

TABLE OF CONTENTS

| | |
|--|-----------|
| Dedication | iv |
| Acknowledgements | v |
| List of publication | vi |
| Abstract | vii |
| Table of contents | viii |
| List of figures | xi |
| List of tables | xvii |
| | |
| Chapter 1: Introduction | 1 |
| 1.1 Role of computer simulation | 1 |
| 1.2 Importance of heterogeneous catalytic reaction (HCR) | 2 |
| 1.3 History of the project | 4 |
| 1.4 Aim of the project | 12 |
| 1.5 References | 13 |
| | |
| Chapter 2: Monte Carlo simulation and Catalytic Surface Reactions | 15 |
| 2.1 Introduction | 15 |
| 2.2 The Monte Carlo simulation method | 15 |
| 2.2.1 The constant coverage ensemble | 17 |
| 2.2.2 Finite-size scaling approach | 17 |
| 2.2.3 The epidemic method (EM) and dynamical scaling | 18 |
| 2.2.4 The standard ensemble | 20 |
| 2.3 References | 21 |
| | |
| Chapter 3: Surface Catalytic Reactions (SCR) | 23 |
| 3.1 Introduction | 23 |
| 3.2 Elementary steps in surface reaction | 23 |
| 3.2.1 Adsorption mechanism | 24 |

| | | |
|---|---|-----------|
| 3.3 | Catalytic Reaction mechanisms | 25 |
| 3.3.1 | Langmuir- Hinshelwood mechanism | 25 |
| 3.3.2 | Precursor mechanism | 27 |
| 3.3.3 | Hot atom mechanism | 28 |
| 3.3.4 | Eley-Rideal mechanism | 30 |
| 3.4 | Basic Modelling of SCR | 31 |
| 3.4.1 | Ziff, Gulari and Barshad (ZGB) Model | 32 |
| 3.5 | Variants of ZGB Model | 36 |
| 3.5.1 | Desorption mechanism | 36 |
| 3.5.2 | Diffusion mechanism | 36 |
| 3.6 | References | 37 |
| Chapter 4: Simulation of CO-O₂ Reaction | | 39 |
| 4.1 | Introduction | 39 |
| 4.2 | Simulation on simple cubic lattice (SCL) with ER | 40 |
| 4.2.1 | Model and simulation | 40 |
| 4.2.2 | Results and discussion | 42 |
| 4.3 | Simulation on BCC with ER | 50 |
| 4.3.1 | Model and simulation | 50 |
| 4.3.2 | Results and discussion | 52 |
| 4.4 | Simulation on SCL with Ballistic-Type Hot Atom | 56 |
| 4.4.1 | Model and simulation | 57 |
| 4.4.2 | Results and discussion | 58 |
| 4.5 | References | 61 |
| Chapter 5: Simulation of CO-NO Reaction | | 63 |
| 5.1 | Introduction | 63 |
| 5.2 | Simulation on square surface with Precursor mechanism | 64 |
| 5.2.1 | Model and simulation | 64 |
| 5.2.2 | Results and discussion | 66 |
| 5.3 | Simulation on square surface with Precursor and diffusion mechanism | 74 |
| 5.3.1 | Model and simulation | 74 |
| 5.3.2 | Results and discussion | 75 |

| | | |
|--|--|------------|
| 5.4 | Simulation on BCC for CO-N ₀ with Precursor mechanism | 79 |
| 5.4.1 | Model and simulation | 79 |
| 5.4.2 | Results and discussion | 81 |
| 5.5 | Simulation on BCC with Eley Rideal and diffusion mechanism | 96 |
| 5.5.1 | Model and simulation | 96 |
| 5.5.2 | Results and discussion | 98 |
| 5.6 | References | 107 |
| Chapter 6: Results and Conclusion | | 109 |
| 6.1 | Conclusion | 109 |
| 6.2 | Future Research Work | 111 |