

# TABLE OF CONTENTS

<b>1 Introduction</b> .....	<b>Error! Bookmark not defined.</b>
1.1 Overview.....	<b>Error! Bookmark not defined.</b>
1.2 Historical background .....	<b>Error! Bookmark not defined.</b>
1.3 Objectives and motivations .....	<b>Error! Bookmark not defined.</b>
1.4 Solution methodologies.....	<b>Error! Bookmark not defined.</b>
1.4.1 Laplace transformation.....	<b>Error! Bookmark not defined.</b>
1.4.2 High resolution finite volume scheme (HR-FVS) .....	<b>Error! Bookmark not defined.</b>
1.5 Achievements of the project.....	<b>Error! Bookmark not defined.</b>
1.6 Thesis layout.....	<b>Error! Bookmark not defined.</b>
1.7 Published and submitted papers.....	<b>Error! Bookmark not defined.</b>
<b>2 Preliminaries</b> .....	<b>Error! Bookmark not defined.</b>
2.1 Chromatography .....	<b>Error! Bookmark not defined.</b>
2.1.1 Basic terminologies in chromatography .....	<b>Error! Bookmark not defined.</b>
2.2 Mathematical modeling of FBLCC .....	<b>Error! Bookmark not defined.</b>
2.3 Model parameters.....	<b>Error! Bookmark not defined.</b>
2.3.1 Column porosities .....	<b>Error! Bookmark not defined.</b>
2.3.2 Adsorption isotherms.....	<b>Error! Bookmark not defined.</b>
2.4 Ideal and non-ideal chromatography.....	<b>Error! Bookmark not defined.</b>
2.5 Continuous chromatographic models.....	<b>Error! Bookmark not defined.</b>
2.5.1 The lumped kinetic model (LKM).....	<b>Error! Bookmark not defined.</b>
2.5.2 The equilibrium dispersive model (EDM) .....	<b>Error! Bookmark not defined.</b>
2.5.3 The ideal model.....	<b>Error! Bookmark not defined.</b>
2.5.4 The general rate model (GRM) .....	<b>Error! Bookmark not defined.</b>

2.6 Temporal moments .....	Error! Bookmark not defined.
2.6.1 Mean .....	Error! Bookmark not defined.
2.6.2 Retention time.....	Error! Bookmark not defined.
2.6.3 Variance .....	Error! Bookmark not defined.
2.6.4 Skewness .....	Error! Bookmark not defined.
2.6.5 Kurtosis.....	Error! Bookmark not defined.
2.6.6 Column efficiency .....	Error! Bookmark not defined.
<b>3 Analysis of linear EDM and LKM .....</b>	<b>Error! Bookmark not defined.</b>
3.1 Single solute LKM .....	Error! Bookmark not defined.
3.2 Single solute EDM .....	Error! Bookmark not defined.
3.3 Analytical solutions of linear LKM and EDM .....	Error! Bookmark not defined.
3.3.1 Analytical solutions of the LKM.....	Error! Bookmark not defined.
3.3.2 Analytical solutions of the linear EDM .....	Error! Bookmark not defined.
3.4 Temporal moments of the linear LKM and EDM .....	Error! Bookmark not defined.
3.5 Numerical test problems.....	Error! Bookmark not defined.
<b>4 Numerical approximation of nonlinear EDM and LKM .....</b>	<b>Error! Bookmark not defined.</b>
4.1 The flux-limiting finite volume schemes .....	Error! Bookmark not defined.
4.2 Numerical test problems.....	Error! Bookmark not defined.
4.3 Single-component elution.....	Error! Bookmark not defined.
4.3.1 Single-component elution with linear isotherm .....	Error! Bookmark not defined.
4.3.2 Single-component model with nonlinear isotherm.....	Error! Bookmark not defined.
4.3.3 Two-component elution .....	Error! Bookmark not defined.
4.3.4 Three-component elutions.....	Error! Bookmark not defined.
<b>5 Analysis of linear GRM for fixed-beds packed with core-shell particles .....</b>	<b>Error! Bookmark not defined.</b>
5.1 The linear GRM for core-shell particles .....	Error! Bookmark not defined.
5.2 Analytical solutions of GRM for Linear Isotherms .....	Error! Bookmark not defined.
5.3 Moments of the general rate model.....	Error! Bookmark not defined.

5.3.1 Heights equivalent to a theoretical plate (HETP) curve for Dirichlet **Error! Bookmark not defined.**

BC ..... **Error! Bookmark not defined.**

5.3.2 HETP curve for Danckwerts BC..... **Error! Bookmark not defined.**

5.3.3 Skewness ..... **Error! Bookmark not defined.**

5.4 Numerical test problems..... **Error! Bookmark not defined.**

**6 Numerical approximation of nonlinear GRM for fixed-beds packed with core shell-particles** ..... **Error! Bookmark not defined.**

6.1 Mathematical model for core breads ..... **Error! Bookmark not defined.**

6.2 Numerical scheme ..... **Error! Bookmark not defined.**

6.2.1 Domain discretization ..... **Error! Bookmark not defined.**

6.2.2 First order scheme ..... **Error! Bookmark not defined.**

6.2.3 The flux-limiting high resolution scheme ..... **Error! Bookmark not defined.**

6.3 Numerical case studies ..... **Error! Bookmark not defined.**

6.3.1 Single-component elution ..... **Error! Bookmark not defined.**

6.3.2 Two-component elution ..... **Error! Bookmark not defined.**

6.3.3 Three-component elution..... **Error! Bookmark not defined.**

**7 Conclusions and future perspectives** ..... **Error! Bookmark not defined.**

7.1 Conclusions ..... **Error! Bookmark not defined.**

7.2 Future perspectives..... **Error! Bookmark not defined.**

**8 References** ..... **Error! Bookmark not defined.**