

Contents

Nomenclature	v
Zusammenfassung	xi
Abstract	xv
1 Introduction	1
2 Numerical approach: Smoothed Particle Hydrodynamics (SPH)	5
2.1 The interpolation	5
2.1.1 Kernel function	6
2.1.2 Discrete interpolation	8
2.1.3 Error estimation	9
2.1.4 Derivatives	10
2.1.5 Consistency	16
2.1.6 Corrected SPH	16
2.2 Conservation laws	18
2.2.1 The Euler equations	18
2.2.2 Linear momentum	19
2.2.3 Angular momentum	20
2.2.4 Mass	21
2.2.5 Energy	22
2.3 Time integration of the incompressible scheme	23
2.3.1 Euler scheme	24
2.3.2 Leap–Frog scheme	25
2.3.3 Time step criteria	25
2.4 Common forms of derivatives in the momentum balance	26

3	Two-phase model	31
3.1	Two-phase interface condition	33
3.2	Three-phase contact line condition	38
3.2.1	Wettability	38
3.2.2	State of the art models	42
3.2.3	Contact Line Force (CLF)	45
4	Present SPH model	51
4.1	Background	51
4.2	Navier–Stokes equations	52
4.3	Surface tension	53
4.4	Boundary conditions	56
4.4.1	Velocity boundary condition	57
4.4.2	Pressure boundary condition	62
4.4.3	Boundary condition for surface tension	63
4.5	Time integration by the predictor–corrector scheme	65
5	Verifications	69
5.1	Time integration scheme	69
5.2	Couette flow	74
5.3	Hagen–Poiseuille flow	76
5.4	Rayleigh–Taylor instability	79
5.5	Surface tension	81
5.5.1	Interfaces	81
5.5.2	Contact angles	84
6	Applications	95
6.1	Qualitative wettability simulations on curved solids	95
6.1.1	Determining equilibrium states in porous materials	95
6.1.2	Rising bubbles in porous structures	98
6.2	Primary bubble formation at an orifice	101
6.2.1	Background	101
6.2.2	Problem setup	105
6.2.3	Bubble detachment results	109

Bibliography 133

List of Figures 149

List of Tables 157