

# Contents

<b>Abstract</b>	<b>v</b>
<b>1 Introduction</b>	<b>1</b>
1.1 A Moving-Boundary Problem: the Carbonation of Concrete . . .	1
1.2 Outline of the Thesis . . . . .	3
<b>2 Moving-Interface Carbonation Models</b>	<b>5</b>
2.1 Problem Statement . . . . .	5
2.1.1 Comments on the Physics of the Situation . . . . .	5
2.1.2 Earlier Studies . . . . .	6
2.2 The Reaction-Diffusion Problem. Modeling Assumptions . . . . .	8
2.2.1 Basic Geometry. Choice of Porosities . . . . .	8
2.2.2 Transport Mechanisms and Coefficients . . . . .	13
2.2.3 Production by Henry's Law . . . . .	13
2.2.4 Production by Dissolution and Precipitation Reactions . .	15
2.2.5 Modeling the Carbonation Reaction Rate . . . . .	17
2.2.6 On the Mass Balance of Humidity . . . . .	19
2.2.7 General Reaction-Diffusion Model . . . . .	22
2.3 The Sharp-Interface Carbonation Model . . . . .	23
2.3.1 An Equation for the Speed of the Interface . . . . .	25
2.4 The Moving-Two-Reaction-Zones Model . . . . .	27
2.5 Notes and Comments . . . . .	32
<b>3 Analysis of Selected Carbonation Models</b>	<b>34</b>
3.1 Basic Notation . . . . .	34
3.2 Function Spaces . . . . .	35
3.3 Elementary Inequalities . . . . .	36
3.4 Well-Posedness of the Sharp-Interface Model . . . . .	38
3.4.1 Fixing the Moving Interface. Definition of the Weak So- lution. Main Results. . . . .	38
3.4.2 Basic Estimates . . . . .	45
3.4.3 Proof of Theorem 3.4.6 . . . . .	52
3.4.4 Proofs of Theorem 3.4.8 . . . . .	61
3.4.5 Proof of Proposition 3.4.10 . . . . .	66
3.5 Well-Posedness of the Moving-Two-Reaction-Zones Model . . . . .	72
3.5.1 Fixing the Moving Layer. Definition of the Weak Solution. Main Results . . . . .	72
3.5.2 Basic Estimates . . . . .	77

3.5.3	Proof of Theorem 3.5.4 . . . . .	82
3.5.4	Proof of Theorem 3.5.5 . . . . .	89
3.6	Notes and Comments . . . . .	93
<b>4</b>	<b>Numerical Simulations</b>	<b>96</b>
4.1	Introduction and Problem Statement . . . . .	96
4.2	Numerical Approach . . . . .	99
4.2.1	Fixed-Domain Transformation. The Problems $\mathcal{P}^{\mathcal{R}\epsilon}$ and $\mathcal{P}_{red}^{\mathcal{R}\epsilon}$ . . . . .	100
4.2.2	FEM Approximation. The Problems $\mathcal{P}^{\mathcal{R}\epsilon n}$ and $\mathcal{P}_{red}^{\mathcal{R}\epsilon n}$ . . . . .	102
4.2.3	Implementation Details . . . . .	104
4.3	Simulation Results . . . . .	105
4.3.1	Typical Questions . . . . .	106
4.3.2	Behavior of Concentrations and Front Position . . . . .	107
4.4	Conclusions on the Validation of the Moving-Interface Carbonation Models . . . . .	113
4.4.1	Interpretation of the Simulation Results . . . . .	113
4.4.2	Conclusions . . . . .	114
4.5	Notes and Comments . . . . .	114
<b>5</b>	<b>Conclusions</b>	<b>115</b>
	<b>Bibliography</b>	<b>118</b>
<b>A</b>	<b>A Non-Dimensionalization Procedure</b>	<b>128</b>
<b>B</b>	<b>Proof of Proposition 3.4.17</b>	<b>136</b>
<b>C</b>	<b>Concise Description of Two Carbonation Tests</b>	<b>138</b>
<b>D</b>	<b>List of Material Parameters and Their Typical Ranges</b>	<b>140</b>
	Acknowledgements . . . . .	145
	Zusammenfassung . . . . .	146
	Version Abrégée . . . . .	147