Contents

1. Introduction **1**

1.1. Aim of this Work . . . 3

1.2. Structure of this Work . . . 4

2. Numerical Simulation of Particulate Flows using CFD-DEM **5**

2.1. Governing Equations of the Discrete Element Method . . . 5

2.2. Governing Equations in Computational Fluid Dynamics . . . 8

2.2.1. Turbulence Modeling . . . 10

2.3. Eulerian-Lagrangian Phase Coupling . . . 10

2.3.1. A Novel, Simple Coupling Algorithm for Massively Parallel Simulations . . . 11

2.3.2. Euler-Lagrange Mapping . . . 14

2.3.3. Momentum Coupling for Dense Particulate Flows . . . 15

2.4. Coarse-Graining Techniques for Dense Particulate Flows . . . 18

2.4.1. Particle Coarsening . . . 18

2.4.2. Fluid Coarsening . . . 18

3. Development of a Segregated Calibration Approach for Handling Wetted Materials in the Discrete Element Method **21**

3.1. Micromechanics of Wetted Granular Matter . . . 21

3.1.1. Capillary Force . . . 22

3.1.2. Viscous Force . . . 26

3.1.3. Liquid Bridge Rupture and Liquid Distribution . . . 27

3.1.4. Liquid Bridge Volume . . . 28

3.1.5. Particle Softening Correction and Coarse Graining Approaches . . . 33

3.2. Liquid Bridge Model Composition and Implementation . . . 34

3.3. Experimental Characterization . . . 37

3.3.1. Basic Material Properties . . . 37

3.3.2. Shear Testing . . . 38

3.3.3. Static Angle of Repose . . . 39

3.3.4. Dynamic Angle of Repose . . . 40

3.4. Sensitivity Analysis of the Numerical Model . . . 42

3.4.1. Restitution Analysis . . . 42

3.4.2. Sensitivity of the Static Angle of Repose . . . 44

3.4.3. Sensitivity of the Shear Test . . . 48
3.4.4. Sensitivity of the Dynamic Angle of Repose . . . 50
3.5. Calibration Workflow for Liquid Bridge Modelling in the Discrete Element Method . . . 54
4. Calibration of a Discrete Element Method Contact Law for Describing a Wetted Granular System 59
4.1. Experimental Characterization . . . 59
4.1.1. Basic Physical Properties . . . 59
4.1.2. Static Angle of Repose . . . 60
4.1.3. Shear Testing . . . 60
4.1.4. Dynamic Angle of Repose . . . 63
4.2. Determination of Model Material Parameters . . . 66
4.3. Calibration of Frictional Contact Model Coefficients . . . 67
4.4. Calibration of Liquid Bridge Model Coefficients . . . 71
4.5. Summary . . . 73
5. Implementation and Validation of a Full-Physics CFD-DEM Solver for the Simulation of Fluidized Bed Spray Granulation 75
5.1. Governing Equations for Heat and Mass Transfer Modeling . . . 76
5.1.1. Governing Equations for the Droplet Phase and the Particle Phase 76
5.2. Closures for Heat and Mass Transfer . . . 78
5.2.1. Heat Transfer . . . 78
5.2.2. Mass Transfer . . . 79
5.3. Surface Coverage Modeling . . . 80
5.3.1. Analytical Surface Coverage Models . . . 81
5.3.2. Surface Coverage Modeling using a Discretized Surface Area . . . 82
5.3.3. Comparison of Surface Coverage Models . . . 82
5.4. Droplet Deposition Modeling . . . 84
5.5. Governing Equations in the Eulerian Frame of Reference . . . 87
5.5.1. Vapor Transport . . . 87
5.5.2. Evaporation Modeling . . . 88
5.5.3. Heat Transfer and Transport . . . 88
5.6. Solver Validation against Drying Experiments . . . 90
5.6.1. Case Analysis . . . 92
5.6.2. Validation against Steady-State Experiments . . . 93
5.6.3. Validation of Mean Temperature Response against Transient Experiments . . . 96
5.7. Summary . . . 97

6. Development of a Novel Approach for Prediction of Particle Properties in Fluidized Bed Spray Granulation **99**
6.1. Theoretical Considerations . . . 99
6.1.1. Macroscopic Experimental Studies . . . 99
6.1.2. Micro-Scale Processes in Layering Granulation . . . 101
6.2. Proposed Approach . . . 103
6.2.1. Requirements . . . 103
6.2.2. Tracked Quantities . . . 104
6.2.3. Evaluation of the Simulations . . . 105
6.2.4. Workflow . . . 105
6.2.5. Limitations and Assumptions . . . 107
6.3. Derivation of a Mapping between Tracked Quantities and Product Properties 107
6.3.1. Fitting of a Linear Regression Model . . . 107
6.4. Demonstration Case according to Hoffmann (2016) . . . 110
6.4.1. Case Setup . . . 111
6.4.2. Drying Behavior and Tracked Quantities . . . 112
6.5. Summary . . . 113
7. Micro-Scale Product-Property Predictors in Fluidized Bed Spray Granulation of a Suspension **117**
7.1. Experimental Procedure . . . 117
7.2. Simulation Setup . . . 118
7.3. Relationship between Shell Porosity and Process Conditions . . . 120
7.4. Correlating Shell Porosity and Tracked Quantities . . . 124
7.5. Summary . . . 124
8. Micro-scale Product-Property Predictors in Fluidized Bed Spray Granulation of a Liquid Solution **127**
8.1. Experimental Procedure . . . 127
8.2. Product Roughness Quantification using Laser-Scanning Confocal Microscopy . . . 130
8.2.1. Post-Processing of Roughness Measurements . . . 130
8.2.2. Roughness Quantification . . . 132
8.3. Simulation Setup . . . 137
8.4. Relationship between Global Process Conditions and Tracked Quantities 141
8.5. Principal Component Analysis of Influence of Global Process Conditions and Tracked Quantities on Product Properties . . . 142
8.6. Derivation of a Mapping between Global Process Conditions and Particle Properties . . . 145
8.7. Derivation of a Mapping between Tracked Quantities and Particle Properties 147
8.8. Summary . . . 149

9. Application of the Product Property Prediction-Approach to Scale-Up 151
9.1. Experimental Design and Simulation Setup 151
9.2. Analysis of Hydrodynamics, Thermodynamics and Tracked Quantities in Scale-Up 154
9.3. Summary 161
10. Conclusion 163
Bibliography 167
A. CFD-DEM Modelling: Verification 175
A.1. Test Case Setup 175
A.1.1. Mass Transport and Conservation 175
A.1.2. Energy Conservation 177
B. Solution Granulation Case: Supplementary Data 181
C. Calculation of Thermophysical Properties in OpenFOAM 185
C.1. Calculation of the Density 185
C.2. Calculation of the Heat Capacity 185
C.3. Calculation of the Viscosity 186
Curriculum Vitae 187