

Contents

Glossary	xxvii
1 Introduction	1
1.1 Motivation	2
1.2 Application examples	4
1.3 State-of-the-art in modeling open-porous structure formation	7
1.3.1 Comparison of numerical methods	7
1.3.2 Mesh-free methods	8
2 The Smoothed Particle Hydrodynamics Method	15
2.1 Basic Smoothed Particle formulations	15
2.1.1 Kernel approximation and kernel function	16
2.1.2 Discretization of the kernel approximation	18
2.1.3 Spatial derivatives of the kernel interpolation	21
2.1.4 Kernel functions and properties	23
2.2 Improved SPH derivatives for continuum mechanics	30
2.2.1 First order derivatives	30
2.2.2 Second order derivative	33
2.3 Consistency of the SPH approximation at boundaries	36
2.4 Boundary treatment within the SPH framework	41
2.5 Corrected SPH approaches	45
2.6 SPH discretization from Variational Principles	50
2.7 SPH algorithms for compressible and incompressible flow	53
2.7.1 Explicit SPH for compressible and weakly compressible materials	54
2.7.2 Incompressible SPH algorithm	56

3	Physical model and numerical solution	61
3.1	Governing equations	61
3.2	Numerical approach	67
3.2.1	The compressible–incompressible multiphase SPH algorithm	67
3.2.1.1	Spatial coupling of the multiphase algorithm	70
3.2.1.2	Time-stepping of the multiphase algorithm	73
3.2.2	Numerical model	76
3.2.2.1	Normalized Corrected SPH model	79
3.2.2.2	Normalized SPH model	93
3.2.3	Simplified treatment of the gaseous phase – the hybrid approach	103
3.2.4	Comparison with the state-of-the-art	107
3.2.5	Roundup of the NCSPH discretized equations	109
3.2.6	Roundup of the NSPH discretized equations	114
4	Validation and Verification	119
4.1	Validation and verification of the single phase algorithm	119
4.1.1	Heat conduction and treatment of free surface boundaries	119
4.1.2	Hydrostatic pressure in a channel with a free surface	129
4.1.3	Collapsing water column after dam break	136
4.1.4	Free surface flow of a fluid droplet	145
4.1.5	Stability of a fluid patch with a free surface	154
4.1.6	Interim conclusion	159
4.2	Verification of material models	160
4.2.1	Viscous material behavior	162
4.2.2	Viscoplastic material behavior	170
4.2.3	Viscoelastic material behavior	174
4.2.4	Elastic materials	186
4.2.5	Interim conclusion	198
4.3	Validation and verification of the multiphase algorithm	199
4.3.1	Hydrostatic pressure in a channel with a free surface	199
4.3.2	Multiphase Poiseuille flow of a viscous fluid	204
4.3.3	Rising gas bubble in a viscous fluid	208
4.3.4	Expansion of a gaseous bubble in a viscous substrate	214

4.3.5	Interim conclusion	223
5	Simulation of the morphogenesis of open-porous materials	225
5.1	Reaction-induced formation of a single open pore	226
5.1.1	Normalized Corrected SPH approach	226
5.1.2	Normalized SPH approach	230
5.1.3	The hybrid–NCSPH approach	234
5.1.4	Interim conclusion	241
5.2	Generation of an open-porous transport pore system	243
5.3	Influence of the polymer, solid and wax phase properties on the structure formation	246
6	Conclusion and outlook	249
6.1	Conclusion	249
6.2	Outlook	254
6.2.1	Possible future developments	254
6.2.2	Additional applications	255
A	Grid-based methods	259
B	Discussion of further particle methods	263
C	SPH discretization from Variational Principles	267
D	Transformation of coordinates	271
E	Corrected second order derivative	275
F	Semi-analytical solution of the evolution of the elliptic fluid drop	279
G	Algorithm for the reconstruction of the pore volume	281
H	Analytical solution of the bubble expansion	283
I	Derivation of balance equations	285