

CHAPTER 1

INTRODUCTION.....	1
1.1. WHAT ARE NANOMATERIALS?.....	1
1.2. NANOMATERIAL PROPERTIES AND RELEVANCE.....	2
1.3. RESEARCH ON NANOMATERIALS	4
1.4. PRODUCTION STRATEGIES OF NANOPARTICLES	5
1.4.1. Aerosol-Flame Synthesis of Nanoparticles.....	7
1.4.2. Flame Spray Pyrolysis Process	8
1.5. MOTIVATION AND SCOPE OF THE WORK.....	12
1.6. STRUCTURE OF THE WORK	14

CHAPTER 2

MODELLING OF TURBULENT COMBUSTION

AND PARTICLE FORMATION	17
2.1. ASSUMPTIONS OF THE MATHEMATICAL MODEL	18
2.2. GOVERNING EQUATIONS FOR THE GAS PHASE.....	19
2.2.1. Mass Conservation.....	19
2.2.2. Momentum Conservation.....	19
2.2.3. Energy Conservation.....	20
2.2.4. Chemical Species Conservation.....	21
2.3. LIQUID ATOMIZATION AND SPRAY FORMATION	21
2.4. GOVERNING EQUATIONS FOR THE DISCRETE PHASE (DROPLETS).....	22
2.4.1. Force Balance for a Single Droplet.....	23
2.4.2. Energy Equation for a Single Droplet.....	23
2.5. EQUATIONS OF STATE AND THERMOPHYSICAL PROPERTIES	25
2.5.1. Ideal Gas Law	25
2.5.2. Thermophysical Properties	25
2.6. TURBULENCE.....	26
2.6.1. Reynolds Decomposition.....	27
2.6.2. Turbulent Kinetic Energy	27
2.6.3. Scales of Turbulent Flows and Dissipation of Turbulent Kinetic Energy	28
2.7. CLOSURE EQUATIONS	29
2.7.1. Mathematical Approaches to Resolve the Turbulence.....	29
2.7.2. Shear-Stress-Transport (SST) $k-\omega$ Model.....	31
2.7.3. Momentum, Heat, and Mass Transfer Between the Phases	33
2.7.4. Radiation.....	35
2.8. COMBUSTION REACTIONS AND INTERACTIONS WITH TURBULENCE.....	35
2.8.1. Eddy Break-Up Model.....	36

2.8.2. Eddy Dissipation Model (EDM).....	36
2.8.3. Eddy Dissipation Concept (EDC) Model	37
2.9. MODELLING NANOPARTICLE SYNTHESIS.....	39
2.9.1. Number-Density Function	39
2.9.2. Population Balance Equation	39
2.9.3. Approaches to Solve the Population Balance Equation.....	42
2.9.4. Nucleation Rate.....	49
2.9.5. Agglomeration Rate.....	49
2.9.6. Sintering Rate	51
2.10. MODELLING PARTICLE DEPOSITION	52

CHAPTER 3

EXPERIMENTAL FACILITY AND MEASUREMENTS..... 57

3.1. EXPERIMENTAL FACILITY.....	57
3.2. MATERIALS AND OPERATING CONDITIONS.....	60
3.3. SPRAY AND FLAME ANALYSIS.....	60
3.3.1. Droplet Size Distribution	60
3.3.2. Temperature Measurements.....	62
3.4. NANOPARTICLE CHARACTERISATION	69
3.4.1. Brunauer-Emmett-Teller (BET) Measurements	69
3.4.2. Transmission Electron Microscopy (TEM) Measurements.....	72

CHAPTER 4

COMBUSTION KINETIC ANALYSIS OF

FLAME SPRAY PYROLYSIS PROCESS..... 77

4.1. BACKGROUND AND OBJECTIVES.....	77
4.2. NUMERICAL SETUP	80
4.2.1. CFD Model	80
4.2.2. Chemical Species and Thermophysical Properties	82
4.2.3. Kinetic Mechanisms	83
4.2.4. Numerical Methodology.....	85
4.3. EFFECTS OF DIFFERENT KINETIC MECHANISMS ON THE FLAME SPRAY AND PARTICLE CHARACTERISTICS	88
4.3.1. Flame Temperature and Droplet Evaporation in the Open FSP Setup	89
4.3.2. Gas Composition in the Open FSP Reactor	93
4.3.3. Flow Behaviour and Flame Temperature Analysis in the Enclosed FSP Reactor.....	97
4.3.4. Gas Composition in the Enclosed FSP Reactor.....	102
4.3.5. Nanoparticle Size Evolution in the Open FSP Reactor.....	105
4.3.6. Nanoparticle Size Evolution in the Enclosed FSP Reactor with Reduced Co-Flow	108

4.4. SUMMARY OF CHAPTER 4	110
---------------------------------	-----

CHAPTER 5

PARTICLE-RESIDENCE-TIME AND PARTICLE-WALL DEPOSITION IN CONFINED

FLAME SPRAY PROCESS 113

5.1. BACKGROUND AND OBJECTIVES.....	113
5.2. NUMERICAL SETUP	115
5.2.1. Reaction Chamber Geometry and Numerical Domain	115
5.2.2. Mathematical Modelling.....	116
5.2.3. Chemical Species and Properties	117
5.2.4. Particle Formation and Growth.....	118
5.2.5. Particle-Wall Deposition.....	119
5.2.6. Numerical Methodology	119
5.2.7. Operating and Boundary Conditions.....	122
5.3. EFFECTS OF DIFFERENT ENCLOSURE GEOMETRIES AND OPERATING CONDITIONS ON THE FLAME SPRAY AND PARTICLE CHARACTERISTICS.....	123
5.3.1. Gas Velocity and Recirculation	123
5.3.2. Temperature of the Gas Phase	127
5.3.3. Particle Formation and Size Distribution with Different Geometries and Operating Conditions	129
5.3.4. Particle Recirculation and Temperature-Particle-Residence-Time.....	131
5.3.5. Particle Deposition on the Reactor Wall.....	136
5.4. SUMMARY OF CHAPTER 5	139

CHAPTER 6

POLYDISPERSE NANOPARTICLE DISTRIBUTIONS

PRODUCED VIA FLAME SPRAY PYROLYSIS 141

6.1. BACKGROUND AND OBJECTIVES.....	141
6.2. NUMERICAL SETUP	143
6.2.1. Geometry and Numerical Domain.....	143
6.2.2. Mathematical Modelling.....	143
6.2.3. Chemical Species and Properties	146
6.2.4. Solution of the Polydisperse Population Balance Model.....	146
6.2.5. Operating and Boundary Conditions.....	147
6.3. NANOPARTICLE FORMATION AND POLYDISPERSITY	148
6.3.1. Primary Particle Diameter in the Open FSP Reactor.....	148
6.3.2. Number of Primary Particles per Agglomerate.....	151
6.3.3. Agglomerate Diameter in the Open FSP Reactor	152
6.3.4. Primary Particle and Agglomerate Diameter in the Enclosed FSP Reactor ..	154
6.4. SUMMARY OF CHAPTER 6	159

CHAPTER 7

CONCLUSIONS AND OUTLOOK 161

7.1. CONCLUSIONS..... 161

7.2. OUTLOOK 164

BIBLIOGRAPHY 165

ACRONYMS I

DIMENSIONLESS NUMBERS IV

GREEK SYMBOLS..... V

LATIN SYMBOLS IX

LIST OF FIGURESXV

LIST OF TABLES..... XXI

APPENDIX

APPENDIX A – MATERIAL PROPERTIESXXIII

APPENDIX B – CO-AUTHORS AND THEIR CONTRIBUTIONS XXIX