Contents

CHAPTER 1 ..... **1**

INTRODUCTION 1

1.1 Background *1*

1.2 Thermal decomposition of methane *2*

1.3 Types of pyrolytic carbon and their importance *4*

1.4 Various manufacturing processes of pyrocarbon *6*

1.5 Advantages of CVD over another manufacturing process *10*

1.6 CVD of pyrocarbon (PyC) *11*

1.6.1. A sequence of events during CVD of PyC 12

1.6.2. Types of CVD 13

1.6.3. Critical components in CVD 18

1.6.4. Advantage of vertical over horizontal CVD reactor 19

1.7 Importance of CFD in designing CVD reactor: *20*

1.8 Techniques used for optimisation of CVD *21*

1.9 Machine learning *23*

1.10 Support vector machines (SVM) *24*

1.11 Objectives of the thesis *25*

1.12 Thesis organisation *26*

CHAPTER 2 ..... **33**

LITERATURE REVIEW 33

2.1 History of the CVD processes *33*

2.2 Modelling approaches in CVD *33*

2.3 Literature based on pyrolysis of methane in CVD reactor *36*

2.4 Use of machine learning (ML) in chemical processes *40*

CHAPTER 3 ..... **46**

CFD MODEL AND OPTIMISATION METHODOLOGY 46

3.1 Basic equation, assumptions, and properties estimation *46*

3.2 Gas and surface reaction models *49*

3.3 Boundary condition and solution procedure *51*

3.3 Machine learning model for prediction of PyC deposition *54*

3.4 Nelder-Mead algorithm *56*

3.6 Objective function *58*

CHAPTER 4 ..... **62**

RESULTS AND DISCUSSION 62

4.1Validation of simulation results *62*

4.2 Effect of reactor temperature *62*

4.3 Effect of operating pressure *66*

4.4 Effect of total flow rate *69*

4.5 Effect of CH_4 mole fraction *71*

4.6 Optimisation of the CVD reactor *74*

CHAPTER 5 ..... **80**

CONCLUSIONS AND FUTURE SCOPE 80
5.1 Conclusions *80*
5.2 Future Scope *80*
APPENDIX A 83
APPENDIX B 88
APPENDIX C 96
APPENDIX D 97
GLOSSARY 98