiable with respect to cat_0 , we will prove that there exist T small enough such that the following items hold:

1. There exist solution η, φ, ζ of system of the equations (3.191), (3.198) and (3.199) with homogeneous initial condition, boundary conditions (3.193)-(3.196), (3.200) and they are linear, bounded with respect to δ .

$$2. \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|r(cat_0 + \delta) - r(cat_0) - \eta\|_{X_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0 \text{ and } \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|c(cat_0 + \delta) - c(cat_0) - \varphi\|_{Y_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0.$$

For this, we present the following results.

Lemma 3.30 *There exist solution η, φ, ζ of system of the equations (3.191), (3.198) and (3.199) with homogeneous initial condition, boundary conditions (3.193)-(3.196), (3.200) and they are linear, bounded with respect to δ .*

Proof. Relying on the proof of Lemma 3.23, Using the similar technique in the sections 3.1 and 3.2, with N_t is some given positive constant we define the set

$$N_T = \left\{ (\eta, \varphi), \eta \in \mathbf{X}_T, \varphi \in \mathbf{Y}_T, \|\eta\|_{\mathbf{X}_T} + \|\varphi\|_{\mathbf{Y}_T} \leq N \right\}. \quad (3.201)$$

And we also define an operator $\mathcal{Z}$

$$\mathcal{Z} : N_t \longrightarrow \mathbf{X}_T \times \mathbf{Y}_T$$

by the following approach: For $(\bar{\eta}, \bar{\varphi}) \in N_t$ define $(\eta, \varphi) = \mathcal{Z}(\bar{\eta}, \bar{\varphi})$ as the solution of following system of the equation

$$\eta(t, x) = \int_0^t \left(-\frac{D_2 \text{cat} \varphi}{\int_0^1 r H_\epsilon(c) dx} + \frac{D_2 \text{cat} c}{(\int_0^1 r H_\epsilon(c))^2} \int_0^1 r H'_\epsilon(c) \bar{\varphi} + H_\epsilon(c) \bar{\eta} - \frac{\delta c}{\int_0^1 r H_\epsilon(c) dx} \right) d\tau, \quad (3.202)$$

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{r_x \varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r H_\epsilon(c) dx} + \frac{D_2 \text{cat}}{\int_0^1 r H_\epsilon(c) dx} \right) \varphi = \\ = - \left(\frac{D_1 c}{r (\int_0^1 r H_\epsilon(c) dx)^2} - \frac{2D_2 \text{cat} c^2}{r (\int_0^1 r H_\epsilon(c))^2} \right) \int_0^1 H_\epsilon(c) \bar{\eta} + r H'_\epsilon(c) \bar{\varphi} dx + \\ + \frac{2c_x \eta_x}{r} - \left(\frac{2r_x c_x}{r^2} + \frac{2r_t c}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r H_\epsilon(c) dx} \right) \eta - \frac{2\delta c^2}{r \int_0^1 r H_\epsilon(c) dx}, \end{aligned} \quad (3.203)$$

where

$$\zeta(t, x) = \int_0^t \int_0^1 H'_{R_0}(y, \tau, \text{cat}_0) \bar{\eta}(y, \tau) G(x - y) dy d\tau. \quad (3.204)$$

The initial condition and boundary conditions on the equations (3.202) and (3.203) remain homogeneous like in (3.193)-(3.196).

Following the idea from Lemma 3.23, we finish the proof of this Lemma. ■

With the same technique in Subsection 3.4.1, we have the following Lemma and Theorem.

Lemma 3.31 *Let η, φ be the solution of system of the equations (3.191), (3.198) and (3.199) with homogeneous initial condition, boundary conditions (3.193)-(3.196), (3.200), then*

- $\lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|r(\text{cat}_0 + \delta) - r(\text{cat}_0) - \eta\|_{\mathbf{X}_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0.$

$$\bullet \lim_{\|\delta\|_{W^{1,\infty}(\Omega)} \rightarrow 0} \frac{\|c(cat_0+\delta)-c(cat_0)-\varphi\|_{Y_T}}{\|\delta\|_{W^{1,\infty}(\Omega)}} = 0.$$

Theorem 3.32 *There exist T small enough such that $r(cat_0) \in \mathbf{X}_T$ and $c(cat_0) \in \mathbf{Y}_T$ are Frechet differentiable with respect to $cat_0 \in W^{1,\infty}(\Omega)$.*

3.8 Formulation and weak solution of the problem II_a

The problem II defined in definition 1.1 with $cat(x)$ catalyst positioning Model after reformulating the two coefficients $\gamma(r, c), \beta(r, c)$ leads to the below system

$$c_t - r^{\frac{2}{3}} c_{xx} + \frac{2r_x c_x}{r^{\frac{1}{3}}} - \frac{(\frac{4}{3}r_t + \frac{D_1}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(c) dx})c}{r} = 0, \quad (t, x) \in Q_T, \quad (3.205)$$

$$r_t = -\frac{D_2}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(c) dx} cat(x)c, \quad (t, x) \in Q_T, \quad (3.206)$$

with the initial and boundary conditions (3.4), (3.12), (3.6):

$$c(0, x) = h(x), \quad (3.207)$$

and mixed boundary conditions

$$c(t, 0) = 1, \quad t \in [0, T], \quad (3.208)$$

$$c_x(t, 1) = 0, \quad t \in [0, T]. \quad (3.209)$$

The conditions on $h(x), cat(x)$ are the same in (3.7)

$$\begin{aligned} h(0) &= 1, h(1) = 0, \\ h &\in W^{2,\infty}(\Omega), \\ cat &\in W^{1,\infty}(\Omega), \end{aligned} \quad (3.210)$$

and $H_\epsilon(x)$ is defined in (3.9). By setting

$$\mathbf{u}(t, x) = c(t, x) - 1, \quad (3.211)$$

we have $\mathbf{u}(t, 0) = \mathbf{u}_x(t, 1) = 0$. We also denote $\mathbf{u}_0(x) = h(x) - 1$. The equation (3.212) leads to

$$\mathbf{u}_t - r^{\frac{2}{3}} \mathbf{u}_{xx} - \frac{2r_x \mathbf{u}_x}{r^{\frac{1}{3}}} + \frac{(\frac{4}{3}r_t + \frac{D_1}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1) dx})\mathbf{u}}{r} = -\frac{(\frac{4}{3}r_t + \frac{D_1}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1) dx})}{r}, \quad (t, x) \in Q_T. \quad (3.212)$$

Putting $r_t = -\frac{D_2}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx} cat(x)(\mathbf{u}+1)$, $(t, x) \in Q_T$ into the right hand side of (3.212), then we have the system

$$\mathbf{u}_t - r^{\frac{2}{3}} \mathbf{u}_{xx} - \frac{2r_x \mathbf{u}_x}{r} + \left(\frac{\frac{4}{3}r_t}{r} + \frac{D_1 - \frac{4}{3}D_2 cat(x)}{r \int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx} \right) \mathbf{u} = \frac{\frac{4}{3}D_2 cat(x) - D_1}{r \int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx}, \quad (t, x) \in Q_T, \quad (3.213)$$

$$r_t = -\frac{D_2}{\int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx} cat(x)(\mathbf{u}+1), \quad (t, x) \in Q_T, \quad (3.214)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (3.215)$$

$$\mathbf{u}(0, x) = u_0(x), \quad x \in \Omega, \quad (3.216)$$

$$\mathbf{u}_x(t, 1) = 0, \quad t \in [0, T]. \quad (3.217)$$

We give the definition of a weak solution.

Definition 3.33 The pair $(r, \mathbf{u}) \in W^{1,\infty}(Q_T) \times W(0, T; H^1(\Omega))$ is said to be a weak solution of (3.213)–(3.217) if the following equalities are satisfied

$$\begin{aligned} (\mathbf{u}_t, v)_{((H^1(\Omega))^*, H^1(\Omega))} + \int_0^1 r^{\frac{2}{3}} \mathbf{u}_x x v dx - \int_0^1 \frac{2r_x \mathbf{u}_x}{r} v dx + \int_0^1 \left(\frac{\frac{4}{3}r_t}{r} + \frac{D_1 - \frac{4}{3}D_2 cat(x)}{r \int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx} \right) \mathbf{u} v dx = \\ = \int_0^1 \frac{\frac{4}{3}D_2 cat(x) - D_1}{r \int_0^1 r^{\frac{1}{3}} H_\epsilon(\mathbf{u}+1)dx} v dx, \\ \forall v \in V, \text{ and with a.e. } t \in [0, T], \end{aligned} \quad (3.218)$$

where

$$V = \{v \in H^1(\Omega), v(0) = 0\},$$

$$\mathbf{u}(0, x) = \mathbf{u}_0(x), \quad x \in [0, 1], \quad (3.219)$$

$$r(t, x) = 1 - \int_0^t \frac{D_2}{\int_0^1 r H_\epsilon(\mathbf{u}+1)dx} cat(x) (\mathbf{u}(\tau, x) + 1) d\tau, \quad t \in [0, T]. \quad (3.220)$$

Relying on the basic results on regularity of parabolic equation for initial mixed boundary condition from Chapter 2, the fixed point theory, following the Sections 3.1-3.7, we can conclude the well-posedness of the weak solution of Problem II_a and II_b , the Frechet differentiability r_{cat} or r_{cat_0} .

Chapter 4

Optimization Problems

In this Chapter we investigate mainly the two optimization problems, which subject to I_a and I_b . The optimization problems subject to II_a and II_b are considered in similar way.

From Chapter 3, we know that for Problems I_a and $II_a(cat(x)$ Model), there exist continuous operator:

$$\begin{aligned}\mathcal{F}_1 : W^{1,\infty}(\Omega) &\longrightarrow \mathbf{X}_T \times \mathbf{Y}_T \\ cat &\longmapsto (r(cat)(t, x), c(cat)(t, x)).\end{aligned}$$

For Problems I_b and $II_b(cat(t, x)$ Model), there exist continuous operator:

$$\begin{aligned}\mathcal{F}_2 : W^{1,\infty}(\Omega) &\longrightarrow \mathbf{X}_T \times \mathbf{Y}_T \\ cat_0 &\longmapsto (r(cat_0)(t, x), c(cat_0)(t, x)).\end{aligned}$$

We have the following remark.

Remark 4.1 *For convenience, we will use notations:*

- (i) $r(cat), c(cat)$ or $r(cat; t, x), c(cat; t, x)$ for $r(cat)(t, x), c(cat)(t, x)$ in $cat(x)$ Model.
- (ii) $r(cat_0), c(cat_0)$ or $r(cat_0; t, x), c(cat_0; t, x)$ for $r(cat_0)(t, x), c(cat_0)(t, x)$ in $cat(t, x)$ Model.

alternatively in relevant situations.

4.1 The first optimization problem

We consider the first optimization problem for the $cat(x)$ model, the $cat(t, x)$ case can be treated similarly.

$$\min_{cat \in A} V(cat) = \min_{cat \in A} \int_0^1 r^2(cat)(T, x) dx.$$

subjects to Problem I_a and II_a .

4.1.1 Frechet differentiability of the objective functional with respect to catalytic function

As $r \in \mathbf{X}_T \subset C(0, T; L^2(\Omega))$, we can define the linear bounded projection operator

$$\begin{aligned} \mathbf{P}_T : \mathbf{X}_T &\longrightarrow L^2(\Omega) \\ r(cat; t, \cdot) &\longmapsto r(cat; T, \cdot). \end{aligned} \quad (4.1)$$

The first optimization problem is to minimize the following objective functional

$$V(cat) = \int_0^1 r^2(cat)(T, x) dx = \int_0^1 (\mathbf{P}_T r(cat)(x))^2 dx. \quad (4.2)$$

We know from Chapter 3 that $r(cat)$ is Fréchet differentiable with respect to $cat \in W^{1,\infty}(\Omega)$, i.e. there exist a linear operator

$$\begin{aligned} r_{cat} : W^{1,\infty}(\Omega) &\longrightarrow L(W^{1,\infty}(\Omega), \mathbf{X}_T) \\ cat &\longmapsto r_{cat}(cat), \end{aligned} \quad (4.3)$$

such that

$$\|r(cat + \delta) - r(cat) - r_{cat}(cat)\delta\|_{\mathbf{X}_T} = o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (4.4)$$

Remark 4.2 We use the abbreviation r_{cat} for $r_{cat}(\cdot)$ like in Chapter 3.

Theorem 4.3 Functional V in (4.2) is Fréchet differentiable with respect to $cat \in W^{1,\infty}(\Omega)$.

Proof. Taking $\delta \in W^{1,\infty}(\Omega)$, denoting by $(\cdot, \cdot)$ the inner product in the Hilbert space $L^2(\Omega)$, we calculate

$$\begin{aligned} V(cat + \delta) - V(cat) &= \|\mathbf{P}_T r(cat + \delta)\|_{L^2(\Omega)}^2 - \|\mathbf{P}_T r(cat)\|_{L^2(\Omega)}^2 = \\ &= \|\mathbf{P}_T r(cat + \delta) - \mathbf{P}_T r(cat) + \mathbf{P}_T r(cat)\|_{L^2(\Omega)}^2 - \|\mathbf{P}_T r(cat)\|_{L^2(\Omega)}^2 = \\ &= 2(\mathbf{P}_T(r(cat + \delta) - r(cat)), \mathbf{P}_T r(cat)) + \|\mathbf{P}_T(r(cat + \delta) - r(cat))\|_{L^2(\Omega)}^2. \end{aligned} \quad (4.5)$$

We see that

$$\begin{aligned} &(\mathbf{P}_T(r(cat + \delta) - r(cat)), \mathbf{P}_T r(cat)) - (\mathbf{P}_T r_{cat}\delta, \mathbf{P}_T r(cat)) = (\mathbf{P}_T(r(cat + \delta) - r(cat)) - \mathbf{P}_T r_{cat}\delta, \mathbf{P}_T r(cat)) \leq \\ &\leq \|\mathbf{P}_T(r(cat + \delta) - r(cat)) - \mathbf{P}_T r_{cat}\delta\|_{L^2(\Omega)} \|\mathbf{P}_T r(cat)\|_{L^2(\Omega)} \leq \|r(cat + \delta) - r(cat) - r_{cat}\delta\|_{L^2(\Omega)} \|r_{cat}\delta\|_{L^2(\Omega)}. \end{aligned} \quad (4.6)$$

Combine (4.4) and (4.6), we have:

$$(\mathbf{P}_T(r(cat + \delta) - r(cat)), \mathbf{P}_T r(cat)) = (\mathbf{P}_T r_{cat} \delta, \mathbf{P}_T r(cat)) + o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (4.7)$$

We continue (4.5), using (4.7) and Theorem about continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to cat in $W^{1,\infty}(\Omega)$ as follows

$$V(cat + \delta) - V(cat) = 2(\mathbf{P}_T r_{cat} \delta, \mathbf{P}_T r(cat)) + o(\|\delta\|_{W^{1,\infty}(\Omega)}). \quad (4.8)$$

Hence, we can define the linear bounded operator

$$\begin{aligned} V_{cat} : W^{1,\infty}(\Omega) &\longrightarrow L(W^{1,\infty}(\Omega), \mathbb{R}) \\ cat &\longmapsto V_{cat}(cat) = 2(\mathbf{P}_T r_{cat} \cdot, \mathbf{P}_T r(cat)). \end{aligned} \quad (4.9)$$

■

Remark 4.4 For convenience, we use the abbreviation V_{cat} for $V_{cat}(\cdot)$ from now on.

4.1.2 The existence of the solution of the first optimization problem

Now we prove the the existence of a minimizer of the functional(4.2) over an admissible set. The idea to choose this admissible set we learn from the papers of Dinh-Nho Hào et al [11] and Rosch et al [31]. We introduce the admissible set A as follows

$$A = \left\{ cat \in C^{1,\lambda}(\Omega), 0 \leq cat \leq 1, M_1 \leq cat_x \leq M_2, \forall x \in [0, 1], \sup_{x_1, x_2 \in [0, 1]} \frac{|cat_x(x_1) - cat_x(x_2)|}{|x_1 - x_2|^\lambda} \leq C \right\}, \quad (4.10)$$

where M_1, M_2 are some given positive numbers and $0 < \lambda < 1$. The set A is compact in $C^1(\Omega)$ (see [31]). Since $V(cat)$ is continuous on $W^{1,\infty}(\Omega)$, therefore we have the following results.

Theorem 4.5 The problem of minimizing $V(cat)$ subjects to Problem I_a (or II_a) over A admits at least one solution.

For the first optimization problem subjects to Problem I_b and II_b , we define another admissible set as follows:

$$A_{cat_0} = \left\{ cat_0 \in C^{1,\lambda}(\Omega), 0 \leq cat_0 \leq 1, M_1 \leq cat_{0x} \leq M_2, \forall x \in [0, 1], \sup_{x_1, x_2 \in [0, 1]} \frac{|cat_{0x}(x_1) - cat_{0x}(x_2)|}{|x_1 - x_2|^\lambda} \leq C \right\}, \quad (4.11)$$

Theorem 4.6 *For the first optimization problem subjects to Problem I_b and II_b , we replace the admission set A_{cat} from (4.10) by the set A_{cat_0} defined in (4.11). Then this problem of minimizing $V(cat)$ over A_{cat_0} admits at least one solution.*

For the proofs of Theorem 4.5 and 4.6, see [11] and [31].

Suppose that in the $cat(x)$ model, there exist the linear bounded operators:

$$\begin{aligned} r_{cat} : L^2(\Omega) &\longrightarrow L^2(Q_T) \\ \delta &\longmapsto r_{cat}\delta, \end{aligned} \quad (4.12)$$

$$\begin{aligned} c_{cat} : L^2(\Omega) &\longrightarrow L^2(Q_T) \\ \delta &\longmapsto c_{cat}\delta \end{aligned} \quad (4.13)$$

and suppose that the projection operator $\mathbf{P}_T$ is bounded from $L^2(Q_T)$ onto $L^2(\Omega)$

$$\begin{aligned} \mathbf{P}_T : L^2(Q_T) &\longrightarrow L^2(\Omega) \\ r(cat; t, x) &\longmapsto r(cat; T, x). \end{aligned} \quad (4.14)$$

We get the following theorem:

Theorem 4.7 *Under assumptions (4.12) – (4.14), the Fréchet derivative V_{cat} in the $cat(x)$ model (Problem I_a , II_a) is defined by $2(r_{cat})^*(\mathbf{P}_T)^*\mathbf{P}_Tr(cat)$.*

Proof. The proof is a result of Theorem 4.3 and the assumptions (4.12) – (4.14). ■ The $cat(t, x)$ model is analogous.

4.2 The second optimization problem

We consider the second optimization problem

$$\min_{cat \in \mathbf{A}} \mathcal{V}(cat) = \min_{cat \in \mathbf{A}} \int_{T_1}^T \int_0^1 r^2(cat; t, x) dx dt, \quad (1.37)$$

subjects to Problem I_a , II_a , and

$$\min_{cat \in \mathbf{A}_{cat_0}} \mathcal{V}(cat_0) = \min_{cat_0 \in \mathbf{A}_{cat_0}} \int_{T_1}^T \int_0^1 r^2(cat_0; t, x) dx dt. \quad (1.38)$$

subjects to I_b , II_b . First, we consider the second optimization problem subjects to Problem I_a and II_a . The one subjects to Problem I_b , II_b will be similarly briefly presented later.

Due to the continuous embedding $L^2(Q_T) \in \mathbf{X}_T$, the projection operator:

$$\begin{aligned} \mathbf{P}_{T_1, T} : \mathbf{X}_T &\longrightarrow L^2([T_1, T] \times \Omega) \\ r(cat; t, x) &\longmapsto r(cat; t, x)|_{[T_1, T]} \end{aligned} \quad (4.15)$$

is linear bounded. Denoting by $\langle \cdot, \cdot \rangle$ the inner product in the Hilbert space $L^2(Q_T)$ and $\langle \cdot, \cdot \rangle_{L^2([T_1, T] \times \Omega)}$ the inner product in the Hilbert space $L^2([T_1, T] \times \Omega)$, we have the following Theorem:

Theorem 4.8 *Operator $\mathcal{V}$ in (1.37) is Frechet differentiable with respect to $cat \in W^{1,\infty}(\Omega)$.*

Proof. Taking $\delta \in W^{1,\infty}(\Omega)$, we have

$$\begin{aligned} \mathcal{V}(cat + \delta) - \mathcal{V}(cat) &= \|\mathbf{P}_{T_1,T}r(cat + \delta)\|_{L^2([T_1,T] \times \Omega)}^2 - \|\mathbf{P}_{T_1,T}r(cat)\|_{L^2([T_1,T] \times \Omega)}^2 = \\ &= \|\mathbf{P}_{T_1,T}r(cat + \delta) - \mathbf{P}_{T_1,T}r(cat) + \mathbf{P}_{T_1,T}r(cat)\|_{L^2([T_1,T] \times \Omega)}^2 - \|\mathbf{P}_{T_1,T}r(cat)\|_{L^2([T_1,T] \times \Omega)}^2 = \\ &= 2 \langle \mathbf{P}_{T_1,T}(r(cat + \delta) - r(cat)), \mathbf{P}_{T_1,T}r(cat) \rangle_{L^2([T_1,T] \times \Omega)} + \|\mathbf{P}_{T_1,T}(r(cat + \delta) - r(cat))\|_{L^2([T_1,T] \times \Omega)}^2. \end{aligned} \quad (4.16)$$

Similarly to the proof of Theorem 4.3, using equation (4.4) and Theorem about continuity of (r, c) in $W^{1,\infty}(Q_T) \times \mathbf{Y}_T$ with respect to cat in $W^{1,\infty}(\Omega)$, we continue (4.17) as follows.

$$\mathcal{V}(cat + \delta) - \mathcal{V}(cat) = 2 \langle \mathbf{P}_{T_1,T}r_{cat}\delta, \mathbf{P}_{T_1,T}r(cat) \rangle_{L^2([T_1,T] \times \Omega)} + o(\|\delta\|_{W^{1,\infty}(\Omega)}) \quad (4.17)$$

Hence, we can define the linear bounded operator:

$$\begin{aligned} \mathcal{V}_{cat} : W^{1,\infty}(\Omega) &\longrightarrow L(W^{1,\infty}(\Omega), \mathbb{R}) \\ cat &\longmapsto \mathcal{V}_{cat}(cat) = 2 \langle \mathbf{P}_{T_1,T}r_{cat} \cdot, \mathbf{P}_{T_1,T}r(cat) \rangle_{L^2([T_1,T] \times \Omega)}. \end{aligned} \quad (4.18)$$

■

Remark 4.9 *For convenience, we use the abbreviation $\mathcal{V}_{cat}$ for $\mathcal{V}_{cat}(\cdot)$.*

We use the admissible set A defined in (4.10), we have the following result:

Theorem 4.10 *The problem of minimizing $\mathcal{V}(cat)$ for $cat(x)$ model over A admits at least one solution.*

For the simplicity to execute the numerical implementation (see Chapter 5), we will consider the original model (without Huber function adjustment) in a Hilbert space approach. We learn from the paper of Gerken and Lechleiter [15] and the book [35] to simplify the adjoint operators of derivative r_{cat} and c_{cat} by artificially changing into a Hilbert space framework. Suppose that there exist the linear bounded operator

$$\begin{aligned} r_{cat} : L^2(\Omega) &\longrightarrow L^2(Q_T), \\ \delta &\longmapsto r_{cat}\delta \end{aligned} \quad (4.19)$$

$$\begin{aligned} c_{cat} : L^2(\Omega) &\longrightarrow L^2(Q_T), \\ \delta &\longmapsto c_{cat}\delta \end{aligned} \quad (4.20)$$

and linear bounded projection operator

$$\begin{aligned} \mathbf{P}_{T_1,T} : L^2(Q_T) &\longrightarrow L^2([T_1, T] \times \Omega) \\ r(cat; t, x) &\longmapsto r(cat; t, x)|_{[T_1, T]}. \end{aligned} \quad (4.21)$$

Then there exist the adjoint operator

$$\begin{aligned} r_{cat}^* : L^2(Q_T) &\longrightarrow L^2(\Omega) \\ z &\longmapsto r_{cat}^* z. \end{aligned} \quad (4.22)$$

We denote function z as follows:

$$z(cat; t, x) = \begin{cases} 0, & \text{if } t \in [0, T_1), \\ r(cat; t, x), & \text{if } t \in [T_1, T]. \end{cases} \quad (4.23)$$

Our objective functional is:

$$\begin{aligned} \mathcal{V}(cat) &= \int_0^1 \int_{T_1}^T (r(cat; t, x))^2 dx dt = \int_0^1 \int_{T_1}^T (\mathbf{P}_{T_1, T} r(cat; t, x))^2 dx dt = \\ &= \int_0^1 \int_0^T z^2(cat; t, x) dx dt. \end{aligned} \quad (4.24)$$

We have the following results.

Theorem 4.11 *The Frechet derivative $\mathcal{V}_{cat}$ is defined by $2(r_{cat})^*(\mathbf{P}_{T_1, T})^* \mathbf{P}_{T_1, T} r(cat)$.*

Remark 4.12 *The Frechet derivative $\mathcal{V}_{cat}$ can also be calculated by $2r_{cat}^* z(cat)$, where $z(cat)$ is defined in (4.23).*

Proof. As r_{cat} is linear, using $z(cat) = 0$ on $[0, T_1)$, from (4.24) we have

$$\begin{aligned} \mathcal{V}(cat + \delta) - \mathcal{V}(cat) &\stackrel{(4.17)}{=} 2 \int_0^1 \int_{T_1}^T r_{cat} \delta r(cat) dx dt + o(\|\delta\|_{W^{1, \infty}(\Omega)}) = \\ &= 2 \langle z_{cat} \delta, z(cat) \rangle + o(\|\delta\|_{W^{1, \infty}(\Omega)}) = 2 \langle r_{cat} \delta, z(cat) \rangle = 2(\delta, r_{cat}^* z(cat)) + o(\|\delta\|_{W^{1, \infty}(\Omega)}). \end{aligned} \quad (4.25)$$

■

Remark 4.13 *From Theorem 4.11 and Remark 4.12, we see that*

$$(\mathbf{P}_{T_1, T})^* \mathbf{P}_{T_1, T} r(cat) = z(cat; t, x) = \begin{cases} 0, & \text{if } t \in [0, T_1), \\ r(cat; t, x), & \text{if } t \in [T_1, T]. \end{cases}$$

4.2.1 Calculation of the adjoint operator r_{cat}^* for Problem I_a

For simplicity we will not work with the reformulated model with Huber function in Chapter 3 in solving optimization problems. We recall original Problem I_a :

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)rc, \quad (t, x) \in Q_T, \quad (4.26a)$$

4. Optimization Problems

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c) \text{cat}(x)c, \quad (t, x) \in Q_T, \quad (4.26b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (4.26c)$$

$$c(0, x) = h(x), \quad (4.26d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (4.26e)$$

$$c_x(t, 1) = 0, \quad (4.26f)$$

With assumption of smoothness on r, c and positivity of r , the above system leads us to

$$c_t = c_{xx} + \frac{2r_x c_x}{r} - \frac{(2r_t + \frac{D_1}{\int_0^1 r c dx})c}{r}, \quad (t, x) \in Q_T, \quad (4.27a)$$

$$r_t = -\frac{D_2}{\int_0^1 r c dx} \text{cat}(x)c, \quad (t, x) \in Q_T, \quad (4.27b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (4.27c)$$

$$c(0, x) = h(x), \quad (4.27d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (4.27e)$$

$$c_x(t, 1) = 0. \quad (4.27f)$$

where γ and β are defined in (1.18).

Now we introduce the following theorem about sensitivity system:

Theorem 4.14 (*Sensitivity system*). *Suppose that there exists a solution of the problem for the original model in space $\mathbf{X}_T \times \mathbf{Y}_T$, suppose also that η and φ are denoted in (3.104). Then for $\delta \in W^{1,\infty}(\Omega)$, we get the sensibility system*

$$\eta_t + \frac{D_2 \text{cat} \varphi}{\int_0^1 r c dx} - \frac{D_2 \text{cat} c}{(\int_0^1 r c dx)^2} \int_0^1 r \varphi + c \eta dx = -\frac{D_2 \delta c}{\int_0^1 r c dx} \quad (4.28)$$

with the initial condition

$$\eta(0, x) = 0 \quad (4.29)$$

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{2r_x \varphi_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r c dx} \right) \varphi &= \frac{2c_x \eta_x}{r} - \frac{2c \eta_t}{r} \\ + \left(\frac{2r_t c}{r^2} - \frac{2r_x c_x}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r c dx} \right) \eta &+ \frac{D_1 c}{r (\int_0^1 r H_\epsilon(c) dx)^2} \int_0^1 c \eta + r c \varphi dx, \end{aligned} \quad (4.30)$$

with initial and boundary conditions

4.2. The second optimization problem

$$\begin{aligned}\varphi(0, x) &= 0, \\ \varphi(t, 0) &= 0, \\ \varphi_x(t, 1) &= 0.\end{aligned}\tag{4.31}$$

Proof. We use the same technique like in Section 3.4.1. ■

We will apply an adjoint technique by introducing an adjoint system corresponding to the sensitivity system in order to calculate $r_{cat}^*z(cat)$. The idea of defining $r_{cat}^*z(cat)$ can be briefly presented in the following Remark.

Remark 4.15 From the Theorem 4.14, we have the sensitivity system:

$$\begin{aligned}D_1\varphi + L_1\eta &= l\delta, \\ D_2\varphi + L_2\eta &= 0,\end{aligned}\tag{4.32}$$

where $l = -\frac{D_2 c}{\int_0^1 r c dx}$ and $D_j, L_j, j = 1, 2$ are the linear differential and integral operators.

Testing system (4.32) by $v(t), w(t)$, with the conditions $v(T) = w(T) = 0$ leads us to:

$$\begin{aligned}\langle \tilde{D}_1 v, \varphi \rangle + \langle \tilde{L}_1 v, \eta \rangle &= \langle l\delta, v \rangle, \\ \langle \tilde{D}_2 w, \varphi \rangle + \langle \tilde{L}_2 w, \eta \rangle &= 0,\end{aligned}\tag{4.33}$$

Summing up the equation from the system (4.33), we deduce:

$$\langle \varphi, \tilde{D}_1 v + \tilde{D}_2 w \rangle + \langle \eta, \tilde{L}_1 v + \tilde{L}_2 w \rangle = \langle \delta, lv \rangle.\tag{4.34}$$

In order to determine $r_{cat}^*z(cat)$, we solve the system

$$\begin{aligned}\tilde{D}_1 v + \tilde{D}_2 w &= 0 \\ \tilde{L}_1 v + \tilde{L}_2 w &= z,\end{aligned}\tag{4.35}$$

then it leads to

$$\begin{aligned}\langle \eta, z \rangle &= \langle \delta, lv \rangle, \\ \Leftrightarrow (\delta, r_{cat}^* z) &= \langle \delta, lv \rangle,\end{aligned}\tag{4.36}$$

Hence we have

$$r_{cat}^*z(cat) = \int_0^T lv dt$$

.

The next Theorem will illustrate the idea mentioned in the above Remark.

Theorem 4.16 (*Adjoint system.*) Suppose that the following system

$$\begin{aligned} -w_t - w_{xx} + \frac{2r_x}{r} w_x + \left(\frac{2r_{xx}r - 2r_x^2 + 2r_t r}{r^2} + \frac{D_1}{r \int_0^1 r c dx} \right) w + \frac{D_2 cat}{\int_0^1 r c dx} v - r \int_0^1 \frac{D_2 catc}{(\int_0^1 r c dx)^2} v dx - \\ - r \int_0^1 \frac{D_1 cw}{r(\int_0^1 r c dx)^2} dx = 0, \end{aligned} \quad (4.37)$$

$$\begin{aligned} -\frac{2c}{r} w_t + \frac{2c_x}{r} w_x - \left(\frac{D_1 c}{r^2 \int_0^1 r c dx} - \frac{2c_{xx}}{r} + \frac{2c_t r}{r^2} \right) w - c \int_0^1 \frac{D_1 c w}{r(\int_0^1 r c dx)^2} dx - \\ - v_t - c \int_0^1 \frac{D_2 catc}{(\int_0^1 r c dx)^2} v dx = z, \end{aligned} \quad (4.38)$$

and the conditions

$$v(T, x) = 0, \quad (4.39)$$

$$\begin{aligned} w(T, x) &= 0, \\ w(t, 0) &= 0, \\ w_x(t, 1) &= 0 \end{aligned} \quad (4.40)$$

has unique solution $(v, w) \in W^{1,\infty}(Q_T) \times W(0, T)$ with some positive T , and z defined in (4.23). Suppose additionally a boundary condition on $cat(x)$

$$cat_x(1) = 0. \quad (4.41)$$

Then we have

$$V_{cat} = \int_0^T \frac{D_2 c}{\int_0^1 r c dx} v dt. \quad (4.42)$$

Proof.

Denoting the coefficients from (4.28) by

$$\begin{aligned} a_1(t, x) &= \frac{D_2 cat}{\int_0^1 r c dx}, \\ a_2(t, x) &= -\frac{D_2 catc}{(\int_0^1 r c dx)^2}, \\ a_3(t, x) &= -\frac{D_2 c}{\int_0^1 r c dx}, \end{aligned} \quad (4.43)$$

and the coefficients from (4.30) by

$$\begin{aligned}
 b_1(t, x) &= -\frac{2r_x}{r}, \\
 b_2(t, x) &= \frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r c dx}, \\
 b_3(t, x) &= \frac{2c_x}{r}, \\
 b_4(t, x) &= -\frac{2c}{r}, \\
 b_5(t, x) &= \frac{2r_t c}{r^2} - \frac{2r_x c_x}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r c dx}, \\
 b_6(t, x) &= \frac{D_1 c}{r(\int_0^1 r c dx)^2}.
 \end{aligned} \tag{4.44}$$

Then (4.28) and (4.30) become

$$\eta_t + a_1 \varphi + a_2 \int_0^1 r \varphi + a_2 \int_0^1 c \eta = a_3 \delta, \tag{4.45}$$

$$\varphi_t - \varphi_{xx} + b_1 \varphi_x + b_2 \varphi = b_3 \eta_x + b_4 \eta_t + b_5 \eta + b_6 \int_0^1 r \varphi dx + b_6 \int_0^1 c \eta dx. \tag{4.46}$$

Testing (4.45) by $v \in W^{1,\infty}(Q_T)$, with the condition (4.39), we deduce

$$\langle \varphi, a_1 v + r \int_0^1 a_2 v dx \rangle + \langle \eta, -v_t + c \int_0^1 a_2 v dx \rangle = \langle \delta, a_3 v \rangle, \tag{4.47}$$

or

$$\begin{aligned}
 \langle \varphi, \frac{D_2 c a t}{\int_0^1 r c dx} v - r \int_0^1 \frac{D_2 c a t c}{(\int_0^1 r c)^2} v dx \rangle + \langle \eta, -v_t - c \int_0^1 \frac{D_2 c a t c}{(\int_0^1 r c)^2} v dx \rangle = - \langle \delta, \frac{D_2 c}{\int_0^1 r c dx} v \rangle,
 \end{aligned} \tag{4.48}$$

Testing (4.46) by the function $w \in W(0, T)$, where w satisfies (4.40), we have

$$\begin{aligned}
 &\langle \varphi_t, w \rangle - \langle \varphi_{xx}, w \rangle + \langle b_1 \varphi_x, w \rangle + \langle b_2 \varphi, w \rangle = \\
 &= \langle b_3 \eta_x, w \rangle + \langle b_4 \eta_t, w \rangle + \langle b_5 \eta, w \rangle + \langle b_6 \int_0^1 r \varphi dx, w \rangle + \langle b_6 \int_0^1 c \eta dx, w \rangle.
 \end{aligned} \tag{4.49}$$

Due to assumption (4.73) and (4.27b), we see that

$$r_x(1) = 0, \quad (4.50)$$

which leads to $b_1(t, 1) = 0$ and $b_3(t, 1) = 0$. We therefore we obtain

$$\begin{aligned} & \langle \varphi, -w_t - w_{xx} + \frac{2r_x}{r} w_x + \left(\frac{2r_{xx}r - 2r_x^2 + 2r_t r}{r^2} + \frac{D_1}{r \int_0^1 r c dx} \right) w - r \int_0^1 \frac{D_1 c}{r(\int_0^1 r c dx)^2} w dx \rangle + \\ & + \langle \eta, -\frac{2c}{r} w_t + \frac{2c_x}{r} w_x - \left(\frac{D_1 c}{r^2 \int_0^1 r c dx} - \frac{2c_{xx}}{r} + \frac{2c_t r}{r^2} \right) w - c \int_0^1 \frac{D_1 c w}{r(\int_0^1 r c dx)^2} dx \rangle = 0. \end{aligned} \quad (4.51)$$

Summing up (4.48) and (4.51), we get

$$\begin{aligned} & \langle \varphi, -w_t - w_{xx} + \frac{2r_x}{r} w_x + \left(\frac{2r_{xx}r - 2r_x^2 + 2r_t r}{r^2} + \frac{D_1}{r \int_0^1 r c dx} \right) w - \\ & - r \int_0^1 \frac{D_1 c}{r(\int_0^1 r c dx)^2} w dx + \frac{D_2 c a t}{\int_0^1 r c dx} v - r \int_0^1 \frac{D_2 c a t c}{(\int_0^1 r c dx)^2} v dx \rangle + \\ & + \langle \eta, -\frac{2c}{r} w_t + \frac{2c_x}{r} w_x - \left(\frac{D_1 c}{r^2 \int_0^1 r c dx} - \frac{2c_{xx}}{r} + \frac{2c_t r}{r^2} \right) w - c \int_0^1 \frac{D_1 c w}{r(\int_0^1 r c dx)^2} dx - \\ & - v_t - c \int_0^1 \frac{D_2 c a t c}{(\int_0^1 r c dx)^2} v dx \rangle = - \langle \delta, \frac{D_2 c}{\int_0^1 r c dx} v \rangle. \end{aligned} \quad (4.52)$$

From the hypothesis of this Theorem that the system (4.67) – (4.40) is solvable. Then

$$\langle \eta, z \rangle = - \langle \delta, \frac{D_2 c}{\int_0^1 r c dx} v \rangle.$$

Hence

$$(\delta, r_{cat}^* z) = - \langle \delta, \frac{D_2 c}{\int_0^1 r c dx} v \rangle. \quad (4.53)$$

We can rewrite (4.53) as

$$\begin{aligned} & \int_0^1 \delta r_{cat}^* z dx = - \int_0^1 \int_0^T \delta \frac{D_2 c}{\int_0^1 r c dx} v dx dt \\ & \Leftrightarrow \int_0^1 \delta \left(r_{cat}^* z - \int_0^T \frac{D_2 c}{\int_0^1 r c dx} v dt \right) dx = 0. \end{aligned} \quad (4.54)$$

As (4.53) is satisfied $\forall \delta \in L^2(\Omega)$, we get

$$r_{cat}^* \mathcal{Z} = - \int_0^T \frac{D_2 c}{\int_0^1 r c dx} v dt. \quad (4.55)$$

Thus we arrive at (4.42). ■

4.2.2 Calculation of the adjoint operator r_{cat}^* for Problem I_b

The Problem I_b leads to system

$$c_t = c_{xx} + \frac{2r_x c_x}{r} - \frac{(2r_t + \frac{D_1}{\int_0^1 r c dx})c}{r}, \quad (t, x) \in Q_T, \quad (4.56a)$$

$$r_t = -\frac{D_2}{\int_0^1 r c dx} cat(t, x)c, \quad (t, x) \in Q_T, \quad (4.56b)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (4.56c)$$

$$c(0, x) = h(x), \quad (4.56d)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (4.56e)$$

$$c_x(t, 1) = 0, \quad (4.56f)$$

where $cat(t, x)$ is defined by (1.25)

$$cat_t(t, x) = \alpha_0 \int_0^1 H_{R_0}(r(cat; y, t))G(x - y) dy, \quad (1.25)$$

and the initial condition

$$cat(0, x) = cat_0(x), \quad (4.57)$$

with given α_0, R_0 . Functions H and G are defined in Appendix A.2 and A.8.

From Chapter 3, we know that $r \in \mathbf{X}_T, c \in \mathbf{Y}_T, cat \in W^{1,\infty}(\Omega)$ are Fréchet differentiable with respect to $cat_0 \in W^{1,\infty}(\Omega)$ for some T small enough, we denote

$$\bar{\eta} := r_{cat_0} \Delta, \quad \bar{\varphi} := c_{cat_0} \Delta, \quad \psi := cat_{cat_0} \Delta.$$

We have the following results.

Theorem 4.17 *Suppose that there exists a solution of the original model of Problem I_b in space $\mathbf{X}_T \times \mathbf{Y}_T$. Then we get the sensitivity system of three equations as follows:*

$$\bar{\eta}_t = -\frac{D_2}{\int_0^1 r c dx} \left(c\psi + cat\bar{\varphi} - \frac{catc}{\int_0^1 r c dx} \int_0^1 r \bar{\varphi} + c \bar{\eta} dx \right), \quad (4.58)$$

with the initial condition

$$\bar{\eta}(0, x) = 0, \quad (4.59)$$

$$\begin{aligned} \bar{\varphi}_t - \bar{\varphi}_{xx} - \frac{2r_x \bar{\varphi}_x}{r} + \left(\frac{2r_t}{r} + \frac{D_1}{r \int_0^1 r c dx} \right) \bar{\varphi} &= \frac{2c_x \bar{\eta}_x}{r} - \frac{2c \bar{\eta}_t}{r} \\ + \left(\frac{2r_t c}{r^2} - \frac{2r_x c_x}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r c dx} \right) \bar{\eta} &+ \frac{D_1 c}{r \left(\int_0^1 r H_\epsilon(c) dx \right)^2} \int_0^1 c \bar{\eta} + r c \bar{\varphi} dx, \end{aligned} \quad (4.60)$$

with initial and boudary conditions

$$\begin{aligned} \bar{\varphi}(0, x) &= 0, \\ \bar{\varphi}(t, 0) &= 0, \\ \bar{\varphi}_x(t, 1) &= 0, \end{aligned} \quad (4.61)$$

and

$$\psi_t = \alpha_0 \int_0^1 G(x-y) H'_{R_0}(r(cat_0; y, t)) \bar{\eta}(y, t) dy, \quad (4.62)$$

with initial condition

$$\psi(0, x) = \Delta(x). \quad (4.63)$$

Proof. The proof of this Theorem follows the same technique in the Section 3.4.1

■

We denote also function $\mathbf{z}$

$$\mathbf{z}(cat_0; t, x) = \begin{cases} 0, & \text{if } t \in [0, T_1) \\ \bar{\mathbf{P}}_{T_1, T} r(cat_0; t, x), & \text{if } t \in [T_1, T] \end{cases} = \begin{cases} 0, & \text{if } t \in [0, T_1) \\ r(cat_0; t, x), & \text{if } t \in [T_1, T] \end{cases} \quad (4.64)$$

Our objective functional is:

$$V(cat_0) := V(cat_0; t, x) = \int_0^1 \int_{T_1}^T (r(cat_0; t, x))^2 dx dt = \int_0^1 \int_0^T (\mathbf{z}(cat_0; t, x))^2 dx dt. \quad (4.65)$$

Theorem 4.18 *Operator $\mathcal{V}$ in (1.38) is Frechet differentiable with respect to cat_0 , and the Frechet derivative is defined by $2(r_{cat_0})^*(\mathbf{P}_{T_1, T})^* \mathbf{P}_{T_1, T} r(cat_0)$.*

Proof. The proof of this Theorem is similar to the one of Theorem 4.11. ■

Remark 4.19 The Frechet derivative $\mathcal{V}_{cat}$ can also be calculated by $2r_{cat_0}^* \mathbf{z}(cat)$, where $\mathbf{z}(cat_0)$ is defined in (4.64).

Proof. Using $\mathbf{z}(cat_0) = 0$ on $[0, T_1)$ and r_{cat_0} are linear

$$\begin{aligned} V(cat_0 + \Delta) - V(cat_0) &= 2 \int_0^1 \int_{T_1}^{T_2} r_{cat_0} \Delta r(cat_0) dx dt + o(\|\Delta\|_{W^{1,\infty}(\Omega)}) = \\ &= 2 \langle \mathbf{z}_{cat_0} \Delta, \mathbf{z}(cat_0) \rangle + o(\|\Delta\|_{W^{1,\infty}(\Omega)}) = 2 \langle r_{cat_0} \Delta, \mathbf{z}(cat_0) \rangle = 2 \langle \Delta, r_{cat_0}^* \mathbf{z}(cat_0) \rangle + o(\|\Delta\|_{W^{1,\infty}(\Omega)}). \end{aligned} \quad (4.66)$$

■

Remark 4.20 From Theorem 4.18 and Remark 4.19, we see that

$$(\mathbf{P}_{T_1, T})^* \mathbf{P}_{T_1, T} r(cat_0) = \mathbf{z}(cat_0; t, x) = \begin{cases} 0, & \text{if } t \in [0, T_1), \\ r(cat_0; t, x), & \text{if } t \in [T_1, T]. \end{cases}$$

In the following Theorem, we will introduce adjoint system to sensitivity in order to calculate $r_{cat_0}^* \mathbf{z}(cat_0)$. The brief idea for this Theorem is similar the one in the Remark 4.15.

Theorem 4.21 Suppose that the following system

$$\begin{aligned} -w_t - w_{xx} + \frac{2r_x}{r} w_x + \left(\frac{2r_{xx}r - 2r_x^2 + 2r_t r}{r^2} + \frac{D_1}{r \int_0^1 r c dx} \right) w + \frac{D_2 cat}{\int_0^1 r c dx} v - \\ - r \int_0^1 \frac{D_2 cat c}{(\int_0^1 r c dx)^2} v dx - r \int_0^1 \frac{D_1 c w}{r (\int_0^1 r c dx)^2} dx = 0, \end{aligned} \quad (4.67)$$

$$\begin{aligned} -\frac{2c}{r} w_t + \frac{2c_x}{r} w_x - \left(\frac{D_1 c}{r^2 \int_0^1 r c dx} - \frac{2c_{xx}}{r} + \frac{2c_t r}{r^2} \right) w - c \int_0^1 \frac{D_1 c w}{r (\int_0^1 r c dx)^2} dx - \\ - v_t - c \int_0^1 \frac{D_2 cat c}{(\int_0^1 r c dx)^2} v dx + \alpha_0 H'_{R_0}(cat_0, x, t) \int_0^1 \zeta(y, t) G(y - x) dy = \mathbf{z}, \end{aligned} \quad (4.68)$$

with the conditions

$$v(T, x) = 0, \quad (4.69)$$

$$\begin{aligned} w(T, x) &= 0 \\ w(t, 0) &= 0 \\ w_x(t, 1) &= 0, \end{aligned} \quad (4.70)$$

and equation

$$\zeta_t = -\frac{D_2 cv}{\int_0^1 rcdx} \quad (4.71)$$

with condition

$$\zeta(T, x) = 0. \quad (4.72)$$

has unique solution $(v, w, cat) \in W^{1,\infty}(Q_T) \times W(0, T) \times W^{1,\infty}(\Omega)$.
Suppose additionally a boundary condition on $cat(x)$

$$cat_{0x}(1) = 0. \quad (4.73)$$

Then

$$V_{cat_0} = -\zeta(0, x). \quad (4.74)$$

Chapter 5

Numerical Implementation

5.1 Forward Problems

In this section we will consider the numerical implementation for forward problems I and II and the two optimization problems for Problem I_a . The optimization problem for Problem I_b shows the similar results as the ones for I_a . First, we introduce the Finite Element Method (FEM) to solve the forward problems and give a short investigation on the greedy algorithm that is presented in [8], where the authors approach to Problems II and II_b by the Finite Difference Method. We will also make some comparisons between the Finite Difference Method and the Finite Element Method for problem II. Finally, the two optimization problems are considered by the sensitivity technique and fast derivative calculation by solving the adjoint systems.

In Problem I, we will find $c(t, x)$ and $r(t, x)$ such that

$$\frac{\partial}{\partial t}(r^2 c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^2 c, \quad (t, x) \in Q_T, \quad (5.1)$$

$$\frac{\partial r}{\partial t} = -\gamma(t, r, c)c, \quad (t, x) \in Q_T, \quad (5.2)$$

$$r(0, x) = r_0(x) = 1, \quad x \in \Omega, \quad (5.3)$$

$$c(0, x) = h(x), \quad (5.4)$$

$$c(t, 0) = 1, \quad t \in [0, T], \quad (5.5)$$

$$c_x(t, 1) = 0, \quad t \in [0, T], \quad (5.6)$$

In the problem *II*, the equation (5.1) is replaced by

$$\frac{\partial}{\partial t}(r^{\frac{4}{3}}c) = \frac{\partial}{\partial x}(r^2 \frac{\partial c}{\partial x}) - \beta(t, r, c)r^{\frac{1}{3}}c, \quad (t, x) \in Q_T, \quad (5.7)$$

Suppose that $r > r_0$, where r_0 is some positive number, we rewrite the equations (5.1), (5.4), (5.5) in the form of parabolic problem:

$$c_t - c_{xx} - \frac{2r_x c_x}{r} + \frac{(2r_t + \beta)c}{r} = 0, \quad (t, x) \in Q_T, \quad (5.8)$$

and the equations (5.7), (5.4), (5.5) in the form

$$c_t - r^{\frac{2}{3}}c_{xx} - \frac{2r_x c_x}{r^{\frac{1}{3}}} + \frac{(\frac{4}{3}r_t + \beta)c}{r} = 0, \quad (t, x) \in Q_T. \quad (5.9)$$

The authors of [8] solved numerically the above system by dealing with every time step Δt starting with the Cauchy equation (5.2) and then the equation (5.9). They applied FDM to Problem *II* and *II_b*. The main idea of the FDM is the approximation of partial derivatives with the difference quotients of values of functions pore radius r and oxygen concentration c . They did experiments with finite explicit method in time and both implicit and explicit methods in space. Finally, they concluded that the greedy algorithm works faster with the implicit one.

N, J are some natural numbers, the equidistant grids are

$$x_j = j \Delta x, \quad j = 0, \dots, J-1$$

$$t_n = n \Delta t, \quad n = 0, 1, \dots$$

where $\Delta x = \frac{1}{J-1}$ and $\Delta t = \frac{1}{N-1}$ are the spacial and time steps alternatively.

The partial differential equation (5.2) determining the decrease of radius r is discretized and the radius in the next time step is calculated via

$$r_j^{n+1} = r_j^n - \Delta t \gamma c_j^n, \quad \text{for } j = 0, \dots, J-1, \quad n = 0, 1, \dots \quad (5.10)$$

with the discrete initial conditions for $n = 0$

$$r_j^0 = 1 \text{ for } j = 0, \dots, J-1, \quad (5.11)$$

the Dirichlet boundary condition for $j = 0$

$$c_0^n = 1 \text{ for } n = 0, 1, \dots \quad (5.12)$$

and the Neumann condition

$$c_{J-2}^n = c_{J-1}^n \text{ for } n = 0, 1, \dots \quad (5.13)$$

In those notions the derivatives are written as

$$r_x \approx \frac{r_j^n - r_{j-1}^n}{\Delta x},$$

$$c_x \approx \frac{c_j^{n+1} - c_{j-1}^{n+1}}{\Delta x},$$

$$c_{xx} \approx \frac{c_{j-1}^{n+1} - 2c_j^{n+1} + c_{j+1}^{n+1}}{(\Delta x)^2},$$

5. Numerical Implementation

Then it leads to solving the following system of $(J - 1)$ algebraic equations

$$Ac^{n+1} = c^n - corr^n$$

where $corr^n = (a_{10}^n \Delta c_0^{n+1}, 0, \dots, 0)^T$ is a correction vector due to the mixed boundary condition. The $(J - 1) \times (J - 1)$ matrix A is given by:

$$A = \begin{bmatrix} a_{11}^n & a_{12}^n & 0 & \cdots & 0 \\ a_{21}^n & a_{22}^n & a_{23}^n & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & a_{J-2J-3}^n & a_{J-2J-2}^n & a_{J-2J-1}^n \\ 0 & \cdots & \cdots & a_{J-1J-2}^n & a_{J-1J-1}^n + a_{J-1J}^n \end{bmatrix}$$

with elements

$$\begin{aligned} a_{jj-1}^n &= \frac{\Delta t}{\Delta x^2} (r_j^n)^{\frac{2}{3}}, \\ a_{jj}^n &= \frac{\Delta t}{\Delta x^2} (r_j^n)^{-\frac{1}{3}} 2(r_{j-1}^n - 2r_j^n) + (r_j^n)^{-1} \left[\frac{1}{3} (7r_j^n - 4r_j^{n+1}) - \beta \Delta t \right], \\ a_{jj+1}^n &= \frac{\Delta t}{\Delta x^2} (r_j^n)^{-\frac{1}{3}} (3r_j^n - 2r_{j-1}^n). \end{aligned}$$

The calculation of β and γ leads to the knowledge of the reaction rate k_s . Dabrowski et al. approximated the integral in k_s via the trapezoidal rule as the following:

$$Q^n(r^n, c^n) = \Delta x \left[\frac{1}{2} ((r_0^n)^{\frac{1}{3}} c_0^n + (r_{J-1}^n)^{\frac{1}{3}} c_{J-1}^n) + \sum_{j=1}^{J-2} (r_j^n)^{\frac{1}{3}} c_j^n r_j^n \right], \quad (5.14)$$

then we got the discrete reaction rate

$$k_s^n = \frac{ir_p^0}{4F\epsilon_0 c_{A,0} l_c} \frac{1}{Q^n(r^n, c^n)}. \quad (5.15)$$

The stability condition for FDM is given by:

$$\frac{\Delta t}{\Delta x} \geq \text{const.} \left[\frac{1}{2} ((r_0^n)^{\frac{1}{3}} c_0^n + (r_{J-1}^n)^{\frac{1}{3}} c_{J-1}^n) + \sum_{j=1}^{J-2} (r_j^n)^{\frac{1}{3}} c_j^n r_j^n \right] \left[\frac{1}{3} (7r_j^n - 4r_j^{n+1}) - (r_j^n)^{-\frac{5}{3}} \right], \quad (5.16)$$

and

$$\frac{\Delta t}{\Delta x} \leq \text{const.} \left[\frac{1}{2} ((r_0^n)^{\frac{1}{3}} c_0^n + (r_{J-1}^n)^{\frac{1}{3}} c_{J-1}^n) + \sum_{j=1}^{J-2} (r_j^n)^{\frac{1}{3}} c_j^n r_j^n \right] \left[\frac{1}{3} (7r_j^n - 4r_j^{n+1}) \right]. \quad (5.17)$$

However, we see that, the condition (5.16) and (5.17) are not explicit, as the two sides of them depends on Δt and Δx .

Now we will develop the Finite Element method (FEM) for numerically solving the system of partial differential equations in the problems *I* and *II*. First denoting $u(t, x) = c(t, x) - 1$, we obtain for the problem *I*:

$$u_t - u_{xx} - \frac{2r_x u_x}{r} + \frac{(2r_t + \beta)u}{r} = -\frac{2r_t + \beta}{r}, \quad (t, x) \in Q_T, \quad (5.18)$$

$$u(0, x) = h(x) - 1, \quad (5.19)$$

$$u(t, 0) = 0, \quad t \in [0, T], \quad (5.20)$$

$$u_x(t, 1) = 0, \quad t \in [0, T], \quad (5.21)$$

and the equation (5.18) is replaced by

$$u_t - r^{\frac{2}{3}} u_{xx} - \frac{2r_x u_x}{r^{\frac{1}{3}}} + \frac{(\frac{4}{3}r_t + \beta)u}{r} = -\frac{\frac{4}{3}r_t + \beta}{r}, \quad (t, x) \in Q_T \quad (5.22)$$

for the problem *II*.

Note that $\beta = \frac{D_1}{\int_0^1 r c dc}$, $\gamma = \frac{D_2}{\int_0^1 r c dc}$ in Problem *I* and $\beta = \frac{D_1}{\int_0^1 r^{\frac{1}{3}} c dc}$, $\gamma = \frac{D_2}{\int_0^1 r^{\frac{1}{3}} c dc}$ in Problem *II*. Define the space

$$V = \{v \in H^1(\Omega), v(0) = 0, v_x(1) = 0\} \quad (5.23)$$

We will employ the backward Euler scheme for the time derivative term and the discretisation in the x variable that is based on the finite element method. The stability of backward Euler scheme method was proved in many text books on FEM or numerical methods on solving PDEs, e.g. [33]. For solving system of PDEs in one dimensional spacial frame, we refer [34].

We define the piecewise basic functions as follows.

5.1.1 Piecewise basic functions of the spaces V_h

Figure 5.1: The subdivision of $\Omega = [0, 1]$, $x_0 = 0$, $x_{J-1} = 1$

In order to solve our problem numerically we subdivide $\Omega = [0, 1]$ into $J-1$ subintervals $[x_i, x_{i+1}]$, $i = 0, \dots, J-2$ by the points $x_i = ih$, where $i = 0, \dots, J-1$ and $h = 1/(J-1)$. The subdivision is expressed

Figure 5.2: The piecewise linear finite element basis function $\Phi_i(x)$, $i \in [1, J-3]$

Figure 5.3: The piecewise linear finite element basis function $\Phi_{J-2}(x)$

in the Figure 5.1.

The weak solution $v \in V$ of the problem (5.19)-(5.53) will be approximated by a linear combination of the finite element basic piecewise linear functions with x -mesh point x_i on the subdivisions $\Phi_i(x)$, depicted in the figures 5.2 and 5.3.

$$\Phi_i(x) = (1 - \left| \frac{x - x_i}{h} \right|)_+, \quad i = 1, \dots, J-3, \quad (5.24)$$

and

$$\Phi_{J-2}(x) = \begin{cases} 1 - \frac{x - x_{J-2}}{h}, & \text{if } x \in [x_{J-3}, x_{J-2}] \\ 1, & \text{if } x \in [x_{J-2}, x_{J-1}] \end{cases} \quad (5.25)$$

It is clear that $\Phi_i(x) \in V$, $i = 1, \dots, J-2$; furthermore $\text{supp}\Phi_i = [x_i, x_{i+1}]$, $i = 1, \dots, J-2$. The space

$$V_h = \text{span}(\Phi_1, \dots, \Phi_{J-2}) \quad (5.26)$$

is an $(J-2)$ dimensional subspace of V .

We have the followings

$$(\Phi_i, \Phi_j) = \begin{cases} \frac{2h}{3}, & \text{if } i = j < J - 2, \\ \frac{4h}{3}, & \text{if } i = j = J - 2, \\ \frac{h}{6}, & \text{if } |i - j| = 1, \\ 0, & \text{if } |i - j| > 1, \end{cases} \quad (5.27)$$

$$((\Phi_i)_x, \Phi_j) = \begin{cases} 0, & \text{if } i = j < J - 2, \\ \frac{1}{2}, & \text{if } i = j = J - 2, \\ -\frac{1}{2}, & \text{if } |i - j| = 1, i < j, \\ \frac{1}{2}, & \text{if } |i - j| = 1, i > j, \\ 0, & \text{if } |i - j| > 1, \end{cases} \quad (5.28)$$

$$((\Phi_i)_x, (\Phi_j)_x) = \begin{cases} \frac{2}{h}, & \text{if } i = j < J - 2, \\ \frac{1}{h}, & \text{if } i = j = J - 2, \\ -\frac{1}{h}, & \text{if } |i - j| = 1, \\ 0, & \text{if } |i - j| > 1. \end{cases} \quad (5.29)$$

5.1.2 The θ scheme for numerical solving the problems *I* and *II*

The finite element approximation of the two problems *I* and *II* via θ scheme is as follows.

Find $u_h^m \in V_h$, $0 \leq m \leq N - 1$, such that

$$\begin{aligned} \left(\frac{u_h^{m+1} - u_h^m}{\delta t}, \vartheta_h \right) + a(u_h^{m+\theta}, \vartheta_h) &= (f(\cdot, t^{m+\theta}), \vartheta_h), \forall \vartheta_h \in V_h, \\ (u_h^0 - u_0, \vartheta_h) &= 0, \forall \vartheta_h \in V_h, \end{aligned} \quad (5.30)$$

where $0 \leq \theta \leq 1$, u_h^m represents the approximation of $u(\cdot, t^m)$, and for the sake of simplicity, we write:

$$u_h^{m+\theta}(x) = \theta u_h^{m+1}(x) + (1 - \theta) u_h^m(x), \quad (5.31)$$

The right hand side for problem *I* is

$$f(\cdot, t^{m+\theta}) = - \left(\theta \frac{2r_t + \beta}{r} \Big|_{t=t^{m+1}} + (1 - \theta) \frac{2r_t + \beta}{r} \Big|_{t=t^m} \right), \quad (5.32)$$

and for the problem *II* is

$$f(\cdot, t^{m+\theta}) = - \left(\theta \frac{\frac{4}{3}r_t + \beta}{r} \Big|_{t=t^{m+1}} + (1 - \theta) \frac{\frac{4}{3}r_t + \beta}{r} \Big|_{t=t^m} \right). \quad (5.33)$$

5. Numerical Implementation

We define the bilinear form:

$$a(u_h^{m+\theta}, \vartheta_h) = ((u_h^{m+\theta})_x, (\vartheta_h)_x) - \left(\frac{2r_x(u_h^{m+\theta})_x}{r}, \vartheta_h \right) + \left(\frac{2r_t + \beta}{r} u_h^{m+\theta}, \vartheta_h \right) \quad (5.34)$$

for problem *I*, and

$$a(u_h^{m+\theta}, \vartheta_h) = \left(r^{\frac{2}{3}} (u_h^{m+\theta})_x, (\vartheta_h)_x \right) - \frac{4}{3} \left(\frac{2r_x(u_h^{m+\theta})_x}{r^{\frac{1}{3}}}, \vartheta_h \right) + \left(\frac{\frac{4}{3}r_t + \beta}{r} u_h^{m+\theta}, \vartheta_h \right) \quad (5.35)$$

for the problem *II*.

Note that as the our forward problem is non-linear, we do not have enough information for $f(\cdot, t^{m+1})$, therefore we approximate $(f(\cdot, t^{m+1}))$ by

$$(f(\cdot, t^{m+1})) = \frac{2 \frac{r^{m+1}(\cdot) - r^m(\cdot)}{\Delta t} + \frac{D_2}{\int_0^1 r^{m+1} c^m dx}}{r^{m+1}(\cdot)} \quad (5.36)$$

and

$$f(\cdot, t^{m+1}) = \frac{\frac{4}{3} \frac{r^{m+1}(\cdot) - r^m(\cdot)}{\Delta t} + \frac{D_2}{\int_0^1 r^{m+1} c^m dx}}{r^{m+1}(\cdot)} \quad (5.37)$$

for problem *I* and *II* correspondingly. Equivalently, (5.30) can be written as

$$\begin{aligned} (v_h^{m+1}, \vartheta_h) + \Delta t a(v_h^{m+1}, \vartheta_h) &= \Delta t (f(\cdot, t^{m+1}), \vartheta_h), \forall \vartheta \in V_h, \\ \forall \vartheta_h \in V_h. \end{aligned} \quad (5.38)$$

Thus, given u_h^m , supposing that

$$u_h^m = \sum_{j=1}^{J-2} \mu_j^m \Phi_j,$$

we will find $u_h^{m+1} = \sum_{j=1}^{J-2} \mu_j \Phi_j$ at the time level t^{m+1} , we have to solve a system of $J - 2$ linear equations obtained after replacing ϑ_h in (5.38) by $\Phi_1, \Phi_2, \dots, \Phi_{J-2}$

$$B\mu = b, \quad (5.39)$$

where B is a $(J - 2) \times (J - 2)$ matrix:

$$B = \begin{bmatrix} bb_1 & cc_1 & 0 & \cdots & 0 \\ aa_1 & bb_2 & cc_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & bb_{J-3} & cc_{J-3} \\ 0 & \cdots & \cdots & aa_{J-2} & bb_{J-2} \end{bmatrix}$$

$$\mu = (\mu_1, \dots, \mu_{J-2}), \quad b = (b_1, \dots, b_{J-2})^T.$$

The elements of the matrix B and the right hand sides b are determined by

$$\begin{aligned}
 bb_i &= \frac{2h}{3} + \frac{2h}{3}\theta\Delta t \frac{2r_t + \beta}{r} + 2\theta \frac{\Delta t}{h}, \quad i = 1, \dots, J-3, \\
 bb_{J-2} &= \frac{4h}{3} + \frac{4h}{3}\theta\Delta t \frac{2r_t + \beta}{r} + \theta \frac{\Delta t}{h} - \theta \frac{\Delta tr_x}{r}, \\
 aa_i &= \frac{h}{6} + \frac{h}{6}\theta\Delta t \frac{2r_t + \beta}{r} - \theta \frac{\Delta t}{h} + \theta \frac{\Delta tr_x}{r}, \quad i = 1, \dots, J-3, \\
 cc_i &= \frac{h}{6} + \frac{h}{6}\theta\Delta t \frac{2r_t + \beta}{r} - \theta \frac{\Delta t}{h} - \theta \frac{\Delta tr_x}{r}, \quad i = 1, \dots, J-3,
 \end{aligned} \tag{5.40}$$

$$\begin{aligned}
 b_1 &= \left[\frac{2h}{3} + \frac{2h}{3}\Delta t(1-\theta) \frac{2r_t + \beta}{r} - 2(1-\theta) \frac{\Delta t}{h} \right] \mu_1^m + \\
 &\quad + \left[\frac{h}{6} - \frac{h}{6}(1-\theta)\Delta t \frac{2r_t + \beta}{r} + (1-\theta) \frac{\Delta t}{h} + (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_2^m - \Delta th(2r_t + \beta) \left(\frac{\theta}{r_1^{m+1}} + \frac{1-\theta}{r_1^m} \right),
 \end{aligned} \tag{5.41}$$

$$\begin{aligned}
 b_i &= \left[\frac{h}{6} - \frac{h}{6}(1-\theta)\Delta t \frac{2r_t + \beta}{r} + (1-\theta) \frac{\Delta t}{h} - (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_{i-1}^m + \\
 &\quad + \left[\frac{2h}{3} - \frac{2h}{3}(1-\theta) \frac{2r_t + \beta}{r} - 2(1-\theta) \frac{\Delta t}{h} + (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_i^m + \\
 &\quad + \left[\frac{h}{6} - \frac{h}{6}(1-\theta)\Delta t \frac{2r_t + \beta}{r} + (1-\theta) \frac{\Delta t}{h} + (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_{i+1}^m - h\Delta t(2r_t + \beta) \left(\frac{\theta}{r_i^{m+1}} + \frac{1-\theta}{r_i^m} \right), \quad i = 1, \dots, J-3,
 \end{aligned} \tag{5.42}$$

$$\begin{aligned}
 b_{J-2} &= \left[\frac{h}{6} - \frac{h}{6}(1-\theta)\Delta t \frac{2r_t + \beta}{r} + (1-\theta) \frac{\Delta t}{h} - (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_{J-3}^m + \\
 &\quad + \left[\frac{4h}{3} - \frac{4h}{3}(1-\theta)\Delta t \frac{2r_t + \beta}{r} - (1-\theta) \frac{\Delta t}{h} + (1-\theta) \frac{\Delta tr_x}{r} \right] \mu_{J-2}^m - \frac{3h}{2}\Delta t(2r_t + \beta) \left(\frac{\theta}{r_{J-2}^{m+1}} + \frac{1-\theta}{r_{J-2}^m} \right)
 \end{aligned} \tag{5.43}$$

for the problem I and

$$\begin{aligned}
 bb_i &= \frac{2h}{3} + \frac{2h}{3}\theta\Delta t \frac{\frac{4}{3}r_t + \beta}{r} + \theta r^{\frac{2}{3}} \frac{2\Delta t}{h}, \quad i = 1, \dots, J-3, \\
 bb_{J-2} &= \frac{4h}{3} + \frac{4h}{3}\theta\Delta t \frac{\frac{4}{3}r_t + \beta}{r} + \theta r^{\frac{2}{3}} \frac{\Delta t}{h} - \frac{2}{3}\theta \frac{\Delta tr_x}{r^{\frac{1}{3}}} \\
 aa_i &= \frac{h}{6} + \frac{h}{6}\theta\Delta t \frac{\frac{4}{3}r_t + \beta}{r} - \theta r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3}\theta \frac{\Delta tr_x}{r^{\frac{1}{3}}}, \quad i = 2, \dots, J-2, \\
 cc_i &= \frac{h}{6} + \frac{h}{6}\theta\Delta t \frac{\frac{4}{3}r_t + \beta}{r} - \theta r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3}\theta \frac{\Delta tr_x}{r^{\frac{1}{3}}}, \quad i = 1, \dots, J-3,
 \end{aligned} \tag{5.44}$$

$$b_1 = \left[\frac{2h}{3} + \frac{2h}{3} \Delta t (1 - \theta) \frac{\frac{4}{3}r_t + \beta}{r} - 2(1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} \right] \mu_1^m + \left[\frac{h}{6} - \frac{h}{6} (1 - \theta) \Delta t \frac{\frac{4}{3}r_t + \beta}{r} + (1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_2^m - \Delta t h \left(\frac{4}{3}r_t + \beta \right) \left(\frac{\theta}{r_1^{m+1}} + \frac{1 - \theta}{r_1^m} \right), \quad (5.45)$$

$$b_i = \left[\frac{h}{6} - \frac{h}{6} (1 - \theta) \Delta t \frac{\frac{4}{3}r_t + \beta}{r} + (1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} - \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_{i-1}^m + \left[\frac{2h}{3} - \frac{2h}{3} (1 - \theta) \frac{\frac{4}{3}r_t + \beta}{r} - 2(1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_i^m + \left[\frac{h}{6} - \frac{h}{6} (1 - \theta) \Delta t \frac{\frac{4}{3}r_t + \beta}{r} + (1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_{i+1}^m - h \Delta t \left(\frac{4}{3}r_t + \beta \right) \left(\frac{\theta}{r_i^{m+1}} + \frac{1 - \theta}{r_i^m} \right), \quad i = 1, \dots, J - 3, \quad (5.46)$$

$$b_{J-2} = \left[\frac{h}{6} - \frac{h}{6} (1 - \theta) \Delta t \frac{\frac{4}{3}r_t + \beta}{r} + (1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} - \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_{J-3}^m + \left[\frac{4h}{3} - \frac{4h}{3} (1 - \theta) \Delta t \frac{\frac{4}{3}r_t + \beta}{r} - (1 - \theta) r^{\frac{2}{3}} \frac{\Delta t}{h} + \frac{2}{3} (1 - \theta) \frac{\Delta t r_x}{r^{\frac{1}{3}}} \right] \mu_{J-2}^m - \frac{3h}{2} \Delta t \left(\frac{4}{3}r_t + \beta \right) \left(\frac{\theta}{r_{J-2}^{m+1}} + \frac{1 - \theta}{r_{J-2}^m} \right) \quad (5.47)$$

for the problem II.

The Pseudo codes of the FEM for the forward problem is presented as the Algorithm 5.1.

5.1.3 Comparison between the implicit FDM and the FEM.

In [9], the authors compare the difference between the implicit FDM and the explicit FDM. They carried out the experiment using electrolyte $DMSO^{Li^+}$, considering the pore clogging occurs when the pore radius goes below than 0.1. The two above methods show very slightly difference: radius, concentration and the deviation between them is below 0.001%, where the deviation is defined by:

$$\sigma_{V_{free}} = \frac{|V_{free}^{exp} - V_{free}^{imp}|}{V_{free}^{exp}}.$$

However, the run time for the explicit FDM is much longer that the one for the implicit FDM. We adapt the table from [9]:

Following [9], we define the stability of a numerical method for this problem by the considering the concentration $c(t, x)$ at every time step $t^n = n\Delta t$. The stability is held if $c \in [0, 1]$ when $r(t, x) > 0.1$.

Algorithm 5.1 FEM for forward problem

Input: $\Delta x, \Delta t, \beta_0, \gamma_0, J, k, EPS$

Output: r_j^N, c_j^N for $j = 0, \dots, J - 1$, time steps M

```

1: for  $j = 0, \dots, J - 1$  do
2:    $r_j^0 = 1$ ;
3:    $c_j^0 = 0$ ;
4:    $u_j^0 = -1$ ;
5: end for
6:  $c_0^0 = 1$ ;
7:  $u_0^0 = 0$ ;
8:  $n = 0$ ;
9: repeat
10:   $k_{tmp} = k \cdot \left[ \Delta x \left( \frac{1}{2} \left( (r_0^n)^{\frac{1}{3}} c_0^n + (r_{J-1}^n)^{\frac{1}{3}} c_{J-1}^n \right) + \sum_{j=1}^{J-2} (r_j^n)^{\frac{1}{3}} c_j^n \right) \right]^{-1}$ 
11:   $\gamma = k \cdot \gamma_0$ ;
12:   $\beta = k \cdot \beta_0$ ;
13:  for  $j = 0, \dots, J - 1$  do
14:     $r_j^{n+1} = r_j^n - \Delta t \gamma c_j^n$ ;
15:  end for
16:   $U_1 = b b_1^n$ ;
17:  for  $j = 2, \dots, J - 2$  do
18:     $L_j = a a_j^n / U_{j-1}$ ;
19:     $U_j = b b_j^n - L_j c_{j-1}^n$ ;
20:  end for
21:   $y_1 = b_1^n$ ;
22:  for  $j = 2, \dots, J - 2$  do
23:     $y_j = b_j^n - L_j y_{j-1}$ ;
24:  end for
25:   $u_{J-2}^{n+1} = y_{J-2} / U_{J-2}$ ;
26:  for  $j = J - 3, \dots, 1$  do
27:     $u_j^{n+1} = (y_j - c c_j^n \cdot u_{j+1}^{n+1}) / U_j$ ;
28:  end for
29:   $u_{J-1}^{n+1} = u_{J-2}^{n+1}$ ;
30:  for  $j = 0, \dots, J - 1$  do
31:     $c_j^{n+1} = u_j^{n+1} + 1$ ;
32:  end for
33: until  $r_j^{n+1} \leq EPS$  for a  $j$ ;
34:  $M = n$ ;

```

5. Numerical Implementation

Figure 5.4: The pore radii and the concentration of oxygen inside pore before pore clogging with $J = N = 100$ solving with FDM and FEM

J	$(\Delta t)^{-1}$		$V_{free} / \%$		$\sigma_{V_{free}} / \%$	t_{run} / s	
	implicit	explicit	implicit	explicit		implicit	explicit
100	100	24000	61.6157	61.6152	0.0008	20.10	4762
200	200	92000	61.7067	61.7063	0.0006	82.01	37165
300	300	201000	61.7335	61.7332	0.0005	182.91	115751
400	400	352000	67.7460	61.7457	0.0004	326.21	268083

Figure 5.5: Free pore volume, relative deviation and runtime for the implicit and explicit FDM

The Table in the Figure 5.5 shows the free volume after pore clogging, the runtime in different time steps as well as the stability in two these methods in spacial discretion of $J = 100$ and for the problem (II). The FEM we use here is in case of $\theta = 1$ and $f(\cdot, t^m)$ in the right hand side in stead of $f(\cdot, t^{m+1})$ in (5.37). The deviation in this Table is defined by:

$$\sigma_{V_{free}}^* = \frac{|V_{free}^{imp} - V_{free}^{FEM}|}{V_{free}^{imp}}.$$

5.2. Some remarks on the Greedy algorithm in Problem II_b and I_b using FDM.

Δt	$N = (\Delta t)^{-1} + 1$	$V_{free}/\%$		$\sigma_{V_{free}}^*/\%$	t_{run}/s	
		FEM	FDM implicit		FEM	FDM implicit
0.010101	100	58.9922	61.6157	4.2578	17.0621	10.498
0.020408	50	58.9929	61.6163	4.2576	8.46296	5.49169
0.025641	40	58.9932	61.6166	4.2576	6.4961	4.25776
0.034482	30	58.9938	61.6591	4.3226	5.1977	3.1829
0.052631	20	58.995	not stable		3.55292	not stable
0.111111	10	58.9986	not stable		1.57534	not stable
0.142857	8	59.0013	not stable		1.34791	not stable
0.2	6	59.0052	not stable		1.01438	not stable
0.333333	4	59.0654	not stable		0.717149	not stable
1	2	58.9986	not stable		0.222847	not stable
2	1.5	59.1416	not stable		0.118924	not stable
5	1.2	59.4254	not stable		0.0469593	not stable

Table 5.1: Free volume and runtime for the implicit FDM and FEM with spacial discretion of $J = 100$

Concern the continuous catalyst positioning model $\text{cat}(x)$ (Problems I_a , II_a) and the continuous catalyst positioning model $\text{cat}(t,x)$ (Problems I_b and II_b) in this Thesis, we care about the runtime in order to implement the different optimization methods such as sensitivity system and adjoint methods. For this, FEM is a potential method. In this table, the deviation shows that there is a certain difference between the two solution of the two methods (deviation is below than 4.4%) with $N = 100, 50, 40, 30$, with $\Delta t = 0.010101, 0.020408, 0.015641, 0.034482$, relatively. The runtime of FDM method is below than the runtime of FEM in these four Δt , as the computation of the coefficients of the matrix B consumes more time for the ones of the matrix A . However, for the other greater Δt in the Table 5.5, the implicit FDM is not stable, while the FEM still shows an acceptable solution.

5.2 Some remarks on the Greedy algorithm in Problem II_b and I_b using FDM.

According to [8] the greedy algorithm in the catalyst positioning problem for Lithium/air battery is the step-by-step selection of the optimal position of catalyst subsequently based on minimizing an objective function, in this case it is the free volume of the pore inside the cathode before pore clogging:

$$V_{\text{free}}^n = \Delta x \left[\frac{1}{2} \left((r_0^n)^2 + (r_{J-1}^n)^2 \right) + \sum_{j=1}^{J-2} (r_j^n)^2 \right].$$

This V_{free}^n is calculated by the trapezoidal rule.

The Greedy algorithm normally does not give a global minimum, as it does not solve the optimal problem globally on the whole original domain [2]. In [8], the authors choose the minimal node in

Figure 5.6: The pore radii and the concentration of oxygen inside pore before pore clogging with $J = 100$ and different N in Problem I

the first step by checking the whole J possible position of the catalyst. Remembering this node, they continue to improve the algorithm in the next step by checking the whole combinations of the previous minimal node with one of the $(J - 1)$ other nodes to select the next optimal position of catalyst. They stop this process when $V_{\text{free}}^n > V_{\text{free}}^{n-1}$ in the n -th iteration. However, we would like to recommend to continue this checking process after this n -th state to globalize the algorithm. We let n run from 1 to J and then selecting the "global" greedy algorithm solution, which is corresponding to the minimum value $\min_n V_{\text{free}}^n$, $n = 1, \dots, J$.

We check with electrolyte DMSO, discretion of space is $J = 100$, threshold of 4% then we get the first local minimum at the 33-th step with $V_{\text{free}}^{37} = 24, 61\%$, and the second local minimum at the 47-th iteration with $V_{\text{free}}^{37} = 23, 46\%$. In the Figure 5.11a, the graph of optimal the numbers of catalyst with the minimal V_{free} volume. We can see from this graph that number of 47 is the better optimal number in this experiment.

Figure 5.11a shows the comparison between the two state of the pore before pore clogging. Radius of the pore at the 33-th iteration (red line) is lower than the radius of the pore at 47-th iteration (blue line) at the center of the pore and they are slightly different at the end of the pore, where the diffusion limited side sited.

Figure 5.10 expresses the distribution of the optimal catalyst number of 47, that is the global greedy algorithm solution in this case.

We also present an experiment for Problem I_b . Figure 5.11 shows the evolutions of pore radii and concentration of oxygen along the pore over time with the optimal catalyst number of 41, which is illustrated in the Figure 5.12. In this experiment, we take $J = N = 100$, threshold of 4%.

Figure 5.7: The optimal numbers of catalysts from 1 to 100 by Greedy algorithm in Problem II_b

5.3 The continuous positioning

As we mentioned in Chapter Introduction of this Thesis, the authors in [9] implements a simple propagation process of the catalytic function to the neighbourhood using a binary function. This function either allows depositing catalyst development to the sites or prevents it. This discrete model gives us the first understandings about the binary distributed catalyst positioning and very good comparison of the effect of different electrolytes concerning to optimizing the capacity of the batteries. However, the natural question is Can we model a more visual catalytic function with a clearer geometrical features in order to acknowledge the distribution of catalyst inside the pore? We wish to aim at the more complex structured catalytic functions:

- Cat(x) Model with fractional function that characterizing the presence of catalyst at the sites, as well as the amount of catalyst at certain positions.
- Cat(t,x) Model, which also is also a fractional catalytic function based on time dependent growth kinetics.

The analytic research on the two above models have been presented in Chapters 3 and 4. In the next Subsections, we would like to show some numerical simulations and comparisons of these two Models.

We first transform the distribution of catalyst sites in the discrete catalyst model using in Greedy method to the continuous one using for the two continuous catalyst models cat(x) and cat(t,x). For this, we will use the convolution to smoothen the catalytic function in the following subsection.

5. Numerical Implementation

(a) The radii of pore at the optimal number of catalyst before pore closing

(b) The concentration of oxygen inside the pore with the two optimal numbers of catalyst before pore clogged

Figure 5.8: Comparison of radii and concentration inside the pore with two optimal numbers of catalyst before pore clogged by Greedy algorithm in Problem II_b

5.3. The continuous positioning

(a) The Li_2O growth profile or the radii of pore over time.

(b) The concentration of oxygen inside the pore over time.

Figure 5.9: radii and concentration inside the pore with 47 optimal number catalyst by Greedy algorithm in Problem II_b .

Figure 5.10: The distribution of optimal number of catalysts of 47 catalyst positions

5.3.1 Transformation of discrete catalytic functions to smooth catalytic functions

Suppose that $cat_{dis}(x) \in L^\infty(\Omega)$ is a discrete catalytic function such that its values $cat_{dis}(x_j)$ at $x_j = j\Delta x$, where $j = 0, \dots, J-1$, $x_0 = 0$, $x_{J-1} = 1$ could be 0 or 1. We defined the extended discrete catalytic function $\mathbb{E}_{cat}(x)$ of $cat_{dis}(x)$ by:

$$\mathbb{E}_{cat}(x_j) = \begin{cases} cat_{dis}(x_j), & \text{if } j = 1, \dots, J-2, \\ cat_{dis}(x_{J-1}), & \text{if } j = J-1, \dots, J-1+m, \end{cases} \quad (5.48)$$

where $m \in \mathbb{N}$.

The smooth transformation $cat_{smooth}(x)$ of $cat_{dis}(x)$ is now defined formally on $[0, 1]$ as follows

$$cat_{smooth}(x) = \left(\alpha_{trans} \int_0^{1+\sigma_{trans}} \mathbb{E}_{cat}(y) G(x-y) dy \right) \Big|_{[0,1]}, \quad (5.49)$$

where $G(x-y)$ is normal Gaussian distribution at center y , α_{trans} is some positive constant and $\sigma_{trans} \geq 0$, $\sigma_{trans} = m\Delta x$.

Remark 5.1 We choose α_{trans} such that the values of $cat_{smooth}(x)$ at $x_j = j\delta x$, where $j = 0, \dots, J-1$ are the real values from 0 to 1.

Example of transformation: are described in Figure 5.13 and Figure 5.14 for two cases: $n = 0$ and $m = 7$.

5.3. The continuous positioning

(a) The Li_2O growth profile or the radii of pore over time.

(b) The concentration of oxygen inside the pore over time.

Figure 5.11: radii and concentration inside the pore i line plotting with 41 optimal number catalyst by Greedy algorithm in Problem I_b .

Figure 5.12: The distribution of optimal number of catalysts of 41 catalyst positions in Problem I_b

5.3.2 $cat(x)$ model (Problems I_a and II_a)

The catalytic function is defined as a function in $W^{1,\infty}(\Omega)$ is discretized via a function $cat_j, j \in [0, \dots, J-1]$, where $cat_j = cat(x_j) \in [0, \dots, 1]$. The increasing pore radius r then is written by:

$$r_j^{n+1} = r_j^n - \Delta t \gamma c_j^n cat_j, \text{ where } j = 0, \dots, J-1, n = 0, 1, \dots \quad (5.50)$$

The continuous catalyst positioning model $cat(x)$ with the catalytic function taken fractional values from 0 to 1 allows us to simulate a smooth growth of Li_2O_2 along the active site in the cathode surface, once we choose smooth values for catalytic function. In this model, the catalyst function always keeps all its value with time, therefore, with the site where the the catalyst function with the value of 0, the radius will not be changed, even in the oxygen entering side.

5.3.3 $cat(t,x)$ model (Problems I_b and II_b)

The $cat(t,x)$ Model is inspired by the model of growth of Li_2O_2 from the Thesis of Tatjana Dabrowski [9] using the Greedy Algorithm. Once the threshold is reached, the growth profile is enhanced to start also around the neighbourhood sites. There are circumstances occurred in the nature like bacteria growth or kinetics growth. Different thresholds R_0 or different α_0 in (1.25) characterize different kind of growths.

5.3. The continuous positioning

(a) The local optimal catalytic function (number of catalyst = 33) by Greedy algorithm before pore reaches to 0.1, $J=100$

(b) The local optimal catalytic function by Greedy algorithm before pore reaches to 0.86, $J=100$

Figure 5.13: The transformation from the local optimal discrete catalytic functions by Greedy algorithm in Problem II_b before pore reaches to 0.1 and 0.86 to continuous ones, with $\sigma_{trans} = 0$ in (5.49)

(a) The local optimal catalytic function (number of catalyst = 33) by Greedy algorithm before pore reaches to 0.1, $J=100$

(b) The local optimal catalytic function by Greedy algorithm before pore reaches to 0.86, $J=100$

Figure 5.14: The transformation from local optimal discrete catalytic functions by Greedy algorithm in Problem II_b before pore reaches to 0.1 and 0.86 to continuous ones, with $\sigma_{trans} = 7\Delta x$ in (5.49)

5.3.4 Comparing the two catalyst positioning models: $cat(x)$ and $cat(t, x)$

We show the numerical tests on the center-catalyst positioning for the two models: $cat(x)$ and $cat(t, x)$. The growth of discharged product Li_2O_2 is presented as following As we have seen in the Figure 5.15,

Figure 5.15: Comparing the two catalyst positioning models, experimenting with the center-catalyst positioning. The crosses show the catalytic function at the initial time. Blue lines present the growth profiles of discharged product Li_2O_2 deposited along the pore surface after pore clogging in Problem I_a . The red lines are the growth of Li_2O_2 according to Problem I_b .

in the the $cat(t, x)$ model, the the growth of Li_2O_2 is increasing more to the side where oxygen entering from the left, as the oxygen concentration and deposition rate due to the electrochemical reaction are higher on the left than on the right sight.

5.4 The optimization problems

We will solve numerically the two optimization problems use alternatively. We rely on the line search method, e.g. in [26]. Suppose that cat^k is given, cat^{k+1} is updated by

$$cat^{(k+1)} = cat^{(k)} - \alpha^{(k+1)} V_{cat} \quad (5.51)$$

for the $cat(x)$ model. The optimization problems for $cat(x,t)$ model is solved by the iterative method

$$cat^{(k+1)} = cat^{(k)} - \theta^{(k+1)} V_{cat_0}, \quad (5.52)$$

where cat^k is given. The iteration stops when the free volume at the certain time step $V(cat^{k+1})$ is greater than the previous one $V(cat^k)$. Even though the $cat(x, t)$ model has the advantage in describing the evolution of the Cathode surface with the sparse catalytic distribution, for the sake of simplicity, we present the numerical results here only for $cat(x)$ model. By choosing the smooth and "less" sparse distributed catalytic initial function $cat(x)$, the difference of the performance between the two models will be accepted.

5.4.1 The first optimization problem for Problem I_a

Figure 5.16: Initial $cat(x)$ and optimal $cat(x)$ for Problem I_a in grid of $J = N = 20$

At the first optimization problem, we consider the minimization problem of remaining pore volume with $T, 0 < T < \infty$ is the some final time:

$$\min_{cat \in A} V(cat) = \min_{cat \in A} \int_0^1 r^2(x, cat(x), T) dx, \quad (5.53)$$

where A is the admission set of catalytic function $cat(x)$. According to Theorem 4.3

$$(\mathbf{P}_{Tr_{cat}})^* \mathbf{P}_{Tr}(cat)$$

Suppose that $\mathbf{P}_T^{(k)} r_{cat}^{(k)}$ is approximated for $\mathbf{P}_T r_{cat}$ at the iteration k of the optimization algorithm, then $\mathbf{P}_T^{(k)} r_{cat}^{(k)}$ is a $J \times J$ matrix, therefore the adjoint operator is obviously defined by its transpose matrix $(\mathbf{P}_T^{(k)} r_{cat}^{(k)})^* = (\mathbf{P}_T^{(k)} r_{cat}^{(k)})^T$. However, this method of defining V_{cat} is very much time-consuming as we have to calculate J directive derivatives in order to get the Fréchet derivative. This progress is relied on the sensitivity system from Theorem 4.14. We rewrite the sensitivity system from previous Chapter

$$\eta_t + \frac{D_2 cat \varphi}{\int_0^1 r c dx} - \frac{D_2 cat c}{(\int_0^1 r c dx)^2} \int_0^1 r \varphi + c \eta dx = \frac{D_2 \delta c}{\int_0^1 r c dx}, \quad (4.28)$$

with the initial condition

$$\eta(0, x) = 0, \quad (4.29)$$

$$\begin{aligned} \varphi_t - \varphi_{xx} - \frac{2 r_x \varphi_x}{r} + \left(\frac{2 r_t}{r} + \frac{D_1}{r \int_0^1 r c dx} \right) \varphi &= \frac{2 c_x \eta_x}{r} - \frac{2 c \eta_t}{r} \\ + \left(\frac{2 r_t c}{r^2} - \frac{2 r_x c_x}{r^2} + \frac{D_1 c}{r^2 \int_0^1 r c dx} \right) \eta &+ \frac{D_1 c}{r (\int_0^1 r H_\epsilon(c) dx)^2} \int_0^1 c \eta + r c \varphi dx, \end{aligned} \quad (4.30)$$

with initial and boundary conditions

$$\begin{aligned} \varphi(0, x) &= 0, \\ \varphi(t, 0) &= 0, \\ \varphi_x(t, 1) &= 0. \end{aligned} \quad (4.61)$$

In order to solve the sensitivity system, we apply FEM, which has been presented for forward problems in Section 5.1, taking $\theta = 1$. We want to find $\varphi_h^{m+1} = \sum_{j=1}^{J-2} \nu_j \Phi_j$ at time step t^{m+1} .

$$S \nu = b^s, \quad (5.54)$$

where S is a $(J-2) \times (J-2)$ matrix

$$S = \begin{bmatrix} bb_1^s & cc_1^s & 0 & \cdots & 0 \\ aa_1^s & bb_2^s & cc_2^s & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & bb_{J-3}^s & cc_{J-3}^s \\ 0 & \cdots & \cdots & aa_{J-2}^s & bb_{J-2}^s \end{bmatrix}$$

$$\nu = (\nu_1, \dots, \nu_{J-2}), \quad b^s = (b_1^s, \dots, b_{J-2}^s)^T.$$

ν and b^s are determined according to the backward Euler and FEM method. Using line search optimization method, we get several results described in the figure 5.16. The grid that we work with for this case is very sparse, only $J = N = 20$, and we get some overview on the optimal catalytic function. Here, the blue lines are initial catalytic functions, the red one are the local optimal catalytic functions. The discretization we use 20 points for the spacial direction ($J=20$) and $\Delta_t = \frac{1}{20-1}$. In this Figure, we can see that there are many local minima of the objective functional.

5.4.2 The second optimization problem

For the convenience to apply the adjoint method we also present the second optimization problem that minimizes the mean value of $V_{free}(r, cat, t)$ in a small interval of time $[T_1, T]$:

$$\min_{cat \in \mathbf{A}_{cat}} \mathcal{V}(cat) = \min_{cat \in \mathbf{A}} \int_{T_1}^T \int_0^1 r^2(x, cat(x), t) dx dt, \quad (5.55)$$

The advantage of sensitivity method is that the executing time takes very long. Therefore we cannot test with many initial catalytic functions, while with this catalyst positioning problem, the objective functions has many local minimizers. Following Chapter 4, under the assumption $cat_x(1) = 0.$, The derivative of $V(cat)$ with respect to cat is

$$V_{cat} = - \int_0^T \frac{D_2 v c}{\int_0^1 r c dx} dt$$

Instead of calculating J directional derivatives by solving the sensitivity system, with this second optimization problem, we only solve once the adjoint system from Theorem 4.16. We use FEM to solve this system. The second optimization problem is applied with $T_1 = T - \Delta t(M - 5)$, where M is number of time steps.

Using the line search algorithm from (5.51), we get numerical result of the adjoint method expressed in the Figures 5.17 and 5.17: The blue lines are initial catalytic functions, the red one are the local optimal catalytic functions. The algorithm considering when the pore radius reaches to 0.81 in the Figure 5.17 and to 0.79 in the Figure 5.18. In both cases, the free Volume of the pore via Adjoint method is below than the one via Greedy method around 3 – 6.5%.

(a) The optimal catalytic function by Adjoint method and by Greedy method

(b) The optimal pore radii via Adjoint method and Greedy method in Problem I_a . The Li_2O_2 is deposited in the upper side in this plot

Figure 5.17: Adjoint method and Greedy method with $J=100$, $N=80$, number of time steps $M=1000000$.

5.4. The optimization problems

(a) The optimal catalytic function by Adjoint method and by Greedy method

(b) The optimal pore radii via Adjoint method and Greedy method

Figure 5.18: Adjoint method and by Greedy method in Problem I_a with $J=100$, $N=60$, number of time steps $M=1000000$. The Li_2O_2 is deposited in the upper side in this plot

Conclusions

In this Thesis, we first have been working with two catalytic positioning model of the reformulated system of the two partial differential equations with initial and mixed boundary conditions. We investigated the well-posedness of the forward problems, the differentiability of the radius and concentration of oxygen inside the pore with respect to catalytic function in $W^{1\infty}(\Omega)$. We also prove the solvability of the two optimization problems. Note that the well-posedness of forward problems is local due to the lack of the comparison principle for the weak solution of parabolic equation including the first derivative of x . In the future, we should research the non-local well-posedness of this forward problem. A new approach for the proof of the well-posedness of the original system of the catalytic positioning in Li/air batteries could be studying the classical solution, with which comparison principle works. The fixed point argument for classical solution is written in the book of Friedman [14]. In comparison with the greedy algorithm in [8], our catalyst positioning model is more advanced with the "smoother" catalytic functions.

The numerical part illustrates the sensitivity and adjoint methods and shows that these algorithms works. However, there exist some limitations:

1. The sensitivity requires long time to calculate all the directional derivative for every catalytic function.
2. In order to proceed the adjoint method we need to solve the backward problems, which leads us to store all values of pore radius and concentration of oxygen inside the pore at every time step. The number of time steps could be up to hundreds of millions if we want to reach till the pore clogged (the pore radius reaches to 0.1).

Therefore, in this Thesis, we deal with the optimization problems only in a small interval of time, when the pore radius reaches to 0.8.

In further study, catalytic function should also be investigated in the first equation which is based on Fickian diffusion, as the part $v_R(C_{O_2}, \epsilon, r_p)$ in (1.4) in the Chapter Introduction represents the rate of Li_2O_2 formation per unit of cathode volume. The deposition of Li_2O_2 is certainly proceeded strongly where catalyst is positioned.

There is one more possible direction for the future work. It is consideration on the 2 or 3- dimensional spacial setting for the pore to gain a deeper understanding about the problems of maximizing capacity of the Li/air batteries during its charging process.

Appendix A

Elementary Theorems, Lemmas and other concepts

A.1 Elementary Lemmas and Theorems

Theorem A.1 [Banach Fixed-Point Theorem (1922)] Suppose that

- (i) we are given an operator $\mathcal{T} : \mathbf{M} \subseteq \mathbf{X} \longrightarrow \mathbf{M}$, i.e. $\mathbf{M}$ is mapped into itself by $\mathcal{T}$
- (ii) $\mathbf{M}$ is a closed non-empty set in a complete metric space $(\mathbf{X}, d)$;
- (iii) $\mathcal{T}$ is a k -contrative, i.e.,

$$d(\mathcal{T}(x), \mathcal{T}(y)) \leq k d(x, y)$$

for all $x, y \in \mathbf{M}$ and for a fixed k , $0 \leq k < 1$.

Then

1. Equation $\mathcal{T}(x) = x$, $x \in \mathbf{M}$ has exactly one solution.
2. The sequence of successive iterations

$$x_{n+1} = \mathcal{T}x_n, n = 0, 1, 2, \dots$$

with arbitrary $x_0 \in \mathbf{M}$ converges to the solution x .

Proof. We refer [39] for the proof. ■

Lemma A.2 (Gronwall's inequality (integral form)). [16] Let $\alpha(t), \beta(t)$ and $u(t)$ be real-valued functions on $[0, T]$. Assume that β and u are continuous and that the negative part of α is integrable on

every closed and bounded subinterval of $[0, T]$. If β is non-negative and $u(t)$ satisfies the inequalities

$$u(t) \leq \alpha(t) + \int_0^t \beta(s)u(s)ds, \quad t \in [0, T] \quad (\text{A.1})$$

then

$$u(t) \leq \alpha(t) + \int_0^t \alpha(s)\beta(s) \exp\left(\int_s^t \beta(r)dr\right)ds, \quad t \in [0, T] \quad (\text{A.2})$$

Lemma A.3 (Holder's inequality). [12] Assume $1 \leq p, q \leq \infty, \frac{1}{p} + \frac{1}{q} = 1$. Then if $u \in L^p(\Omega)$, $v \in L^q(\Omega)$, we have

$$\int_{\Omega} |uv|dx \leq \|u\|_{L^p(\Omega)} \|v\|_{L^q(\Omega)}. \quad (\text{A.3})$$

Lemma A.4 (ϵ - Cauchy inequality). [12]

$$ab \leq \epsilon a^2 + \frac{b^2}{\epsilon} \quad (a, b > 0, \epsilon > 0) \quad (\text{A.4})$$

Lemma A.5 (Poincare's inequality for $H_0^1(\Omega)$). There exists a constant C depending on Ω such that with $u \in H_0^1(\Omega)$, we have

$$\|u\|_{L^2(\Omega)} \leq C \|\nabla u\|_{L^2(\Omega)}$$

Proof. Using Holder's inequality, we have

$$u^2(x) = \left(\int_{\partial\Omega} u_x(x)dx \right)^2 \leq C(\Omega) \int_{\partial\Omega} (u_x)^2 dx$$

Hence we deduce the results. ■

Remark A.6 (Other necessary inequalities). Suppose $u \in L^\infty(Q)$, then the following inequalities hold

$$\|u\|_{L^2(Q)} \leq \sqrt{T} \|u\|_{L^2(0,T;L^\infty(\Omega))}, \quad (\text{A.5})$$

$$\|u\|_{L^2(Q)} \leq \sqrt{T} \|u\|_{L^\infty(Q)}. \quad (\text{A.6})$$

A.2 Huber functions

A.2.1 Continuously differentiable Huber C^1 function

We present Huber functions, that we will need further for building a continuous propaganda model of catalyst problem within the pore, and for reforming problem. According to [10] the continuously

Figure A.1: The graphic of Huber C^1 function $h_{1,\gamma}(x)$ with $g = 1$ and $\gamma = 2$

differentiable Huber function is given by

$$h_{1,\gamma}(x) = \begin{cases} g, & \text{if } x > \frac{g}{2\gamma} + \frac{1}{2\gamma^2}, \\ g - \frac{\gamma}{2} (g - \gamma x + \frac{1}{2\gamma})^2, & \text{if } \frac{g}{2\gamma} - \frac{1}{2\gamma^2} < x \leq \frac{g}{2\gamma} + \frac{1}{2\gamma^2}, \\ \gamma x, & \text{if } -\frac{g}{2\gamma} + \frac{1}{2\gamma^2} < x \leq \frac{g}{2\gamma} - \frac{1}{2\gamma^2}, \\ -(g - \frac{\gamma}{2} (g + \gamma x + \frac{1}{2\gamma})^2), & \text{if } -\frac{g}{2\gamma} - \frac{1}{2\gamma^2} < x \leq -\frac{g}{2\gamma} + \frac{1}{2\gamma^2}, \\ -g, & \text{if } x \leq -\frac{g}{2\gamma} - \frac{1}{2\gamma^2}. \end{cases} \quad (\text{A.7})$$

The plot of $h_{1,\gamma}(x)$ when $g = 1$ and $\gamma = 2$ is shown in the Figure A.1. In particular, the following properties are satisfied:

- $h(1, \gamma) : \mathbb{R} \rightarrow \mathbb{R}$ is monotone, Lipschitz continuous and differentiable.
- $\|h(1, \gamma)(x)\| \leq g$, for $\forall \gamma > 0$ and $\forall x \in \mathbb{R}$

Using translation along the axis Ox , Oy , we get

$$h_{1,\gamma}^*(x) = \begin{cases} 2g, & \text{if } x > \frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0, \\ 2g - \frac{\gamma}{2} (g - \gamma x + \gamma R_0 + \frac{1}{2\gamma})^2, & \text{if } \frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0 < x \leq \frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0, \\ g + \gamma x - \gamma R_0, & \text{if } -\frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0 < x \leq \frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0, \\ \frac{\gamma}{2} (g + \gamma x - \gamma R_0 + \frac{1}{2\gamma})^2, & \text{if } -\frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0 < x \leq -\frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0, \\ 0, & \text{if } x \leq -\frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0. \end{cases} \quad (\text{A.8})$$

Taking axial symmetry via $x = 0.94$, we get

$$H_{1,\gamma,R_0}(x) = \begin{cases} 0, & \text{if } x > \frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0 \\ \frac{\gamma}{2} (g - \gamma x + \gamma R_0 + \frac{1}{2\gamma})^2, & \text{if } \frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0 < x \leq \frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0 \\ g - \gamma x + \gamma R_0, & \text{if } -\frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0 < x \leq \frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0 \\ 2g - \frac{\gamma}{2} (g + \gamma x - \gamma R_0 + \frac{1}{2\gamma})^2, & \text{if } -\frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0 < x \leq -\frac{g}{2\gamma} + \frac{1}{2\gamma^2} + R_0 \\ 1, & \text{if } x \leq -\frac{g}{2\gamma} - \frac{1}{2\gamma^2} + R_0, \end{cases} \quad (\text{A.9})$$

Figure A.2: The graphic of C^1 Huber function $H_{1,\gamma,R_0}(x)$ with $g = 1/2$, $\gamma = 50$, and $R_0 = 0.94$

Equation (A.9) has plot given in the Figure A.2 with $g = 1/2$, $\gamma = 50$, $R_0 = 0.94$

A.2.2 Continuously differentiable C^2 Huber function

Referring [6], we present the C^2 Huber function $h_{2,\gamma} : \mathbb{R} \rightarrow \mathbb{R}$, that is given by:

$$h_{2,\gamma}(x) = \begin{cases} 1, & \text{if } x > \frac{b}{\gamma}, \\ \left[\frac{2\gamma-1}{4\gamma} + \frac{\gamma x}{2} - \frac{\gamma}{2}(\gamma x - a)(\gamma x - b) + \frac{\gamma^3}{2}(\gamma x - a)^2(\gamma x - b)^2 \right], & \text{if } \frac{a}{\gamma} < x \leq \frac{b}{\gamma}, \\ \gamma x, & \text{if } -\frac{a}{\gamma} < x \leq \frac{a}{\gamma}, \\ -\left[\frac{2\gamma-1}{4\gamma} - \frac{\gamma x}{2} - \frac{\gamma}{2}(\gamma x + a)(\gamma x + b) + \frac{\gamma^3}{2}(\gamma x + a)^2(\gamma x + b)^2 \right], & \text{if } -\frac{b}{\gamma} < x \leq -\frac{a}{\gamma}, \\ -1, & \text{else} \end{cases} \quad (\text{A.10})$$

where $a := 1 - \frac{1}{2\gamma}$, $b := 1 + \frac{1}{2\gamma}$. The graphic of $h_{2,\gamma}(x)$ is given in Figure A.3.

We also have a characteristic of this C^2 Huber function as following:

Figure A.3: Graphic of C^2 Huber function with $\gamma = 2$

Lemma A.7 *The first and second derivative of the function $h_{2,\gamma} : \mathbb{R} \rightarrow \mathbb{R}$ are Lipschitz continuous functions, with Lipschitz constants depending only on γ .*

Relying on the form of $h_{2,\gamma}(x)$, we would like to deduce a C^2 function $H(2, \gamma)$ that is increase, always greater than ϵ , taking the value of x , where x greater than c_0 . The condition on c_0 and ϵ here is:

$$0 < \epsilon < c_0 < 1 \quad (\text{A.11})$$

$$H_{2,\gamma}(x) = \begin{cases} x, & \text{if } x \geq -\frac{a}{\gamma} + c_0 \\ 2\epsilon - \epsilon \left[\frac{2\gamma-1}{4\gamma} - \frac{\gamma x}{2} - \frac{\gamma}{2}(\gamma x - \gamma c_0 + a)(\gamma x - \gamma c_0 + b) + \frac{\gamma^3}{2}(\gamma x - \gamma c_0 + a)^2(\gamma x - \gamma c_0 + b)^2 \right], & \\ \text{if } -\frac{b}{\gamma} + c_0 < x \leq -\frac{a}{\gamma} + c_0 \\ \epsilon, & \text{else} \end{cases} \quad (\text{A.12})$$

where $\epsilon = \frac{1}{\gamma}$ and $c_0 = \frac{1}{\gamma}$. Graphic of $H_{2,\gamma}(x)$ is expressed in the Figure A.4.

A.3 The Gaussian distribution (Normal distribution)

In the introduction, we recall the discrete propagation model for the deposited Li_2O during the pore of the cathode in [8]. In this work we would like to introduce a continuous propagation model based on Gaussian distribution. There are some several reasons why we choose this distribution for describing the propagation among the active surface of the pore: the central natural distribution of data that could express the propagation of the increasing oxygen reaction product among neighborhood and its convenience to use in mathematical calculation. For more understanding on this distribution, we refer

Figure A.4: Graphic of C^2 function $H_{2,\gamma}(x)$ with $\gamma = 2$, $\epsilon = \frac{1}{\gamma}$, $c_0 = \frac{1}{\gamma}$

readers to a text book on statistics like the one from Hogg and his colleagues [18].

Definition A.8 We say a random variable X has a normal distribution if its probability density function (pdf) is

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right\}, \quad -\infty < x < \infty. \quad (\text{A.13})$$

The parameters μ and σ^2 are the mean and variance of X , respectively. We write that X has a $N(\mu, \sigma^2)$ distribution.

It is easy to see that the integral in (A.13) exist and bounded. Moreover the integral is equal to 1.

The graph in Figure A.5 shows that the normal pdf has symmetrical characteristics about a vertical axis through $x = \mu$. Besides, it is easily to see that there is approximately 99.7 per cent within three standard deviations from the mean. That means that the data that has normal pdf is distributed mostly among three-standard-deviation difference.

$$\int_{\mu-3\sigma}^{\mu+3\sigma} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right\} dx \approx 0.997$$

Figure A.5: The normal density $f(x)$

Remark A.9 For the normal distribution that is defined in the definition A.8, we have:

$$\begin{aligned}
 f(\mu) &= \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + \frac{1}{2}\sigma) &= f(\mu - \frac{1}{2}\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{1}{4}\} \approx 0.7788 \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + \sigma) &= f(\mu - \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{1}{2}\} \approx 0.6065 \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + \frac{3}{2}\sigma) &= f(\mu - \frac{3}{2}\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{9}{4}\} \approx 0.4724 \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + 2\sigma) &= f(\mu - 2\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-1\} \approx 0.3679 \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + \frac{5}{2}\sigma) &= f(\mu - \frac{5}{2}\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{25}{4}\} \approx 0.2865 \frac{1}{\sqrt{2\pi}\sigma}, \\
 f(\mu + 3\sigma) &= f(\mu - 3\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\{-\frac{9}{2}\} \approx 0.0111 \frac{1}{\sqrt{2\pi}\sigma}.
 \end{aligned} \tag{A.14}$$

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