

# Content

<b>Acknowledgement .....</b>	<b>I</b>
<b>Abstract.....</b>	<b>III</b>
<b>Zusammenfassung .....</b>	<b>V</b>
<b>1      Introduction .....</b>	<b>1</b>
<b>2      Improvement of the applicability of d<sup>3</sup>f++ .....</b>	<b>5</b>
2.1     Governing equations for density driven flow in partially saturated media ...	5
2.2     Inverse modelling and calibration.....	6
2.2.1     Optimization algorithms.....	6
2.2.2     Numerical Experiments .....	12
2.3     Coupling with rivers .....	22
2.3.1     Saint-Venant Equations .....	22
2.3.2     Validation Experiments for Saint-Venant.....	22
2.3.3     Coupling of Surface and Subsurface .....	24
2.3.4     Complex river networks.....	26
2.4     Groundwater flow with phreatic surface in fractured media .....	26
2.5     Technical improvements .....	30
2.5.1     Restart with section of higher resolution .....	30
<b>3      Groundwater flow in permafrost conditions.....</b>	<b>31</b>
3.1     General remarks .....	31
3.2     Motivation.....	31
3.3     Relevant physics .....	34
3.4     Mathematical model .....	36
3.4.1     General remarks .....	36
3.4.2     Balance equations.....	37
3.4.3     Processes .....	39
3.4.4     Constitutive Equations .....	40

3.4.5	Equations of state .....	41
3.4.6	Amendments .....	41
3.4.7	Mathematical model for the INTERFROST benchmarks (The Game) .....	42
3.5	Implementation Aspects and Model Validation .....	44
3.5.1	TH2 Benchmark .....	45
3.5.2	TH3 Benchmark .....	47
3.5.3	Discussion .....	50
<b>4</b>	<b>Numerical improvements in d<sup>3</sup>f++ .....</b>	<b>51</b>
4.1	Improvement of the robustness of solvers/AMG-GMG-combination .....	51
4.2	Software integration and re-structuring .....	51
4.3	Stabilization of the level-set method .....	53
4.4	Phase-field modeling of phreatic groundwater surfaces .....	58
4.4.1	Unsaturated porous media .....	58
4.4.2	Capillary pressure .....	59
4.4.3	Retention curves .....	59
4.4.4	Relationship to the level-set method .....	61
4.5	Numerical Experiments .....	62
4.5.1	Henry test case .....	62
4.5.2	Seawater pumping .....	63
<b>5</b>	<b>Applications and benchmarks .....</b>	<b>65</b>
5.1	The Äspö Site Descriptive Model .....	65
5.1.1	Model geometries .....	65
5.1.2	Parameters, initial and boundary conditions .....	67
5.1.3	Simulation results .....	69
5.1.4	Summary .....	76
5.2	Kraví Hora groundwater model .....	77
<b>6</b>	<b>Summary .....</b>	<b>83</b>
	<b>References .....</b>	<b>87</b>

<b>Table of figures .....</b>	<b>95</b>
<b>List of tables .....</b>	<b>99</b>