



Paul Kieckhefen (Autor)
A Novel Method for Predicting Product Properties in Fluidized Bed Spray Granulation



<https://cuvillier.de/de/shop/publications/8575>

Copyright:
Cuvillier Verlag, Inhaberin Annette Jentsch-Cuvillier, Nonnenstieg 8, 37075 Göttingen,
Germany
Telefon: +49 (0)551 54724-0, E-Mail: info@cuvillier.de, Website: <https://cuvillier.de>

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