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Parameterisation of an integrated groundwater-surface water model for hydrological analysis of boreal aapa mire wetlands

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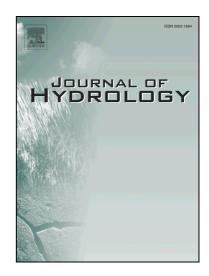
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Hydrological connections between aquifers and boreal mires need to be better understood for protection of this type of wetland. Three-dimensional (3D) models have so far been sparsely used for such systems. This study investigated the effect of parameterisation with global sensitivity analysis on groundwatersurface water (GW-SW) interactions in a boreal esker-aapa mire system. Sensitivity analysis by the elementary effect (Morris) method was applied to a 3D steady-state hydrological model built with the fully-integrated HydroGeoSphere code. Parameter sensitivity with respect to various model outputs was explored, providing comprehensive insights into the most hydrologically relevant parameters. The results indicated that depending on model outputs the most influential model parameters varied. They also revealed existence of feedback in terms of interdependence of parameters between the esker aguifer and surrounding aapa mires. The properties of the mire (or peatland) landscape affected groundwater levels in the unconfined aguifer and, conversely, esker-mire interactions depended on esker hydraulic characteristics. This implies that accurate representation of both systems is required and that reliable determination of GW-SW interactions may be impeded by parameter interactions. In this study, the van Genuchten functions were used to represent hydraulic properties of unsaturated flow domain and the results revealed that formal sensitivity analysis methods based on random sampling might not be appropriate for evaluating parametric sensitivity. If the van Genuchten parameters ranges are large, randomly sampled values may not always produce physically realistic water retention characteristics. Overall, our results demonstrate that the computationally efficient elementary effect method is a suitable tool for investigating the parametric sensitivity of integrated models, enhancing modelling of boreal groundwater-dependent ecosystems.

Table 1. Porous media domain parameter ranges used in the global sensitivity analysis (GSA).

Porous media Parameter Un domain	nit Abbreviation	Minimum value	Maximum value	Sources
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	Hydraulic conductivity K_{XY}	ms - 1	K_{XY_sand}	4.0×10^{-5}	1.0×10^{-2}	Pumping tests of the Kälväsvaara aquifer, unpublished $(n = 3)$
Sand	Anisotropy ratio K_{XY} : K_Z		A_{sand}	1	20	Freeze and Cherry (1979); Weeks (1969)
	Specific storage S_S	m - 1	S_{S_sand}	1.0 × 10 ⁻⁶	1.0×10^{-3}	Dingman (2002); Domenico and Schwartz (1998; Freeze and Cherry (1979)
	Porosity ϕ		ϕ_{sand}	0.25	0.53	Dingman (2002); Freeze and Cherry (1979)
	Residual saturation S_{wr}		S_{wr_sand}	0.03	0.8	Dingman (2002); Jauhiainen (2004. n = 18)
	van Genuchten α	m - 1	α_{sand}	1.1	80	Jauhiainen (2004. n = 18)
	van Genuchten β		β_{sand}	1.4	5.1	Jauhiainen (2004. n = 18)
	Minimum relative permeability $k_{r,min}$		$k_{r, \mathrm{min} _sand}$	1.0×10^{-27}	1.0×10^{-9}	Arbitrary value
	Hydraulic conductivity K_{XY}	ms - 1	K_{XY_till}	1.0 × 10 ⁻⁸	1.0×10^{-4}	Nieminen (1985);
	Anisotropy ratio $K_{XY}:K_Z$		A_{till}	0.2	20	Edwards and Jones (1993)
	Specific storage S_S	m - 1	S_{S_till}	1.0×10^{-4}	1.0×10^{-2}	Leap (1999)
	Porosity ϕ		ϕ_{till}	0.23	0.52	Bouwer (1978); Fetter (1994); Tielaite (1993)
Glacial till	Residual saturation S_{wr}		S_{wr_till}	0.08	0.8	Dingman (2002); Jauhiainen (2004. $n = 4$)
	van Genuchten α	m - 1	$lpha_{till}$	1.4	5.1	Jauhiainen (2004. $n = 4$)
	van Genuchten β		eta_{till}	1.5	2.4	Jauhiainen (2004. $n = 4$)
	Minimum relative permeability $k_{r,min}$		$k_{r, \mathrm{min} _till}$	1.0×10^{-27}	1.0×10^{-7}	Arbitrary value
	Hydraulic conductivity K_{XY}	ms - 1	K _{XY_high_K_peat}	1.9×10^{-4}	2.9×10^{-3}	Ronkanen and Kløve (2005)
	Anisotropy ratio K_{XY} : K_Z		$A_{high_K_peat}$	0.1	1000	Beckwith et al. (2003); Chason and Siegel (1986)
Ton nost	Specific storage S_S	m - 1	$S_{S_high_K_peat}$	1.0×10^{-3}	5.0×10^{-2}	Reeve et al. (2006)
Top peat layers (High K)	Porosity ϕ		φ _{high_K_peat}	0.8	0.99	Defined from unpublished data
	Residual saturation S_{wr}		$S_{wr_high_K_peat}$	0	0.66	Defined from unpublished data
	van Genuchten α	m - 1	$\alpha_{high_K_peat}$	1.5	37	Defined from unpublished data
	van Genuchten β		$eta_{high_K_peat}$	1.1	4.2	Defined from unpublished data
	Minimum relative permeability $k_{r,min}$		$k_{r,\min}$ _high_K_peat	1.0×10^{-27}	1.0×10^{-7}	Arbitrary value
	Hydraulic conductivity K_{XY}	ms ⁻¹	$K_{XY_low_K_peat}$	1.0×10^{-9}	1.0×10^{-5}	Ronkanen and Kløve (2005)
	Anisotropy ratio $K_{XY}:K_Z$		$A_{low_K_peat}$	0.1	10	Beckwith et al. (2003)
Bottom	Specific storage S_S	m ⁻¹	S _{S_low_K_peat}	1.0×10^{-3}	5.0×10^{-2}	Reeve et al. (2006)
peat	Porosity ϕ		$\phi_{low_K_peat}$	8.0	0.97	Defined from unpublished data
layers	Residual saturation S_{wr}		$S_{wr_low_K_peat}$	0	0.79	Defined from unpublished data
(Low K)	van Genuchten α	m - 1	$\alpha_{low_K_peat}$	1.1	7	Defined from unpublished data
	van Genuchten β		$eta_{low_K_peat}$	1.2	3.5	Defined from unpublished data
	Minimum relative permeability $k_{r,min}$		$k_{r, \min_low_K_peat}$	1.0×10^{-27}	1.0×10^{-7}	Arbitrary value
	Hydraulic conductivity K_{XY}	ms - 1	$K_{XY_drained}$	1.0×10^{-9}	1.0×10^{-5}	Mustamo et al. (2016)
Drained peatland	Anisotropy ratio $K_{XY}:K_Z$		$A_{drained}$	1	10	Beckwith et al. (2003)
	Specific storage S_S	m - 1	$S_{S_drained}$	1.0×10^{-3}	5.0×10^{-2}	Reeve et al. (2006)
	Porosity ϕ		$\phi_{drained}$	8.0	0.99	Defined from unpublished data
	Residual saturation S_{wr}		$S_{wr_drained}$	0	0.84	Defined from unpublished data
	van Genuchten α	m - 1	$\alpha_{drained}$	0.6	30	Defined from unpublished data
	van Genuchten β		$eta_{drained}$	1.05	2.9	Defined from unpublished data
	Minimum relative permeability $k_{r,min}$		$k_{r,\min_drained}$	1.0×10^{-27}	1.0×10^{-7}	Arbitrary value

n = number of samples.

Table 2. Overland flow domain and other parameter ranges used in the global sensitivity analysis (GSA).

^{*}One order higher value to represent sand lenses.

^{**}Peat van Genuchten parameters based on studies at the Water Resources and Environmental Engineering Research Unit, University of Oulu, Finland.

Overland flow domain	Parameter	Unit	Abbreviation	Minimum value	Maximum value	Sources
Forest	Manning's n	$m^{-1/3}$ s	n_{forest}	0.4	0.6	Jones et al. (2008); Smerdon et al. (2007)
	Rill storage height h_{RS}	m	h_{RS_forest}	0.05	0.15	Ala-aho et al., (2015a)
	Obstruction storage height h_{OS}	m	h_{OS_forest}	0.05	0.3 *	Ala-aho et al., (2015a)
	Coupling length l_e	m	l_{e_forest}	1.0×10^{-4}	1.0×10^{-1}	Ebel et al. (2009); Liggett et al. (2012)
Drained Peatlands	Manning's n	m ^{-1/3} s	$n_{drained}$	0.4	0.6	Jones et al. (2008); Smerdon et al. (2007)
	Rill storage height h_{RS}	m	$h_{RS_drained}$	0.01	0.15	Ala-aho et al., (2015a)
	Obstruction storage height h_{OS}	m	$h_{OS_drained}$	0.01	0.3 *	Ala-aho et al., (2015a)
	Coupling length l_e	m	$l_{e_drained}$	1.0×10^{-4}	1.0×10^{-1}	Ebel et al. (2009); Liggett et al. (2012)
Pristine peatlands	Manning's n	$m^{-1/3}$ s	$n_{natural}$	0.01	0.1	Bolger et al. (2011); Frei and Fleckenstein (2014); Jones et al. (2008)
	Rill storage height h_{RS}	m	$h_{RS_natural}$	0.01	0.5	Bolger et al. (2011); Seppä (2002)
	Obstruction storage height h_{OS}	m	$h_{OS_natural}$	0.01	0.2	Bolger et al. (2011); Luoto and Seppälä (2002)
	Coupling length l_e	m	$l_{e_natural}$	1.0×10^{-4}	1.0×10^{-1}	Ebel et al. (2009); Liggett et al. (2012)
Channels	Manning's n	$m^{-1/3}$ s	$n_{channel}$	0.01	0.05	Bolger et al. (2011); Jones et al. (2008); Pérez et al. (2011); Smerdon et al. (2007)
	Rill storage height h_{RS}	m	$h_{RS_channel}$	0.01	0.15	Ala-aho et al., (2015a); Bolger et al. (2011)
	Obstruction storage height h_{OS}	m	$h_{OS_channel}$	0.01	0.3	Site specific estimate
	Coupling length l_e	m	$l_{e_channel}$	1.0×10^{-4}	1.0×10^{-1}	Ebel et al. (2009); Liggett et al. (2012)
Other parameter s	Effective rainfall	mm	P_{eff}	310	410	Ranges determined from meteorological data and evapotranspiration estimates by Ala-aho et al., (2015a); Vakkilainen (1986); Solantie and Joukola (2001)
	Depth of the interface between peat layers of high and low hydraulic conductivity K_{high_Kpeat} and $K_{low_K_peat}$	m	$d_{low_K_peat}$	0.5	1	Estimated from Isokangas et al. (2017)

^{*}Approximate height of blueberry/lingonberry bushes

Table 3. The most influential and most interactive/non-linear parameters for various types of outputs, based on the ranked values of the Morris μ^* and σ . The numbers in brackets indicate how many times the parameter was ranked as one of the five most important parameters.

	Groundwater levels	Lakes	Fluxes	Springs	Discharges and predefined reaches	Saturation degree of peat surface*
	$K_{XY_sand}(47)$	$K_{XY_sand}(4)$	$K_{XY_sand}(4)$	$A_{till}(7)$	$K_{XY_till}(48)$	$K_{XY_high_K_peat}(14)$
r ffi	$A_{sand}(46)$	$A_{sand}(4)$	$A_{sand}(3)$	$A_{high_K_peat}(6)$	$A_{high_K_peat}(44)$	$A_{high_K_peat}(14)$
uential ieter	$A_{\text{high_K_peat}}(33)$	$K_{XY_till}(4)$	$A_{till}(2)$	$K_{XY_till}(4)$	$A_{till}(33)$	$S_{wr_high_K_peat}(14)$
in fj	$\alpha_{\mathrm{high_K_peat}}(29)$	$\alpha_{high_K_peat}(4)$	$A_{high_K_peat}(2)$	$h_{RS_natural}(4)$	$K_{XY_sand}(28)$	$\beta_{high_K_peat}(14)$
Most par	$\alpha_{sand}(22)$	$K_{XY_high_K_peat}(2)$	$K_{XY_low_K_peat}$ (2)	$h_{OS_natural}(4)$	$K_{XY_low_K_peat}(23)$	$\alpha_{high_K_peat}(13)$
=	$K_{XY_till}(17)$	$A_{high_K_peat}(2)$	$A_{drained}(2)$	$l_{e_forest}(3)$	$l_{e_channel}(15)$	$K_{XY_drained}(6)$

	$K_{XY_drained}(16)$ $\beta_{sand}(9)$ $K_{XY_low_K_peat}(7)$ $A_{till}(5)$ $A_{drained}(3)$ $\beta_{high_K_peat}(1)$	$lpha_{sand}(1)$ $A_{till}(1)$ $K_{XY_low_K_peat}(1)$ $h_{RS_forest}(1)$ $l_{e_{forest}}(1)$	$lpha_{sand}(1)$ $lpha_{high_K_peat}(1)$ $eta_{highKpeat}(1)$ $K_{XY_{drained}}(1)$ $P_{eff}(1)$	$h_{RS_channel}(3)$ $n_{natural}(2)$ $\beta_{high_K_peat}(1)$ $h_{RS_{forest}}(1)$	A_{sand} (9) $K_{XY_high_K_peat}$ (9) $K_{XY_high_K_peat}$ (5) $R_{high_{K_peat}}$ (5) $R_{natural}$ (5) R_{sand} (4) $R_{s_natural}$ (4) $R_{s_natural}$ (3) $R_{s_natural}$ (3) $R_{s_natural}$ (3) $R_{s_natural}$ (2) $R_{s_natural}$ (1)	$S_{Wr_drained}(6)$ $\alpha_{drained}(6)$ $\beta_{drained}(6)$ $A_{drained}(5)$ $K_{XYtill}(2)$
	$K_{XY_sand}(47)$ $A_{sand}(43)$ $A_{high_K_peat}(30)$ $\alpha_{highKpeat}(29)$	K _{XY_sand} (4) A _{sand} (4) α _{high_K_peat} (4) K _{XY_high_K_peat}	$K_{XY_sand}(4)$ $A_{till}(3)$ $A_{sand}(2)$ $A_{high_K_peat}(2)$	A _{till} (6) A _{high_K_peat} (6) K _{XY_till} (4) h _{RS_natural} (4)	$K_{XY_till}(46)$ $A_{hlgh_K_peat}(43)$ $A_{till}(36)$ $K_{XY_sand}(27)$	A _{high_K_peat} (15) K _{XY_high_K_peat} (14) S _{wr_high_K_peat} (14) β _{high_K_peat} (14)
Most non-linear /interactive parameters	α _{sand} (19) K _{XY_till} (19) K _{XY_drained} (18) β _{sand} (12) K _{XY_low_K_peat} (7) A _{till} (5) A _{drained} (3) β _{high_K_peat} (2) K _{high_K_peat} (1)	(3) $K_{XY_till}(2)$ $\alpha_{sand}(1)$ $A_{till}(1)$ $A_{high_K_peat}(2)$ $K_{XY_low_K_peat}(1)$ $K_{XY_drained}(1)$ $\theta_{r_drained}(1)$ $h_{OS_forest}(1)$ $l_{e_forest}(1)$	$\alpha_{high_K_peat}(2)$ $K_{XY_low_K_peat}(2)$ $A_{drained}(2)$ $\alpha_{sand}(1)$ $\beta_{high_K_peat}(1)$ $\alpha_{drained}(2)$	hos_natural(4) le_forest(3) h _{RS_channel} (3) βhigh_K_peat(2) n _{natural} (2) h _{RS_forest} (1)	KχY_low_K_peat(20) le_channel(17) KχY_high_Kpeat(11) KχY_drained(10) Asand(6) αsand(5) nnatural(5) hRS_natural (5) βhigh_K_peat(4) hOS_natural(4) le_forest (3) αhigh_K_peat(2) nchannel(2) hRS_channel(2) αtill(1) Alow_K_peat(1) Adrained(1) hRS_drained(1) le_drained(1) hOS channels(1)	$\alpha_{high_K_peat}(12)$ $K_{XY_drained}(6)$ $S_{wr_drained}(6)$ $\alpha_{drained}(6)$ $\beta_{drained}(6)$ $A_{drained}(3)$ $\alpha_{sand}(2)$ $K_{XY_till}(2)$

^{*}Six observation points in drained peat (3 Leväsuo, 3 Olvassuo) and 14 observation points in the mire area (7 Leväsuo and 7 Olvassuo).

Highlights

- Parametric sensitivity of a fully-integrated hydrological model was evaluated
- Morris method provided insights on modelling esker-mire systems at wetland scale
- Hydraulic conductivity and anisotropy dominated flow processes in the system

- Groundwater levels and fluxes to mire are coupled through their hydraulic properties
- Study promote use of integrated models for groundwater/ecosystem management

1. Introduction

Boreal aapa mires, also referred to as patterned fens, are typical groundwater-dependent, large-scale wet fens occurring mainly in central and northern boreal zones of Fennoscandia (Laitinen et al., 2005; Pakarinen, 1995), north-western Russia (Botch et al., 1995; Yurkovskaya, 2012), Canada (Vitt et al., 2000) and Alaska (Bedford and Godwin, 2003). Aapa mires are characterised by vast treeless massifs and a specific pattern of ponds, wet flarks and dry hummocky strings (Seppä, 2002). They are often connected to glaciofluvial eskers, which are the most important type of groundwater aquifers in Finland (Katko et al., 2006) and in the entire Fennoscandia area (Knutsson, 2008). Current water policy in the study area promotes the use of groundwater and puts pressure on the ecologically sensitive groundwater-dependent mires and other groundwater-dependent ecosystems located within the aquifer area, such as lakes and springs (Britschgi et al., 2009). Climate change adds to the demand for a better understanding at 'ecosystem scale'.

Understanding the hydrology of groundwater-dependent ecosystems requires a thorough understanding of groundwater-surface water relationships (Barthel and Banzhaf, 2016; Kalbus et al., 2006; Winter et al., 1998). Such interactions occur not only in boreal landscapes but in nearly all landscapes and climates, at a wide range of scales (Winter et al., 1998). Despite this, few studies have addressed the interactions between groundwater (GW) and surface water (SW) at larger or regional scales (≥100 km²) (Barthel and Banzhaf, 2016). Most existing knowledge is based on small-scale experimental studies and point measurements, without including the link to aquifers or catchments as an integral part of the ecosystem.

This is often the case for studies of esker-mire landscapes; accurate characterisation of GW-SW interactions in aapa mire complexes is challenging due to the large spatial extent, remoteness and heterogeneity of the mires, increasing the importance of modelling when studying these landscapes.

Fully-coupled physically-based modelling is a unique tool to explore GW-SW interactions at various scales. This modelling approach describes all major processes of the hydrological cycle occurring in overland flow and variable saturated porous domains using physics-based descriptions, while at the same time avoiding implementation of artificial interfaces between surface and subsurface. These features make the fully-integrated modelling approach particularly useful for studying spatially distributed GW-SW interactions at regional scales. The most commonly used models include ParFlow (Kollet and Maxwell, 2006), HydroGeoSphere (Aquanty, 2015), CATHY (Camporese et al., 2010), PAWS (Shen and Phanikumar, 2010) and OpenGeoSys (Kolditz et al., 2012).

The current main drawbacks of fully-integrated models include long execution times (Goderniaux et al., 2009; von Gunten et al., 2014) and lack of spatially and temporary distributed data required for proper model domain representation, parameterisation and calibration (Barthel and Banzhaf, 2016; Semenova and Beven, 2015). Long computing times constrain the spatial and temporal resolution of such models (Goderniaux et al., 2009) and make the application of automated calibration techniques infeasible. These downsides hamper application, especially at larger scales encompassing wetlands as ecosystems. Due to advances in computer resources, it has become possible to partly overcame these drawbacks by combining extensive computational power of high performance computing with formal sensitivity analysis, automated calibration and uncertainty estimation methods (Bürger et al., 2012; Kurtz et al., 2017; Miller et al., 2018). The role of sensitivity analysis is to identify the key parameters that affect model performance and add most to the uncertainty of the model outputs. It is widely agreed that

sensitivity analysis methods should be an integral part of hydrological modelling studies as one of the steps to produce high quality models (Shin et al., 2013; Song et al., 2015). In particular, global sensitivity analysis (GSA) techniques facilitate hydrological model parameterisation, calibration and uncertainty quantification by reducing the number of parameters that need to be considered (see e.g. Anderson et al., 2015; Doherty, 2015; Hill and Tiedeman, 2007). In comparison with simpler local sensitivity techniques, the GSA methods do not assume model linearity, allow interactions between parameters to be characterised and aim to cover completely relevant parameter space. However, the use of such techniques in fully-integrated physically-based modelling has been limited to date by long computational times for this type of model and large amounts of model parameters. The latter results in a multi-dimensional space to investigate and a large amount of samples to run, which are the primary reasons for the very few GSA applications. To our knowledge, only two studies have implemented GSA into a fully-integrated physically-based models: the regional scale study for the Santa Fe River basin conducted by Srivastava et al. (2014) and reach-scale investigation of river-groundwater interface by Munz et al. (2017). Otherwise, there is a general tendency to use local sensitivity measures (e.g. von Gunten et al., 2014; Wildemeersch et al., 2014).

The main objective of this work was to enhance modelling of aapa mires in order to better understand the hydrology of these systems. We investigated the effect of parameterisation of esker aquifer and an aapa mire complex and sought to identify the parameters that need most attention in the calibration process. We also examined how a qualitative GSA method can be applied to a conceptually expensive fully-integrated model. The effects of parameter relevance on esker-aapa mire interactions were investigated for a case study of the protected and well-preserved Olvassuo aapa mire system, a Natura 2000 site, using the fully-integrated surface-subsurface software HydroGeoSphere (Aquanty, 2015). The parametric sensitivity of the various model outputs was evaluated using an elementary effects method

known in the literature as the Morris method (Morris, 1991). Due to limited data availability, we focused on steady-state investigation and representation of overland and subsurface properties by simple zonation of the model domain that could serve as a starting point for further transient state simulations.

2. Materials and methods

2.1 Study site

The study area, the Kälväsvaara esker aquifer and the adjacent Olvassuo and Leväsuo aapa mire complexes, is located in Northern Finland (**Fig. 1**). The site is situated in the temperate coniferous-mixed forest zone, characterised by cold, wet winters according to the Köppen climate classification (Kersalo and Pirinen, 2009). Mean annual temperature in the region is around 1.4 °C (Finnish Meteorological Institute, 2016a), mean annual precipitation is 585 mm (Finnish Meteorological Institute, 2016b) and mean annual potential evapotranspiration is estimated to be around 235-300 mm (Ala-aho et al., 2015b; Solantie and Joukola, 2001; Vakkilainen, 1986).

Fig. 1.

The Olvassuo mire complex (~60 km²) is mainly in pristine state, although some parts of the wetland were drained for forestry cultivation in the late 1960s (Heikkilä and Lindholm, 1997) and 1970s (Rehell and Tahvanainen, 2006), but have been partly restored during recent years (Rehell, 2013). In contrast, the Leväsuo mire has been drained to a greater extent, but some of the open mire areas have remained in pristine state. Both complexes have typical structures of southern aapa mires, i.e. their marginal zones are dry pine mires with relatively thin peat layers (a few centimetres) and the main massifs are wet flark fens with moderately to weakly decomposed peat several metres deep (Rehell and Tahvanainen, 2006). The peat layer thickness in both mires extends to 5 m (Rundelin, 1999), with average thickness ~1.35 m

(Geological Survey of Finland, 2015; Rundelin, 1999). The mineral soil below the peat is relatively uniform and consists mainly of glacial till, but sand deposits in the western part of Leväsuo (Geological Survey of Finland, 2015) indicate that the aquifer stretches out under the peat beyond the aquifer borders. The bedrock below the wetlands is shallow, with depth ranging from zero (exposures) to over 15 (mean depth 7.5 m.

The Kälväsvaara aguifer is a complex unconfined esker with a recharge area of 14.47 km² (Finnish Environmental Institute, 2014). The majority of groundwater discharge from the Kälväsvaara esker occurs by diffusive upwelling (Heikkilä et al., 2001; Maa ja Vesi Oy, 1993; Natura Borealis Oy, 1995; Rehell and Tahvanainen, 2006), but several springs emerge from the outskirts of the aquifer. The aquifer is covered by Scot pine stands and rises 50 m above the surrounding peatland landscape, to 180 m a.s.l. at its highest (National Land Survey of Finland, 2014a). The esker area includes numerous kettle holes, the majority of which are dry, but a few small lakes and fens intersperse the main esker body. The study area also includes the small Kokkomaa esker, with a recharge area of 0.71 km² (Finnish Environmental Institute, 2014), situated north of the western-most part of the Kälväsvaara aquifer. The Kokkomaa aguifer does not supply water to the Olvassuo mire, but rather drains water from the aapa mire towards the lake Iso Olvasjärvi (Heikkilä et al., 2001). The mineral soil of the Kälväsvaara esker consists predominantly of interspersed layers of sand, gravel and boulders, but numerous glacial till and silt lenses are also present (Rehell and Tahvanainen, 2006). These low hydraulic conductivity layers create some local perched watertables that feed temporal springs and the lake Pieni Kirkaslampi (Fig. 1). Overall, the stratigraphy of the aquifer is complex and large-scale continuous hydrological units have not been defined. Previous surveys indicate that groundwater flow in the esker is partly disconnected by bedrock features (Natura Borealis Oy, 1995).

Owing to the plan for using the Kälväsvaara aquifer for the water supply of the nearby city of Oulu (Rantala et al., 2014) and protection of the Olvassuo and Leväsuo areas under Natura 2000 and national protection programmes, the esker and the adjacent peatlands have been relatively well surveyed. The geology of the site has been investigated using various geophysical methods, including seismic refraction/reflection measurements (Ahonen et al., 1999; Maa ja Vesi Oy, 1993), gravimetric measurements (Ahonen et al., 1999) and ground-penetrating radar (GPR) measurements (Rundelin, 1999). In addition, extensive shallow and deep boreholes have been drilled to complement geophysical measurements and to define aquifer transmissivity properties through pumping tests. The hydrological monitoring of the site has been mainly conducted by the Centre for Economic Development, Transport and the Environment of North Ostrobothnia. The available hydrological dataset used in this study includes:

- water level measurements of the eight largest lakes and ponds (1989-2012; 19-68 observations per lake; median=28 measurements)
- manual groundwater observations from 48 groundwater pipes (2001-2015; 20-48 measurements per pipe; median=32 measurements)
- discharge gauging at the eight major springs (1992-2015; 1-36 observations per spring; median=3 observations)
- discharge from main streams/ditches (few measurements in 2000-2001 and 2015-2016; 1-4 observations per site; median=2 observations).

The temporal coverage of this dataset is irregular, restricting the functionality of data for transient state simulations. For a more detailed description of the data, see Supplementary Materials, Section 1.

2.2 Numerical model

Analysis of the effect of parameterisation on GW-SW interactions was conducted with the fully-integrated physically-based code HydroGeoSphere (HGS; Aquanty, 2015). In this control-volume finite-element model, the subsurface flow equations (three-dimensional (3D) modified Richard's equation; Richards, 1931) and overland flow equation (2D diffusion-wave Saint-Venant approximation) are solved simultaneously in a fully implicit manner. This allows direct representation of feedbacks between porous domain and surface domain, thus enabling genesis of surface water body features, i.e. rivers and lakes are formed in topographical depressions in a physically-based manner, without use of additional predefined boundary conditions (Brunner and Simmons, 2012).

A 3D steady-state numerical model for the Olvassuo and Kälväsvaara study area was developed using information from previous surveys and geographical datasets available for the region. The conceptual cross-section of the study site is presented in **Fig. 2.** The model borders were defined using natural boundaries, i.e. lakes, streams and rivers and natural water divides (see **Fig. 1**). In addition to the esker and close surroundings, the model domain comprised the whole Olvassuo mire massif and a major part of the Leväsuo aapa mire south of the esker. This allowed us to treat the model area as a hydrological entity.

Fig. 2.

The delineated model area (107 km^2) was discretised into a 2D triangular element mesh comprising 22 668 elements and 11 506 nodes. The size of elements varied within the mesh, with a more refined grid containing the esker recharge areas, streams, lakes and the areas surrounding predefined groundwater wells. The mesh was used to build a 3D 7-layer triangular prism grid for the subsurface flow domain and to define the 2D overland flow domain. The undersides of the five top model subsurface

layers followed the surface topography at depths of i) 0.05 m, ii) 0.1 m, iii) 0.25 m, iv) the depth of the interface between hydrologically active high hydraulic conductivity (K) layer and low K layer (see explanation below) and v) 1.35 m (the average depth of peat within the area). The remaining sediment thickness was subdivided vertically, to create two layers of proportions vi) 34% and vii) 66%. Hydraulic properties of pristine peat show significant vertical variation, with low K values in highly decomposed layers at the bottom of peat column and significantly higher values in the top peat layers (Boelter, 1968; Päivänen, 1973). Thus, realistic modelling of peatland hydrology can be accomplished by differentiation of at least two layers to adequately represent pristine peat characteristics. Here, the higher hydraulic conductivity zone consisted of the four top layers of the grid (referred to hereafter as top peat) and the low hydraulic conductivity zone consisted of the fifth layer (referred to hereafter as bottom peat). The depth of the transition from highly decomposed to highly conductive porous peat varies in various mire systems and climate zones. Because of unknown depth of the interface, we treated the variable as one of the parameters for the GSA by varying the thickness of the fourth and fifth layers of the grid.

Fig. 3.

The bedrock topography (**Fig. 3a**) was defined by combining the results from previous geological surveys and bedrock outcrop information from basic maps (National Land Survey of Finland, 2014b). The surface elevation of the model domain (**Fig. 3b**) was defined by combining 2 m x 2 m Lidar-based data (available only for the Olvassuo area) and 10 m x 10 m conventional digital elevation models (DEMs) provided by the National Land Survey of Finland (2014a, 2014c). The use of combined DEMs can introduce topographical artefacts into the 'connection' zone, due to differences in measurement accuracy. However, it was assumed that the benefits of using a 2 m x 2 m DEM for the Olvassuo mire would significantly outweigh the error related to lower accuracy of a 10 m x 10 m DEM. Node elevations within

surface water bodies (major streams and lakes) were adjusted to represent more realistically the actual land surface. This was done either using available bathymetry data or by lowering the land elevation within the lakes and ponds by 6 m (the average lake depth in Finland). The nodes within streambeds were moved 0.5 m downwards and smoothed manually.

The model domain was divided into zones representing the most relevant soil and vegetation features for subsurface and overland media (**Fig. 3c** and **Fig. 3d**). The zonation scheme applied used fewer parameters, shortening the total computation time required. The relationships between pressure head ψ , saturation S_w and relative permeability k_r of various soils were specified using the following van Genuchten-Mualem functions (Mualem, 1976; van Genuchten, 1980):

$$S_w = S_{wr} + (1 - S_{wr})[1 + |\alpha\psi|^{\beta}]^{-\nu} \quad \text{for } \phi < 0$$

 $S_w = 1 \quad \text{for } \phi > 0$ (1)

$$k_r = S_e^{(l_p)} \left[1 - \left(1 - S_e^{1/\nu} \right)^{\nu} \right]^2 \tag{2}$$

where l_p is a dimensionless pore connectivity parameter (here we used 0.5, i.e. the typical value for most soils), S_{wr} represents residual water saturation and S_e indicates effective saturation, defined as:

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} \tag{3}$$

where α and β are experimentally defined parameters and parameter ν is defined in relation to β as:

$$\nu = 1 - \frac{1}{\beta}, \beta > 1 \tag{4}$$

The van Genuchten-Mualem model is one of the most widely used empirical formulae describing unsaturated soil hydraulic properties and it has been found to closely fit the measurement data for a wide range of unstructured mineral soils (Leij et al., 1997). The performance of unimodal van Genuchten-Mualem models is often found to be inferior for peat soils, due to their structural complexity (Weber et al., 2017), presence of macropores (Dettmann et al., 2014) and mire breathing phenomenon (Camporese et al., 2006). However, the hydraulic functions have been previously applied in integrated models to peat soils with good results (Ala-aho et al., 2017, 2015a; Haahti et al., 2016).

The constant head boundary conditions with values of the average surface water levels were assigned to the subsurface domain restricted by lakes (**Fig. 1**). Other segments of the model perimeter and the bottom of the domain (impermeable bedrock) were described as no flow boundaries. For the surface domain, we used critical depth boundary conditions to allow water to freely leave the model domain. In addition, we applied effective rainfall (mean annual precipitation minus estimated actual evapotranspiration) as a constant flux boundary condition to incorporate into the model the effect of evapotranspiration. It is clear that this lumped treatment of evapotranspiration does not represent correctly differences between loss of vapour in forested and peatland landscapes. However, the conflicting literature regarding quantification of evapotranspiration in peatlands restricted reliable partitioning of the area into evapotranspiration zones (as discussed briefly by e.g. Drexler et al., 2004; Mitsch and Gosselink, 2007; Wu et al., 2010). Therefore, we treated effective precipitation in a lumped manner as one of the parameters for the GSA. Steady-state conditions were accomplished by applying unchanged boundary conditions for a long period of 1000 years.

2.3 Global sensitivity analysis method and applied procedure

In order to study the effect of parameterisation on model output, we selected the elementary effects method called also Morris approach (Morris, 1991). It is a qualitative global sensitivity approach suitable for screening large models (Campolongo et al., 2007; Herman et al., 2013). In contrast to quantitative methods, the main aim of screening techniques is not to quantify the overall effect that the parameters have on the model output, but to identify a few parameters that have a substantial influence on the model results, using a relatively small number of model evaluations. This method allows identification of the most crucial parameters in respect of the model's predictive response that require further measurements or calibration, whereas the identified insensitive parameters can be fixed at any value within the evaluated range without significantly affecting model outputs (Saltelli et al., 2004). Despite relatively low coverage of the input space in comparison with quantitative methods, previous studies (Herman et al., 2013; Shin et al., 2013; Wainwright et al., 2014, 2013) have shown that the results of elementary effects analysis are consistent with output of the variance-based Sobol method (Sobol', 1993).

The elementary effects analysis is a one-factor-at-a-time method. The core of the analysis comprises repeatedly calculating so-called elementary effects EE_i in the whole k-dimensional input space domain sampled in p-level grid (usually equal 4). The elementary effect of the model y with k parameters is defined for ith parameter as:

$$EE_{i} = \frac{y(x_{1}, x_{2}, ..., x_{i-1}, x_{i} + \delta_{i}, x_{i+1}, ..., x_{k})}{\delta_{i}} - \frac{y(x_{1}, x_{2}, ..., x_{i-1}, x_{i}, x_{i+1}, ..., x_{k})}{\delta_{i}},$$
(5)

where δ is a multiple of 1/(p-1). To obtain r elementary effects for each parameter, r trajectories are formed by randomly altering each successive parameter by a fixed δ . The global relative importance of each factor is then assessed by analysis of the distribution of r elementary effects EE_i by calculating mean μ_i and standard deviation σ_i for each parameter. A strong influence of the input parameters on the output of model is indicated by high mean μ_i , whereas a high value of σ_i is a sign that the parameter

induces a significant non-linear effect on the model output or is involved in interactions with other parameters. In order to include the effect of model non-monotonicity, Campolongo et al. (2007) proposed a new measure μ_i^* , used in this work, defined as a mean of absolute elementary effects:

$$\mu_{i}^{*} = \frac{1}{r} \sum_{j=1}^{r} |EE_{i}^{j}|. \tag{6}$$

The elementary effects approach is a computationally cheap method, requiring only n = r(k + 1) model evaluations. According to previous studies, using 10 to 20 trajectories is usually sufficient to provide valuable insights (Campolongo et al., 2007, 1999; Campolongo and Saltelli, 1997; Herman et al., 2013). However, Ruano et al. (2012) showed that in some cases a greater amount of trajectories is required due to very high non-linearity of the model or large uncertainty of model input. A common practice to analyse the results of elementary effects method is to present the results visually in the form of μ_i or μ_i^* versus σ plots, so-called Morris plots.

The global sensitivity analysis was performed for the whole model space of 58 parameters. This included all model parameters concerning porous zone and surface zone properties, as well as two model inputs: effective rainfall and depth of the interface between peat layers of high and low hydraulic conductivity K_{high_Kpeat} and $K_{low_K_peat}$. Running a large-scale physically-based model numerous times is a computationally demanding task. To decrease the total time required, we ran all sets on the supercluster of CSC Computing Services of Finland and the elementary effects method was implemented using the numerical computing environment MATLAB. Furthermore, we applied several enhancements to speed up the analysis. First, to decrease the number of model evaluations required for the sensitivity analysis and to reduce the computational burden, we narrowed the investigated parameter ranges by excluding

physically non-feasible values from the GSA. The upper and lower bounds for each parameter were defined using a wide range of values found in the literature, or computed using experimental data. To better capture the site-specific parameter variability of the boreal site, we prioritised the results of local/regional studies and measurements conducted in Finland and other high-latitude areas. The assigned parameter ranges are presented in **Table 1** for subsurface domain and in Table 2 for the overland flow domain. In a few cases, information on parameter variability was not available, and then we defined reasonable hydrological value ranges. Note that the effect of simplified process representation was not accounted for in the predefined ranges.

The second step is sampling of parameter space. This step is crucial for applying any formal GSA. Multiple sampling methods to enhance the elementary effects method for applications involving large models have been proposed (e.g. Campolongo et al., 2007; Khare et al., 2015; Ruano et al., 2012; Xiao et al., 2016). However, as little evidence exists on the superiority of any of these methods for models with very large amounts of parameters, we decided to apply the original sampling method proposed by Morris (1991) based on random generation strategy, due to its low time requirements and simplicity. Sampling consisted of r = 20 trajectories and four p-levels corresponding to the 12.50^{th} , 37.50^{th} , 62.50^{th} and 87.50^{th} quantiles (Saltelli et al., 2004). For any parameter that varied by more than two orders of magnitude, e.g. hydraulic conductivity, coupling length was first transformed to logarithmic scale before sampling.

Table 4

Table 2

We then applied the model for the $\left\lceil \frac{k+1}{2} \right\rceil$ sample of each trajectory to decrease the total evaluation time. The solutions were used as the initial conditions for other samples within the same trajectory. In this way, we attempted to ensure that initial conditions were relatively close to samples of each trajectory. For a

few trajectories, we did not obtain any solution during the computing time permitted by the supercluster settings. For these trajectories, we decided to use the output of the model computed for average parameter

values.

The running time of various parameter sets varied significantly depending how far the initial conditions were from obtained steady-state solution and the overall effect of parameters on model behaviour. Each parameter set was allowed to run on the supercluster for the maximum period of three days defined as the default maximum run time of the supercluster. Models that did not converge in this period were assumed to be flawed and were excluded from the analysis. The reasons for poor convergence are further discussed in the section 4.3 of this paper.

After running all parameter sets, the elementary effects were evaluated for various outputs in order to determine the most relevant parameters for various variables that may be of interest to modellers. The elementary effects for each output type were assessed at multiple locations, in order to analyse the spatial variability associated with each type of variable. Groundwater level outputs and part of discharge observation points were positioned in the actual monitoring locations, in order to compare them later with the measured data. In total, the parametric sensitivity was evaluated at 133 outputs corresponding to i) the locations of the actual monitoring wells (47 outputs), ii) lakes (5 outputs), iii) fluxes between esker and major peatland areas (4 outputs: Olvassuo, Leväsuo, Hetesuo and Hongansuo), iv) springs (7 outputs), v) other locations of discharge measurements (6 outputs) and predefined reaches of major

streams located every 500 m (43 outputs) and vi) saturation of the predefined observation points within natural (14 outputs) and drained areas (6 outputs) of the Olvassuo and Leväsuo peatlands. The exact locations of the output points are presented in Supplementary Materials **Fig. S5** and **Fig. S6**.

Finally, model performance for each set was evaluated using root mean square error (RMSE) values between the simulated outputs and available monitoring data for hydraulic pressure (measured from groundwater wells) and lake levels (excluding the known perched lake Pieni Kirkaslampi). The best model in terms of the minimum RMSE of groundwater and lake levels and fulfilling the chosen saturation threshold for peatland areas was further investigated and served as a base to calibrate the model by refining the most sensitive parameters by trial-and-error method. The threshold value for saturation was set at 80%, based on the knowledge that the peatlands at the site are in nearly saturated state. The RMSE for stream and spring data was also calculated, but not used as a performance criterion due to poor temporal data coverage (see Supplementary Materials: Section 1).

3. Results

3.1 Model performance

The best model in terms of the lowest RMSE and fulfilling saturation criteria produced a reasonable fit with measured data. The model was further refined by adjusting the hydraulic conductivity and anisotropy ratio of sand $K_{XY_{sand}}$ and A_{sand} i.e. parameters found to be most sensitive for groundwater and lake water levels. The calibrated groundwater and lake level hydraulic heads versus measured data are shown in **Fig 4** and the calibrated parameter values are presented in **Supplementary Tables S4** and **S5.** In the refined model, the RMSE for lakes and groundwater was equal to 1.91 m and mean residual error (MRE) was 0.04 m. The model produced a physically realistic esker-mire system; for peatland

areas the saturation varied from 93% to 100%, and the groundwater levels followed the topographical gradient in the area (**Fig. 5**). In terms of GW-SW interactions, the simulated exchange fluxes formed a complex pattern; the groundwater discharge was mostly localized in the proximity of the esker borders, especially areas in which hydraulic gradient was found to be steep. However, the GW-SW exchange was not only limited to the esker boundaries but occurred also in more central parts of both peatlands. The locations of groundwater discharge corresponded to the previous field observations presented by Heikkilä et al. (2006) and Rehell (2013) and are in line with the tracer study quantifying spatial groundwater dependence in boreal peatland by Isokangas et al. (2017). The simulated groundwater table within peatlands was predominantly shallow and in around 30% of the model peatland areas groundwater level was equal or higher than land elevation which is common in wet aapa mire environments (Laitinen et al., 2007; Tahvanainen, 2011)

Fig 4.

Fig 5.

A summary of the parameters found to be most influential and most involved in model non-linear behaviour/interaction (**Table 3**) clearly illustrated that the constructed model was sensitive to a wide range of parameters, especially in respect of the various model outputs. In most cases, the most influential parameters were also found to be the most non-linear/interactive. From 1180 sets tested, 1114 simulations converged during the running time permitted by the cluster maximum running time of three days. All results of converged simulations were used to compute elementary effects measures μ^* and σ for predefined outputs. The model output locations, computed elementary effects μ^* and σ_i and their

rankings from the largest to the smallest, and examples of Morris plots for various types of outputs are presented in Supplementary Materials.

Table 3.

3.2 The most important parameters for modelling GW-wetland interactions

The results of the GSA indicated that the groundwater levels within the Kälväsvaara aquifer were strongly controlled by sand hydraulic properties, with the greatest impact from the hydraulic conductivity of sand K_{XY_sand} , the van Genuchten parameters α_{sand} and β_{sand} , and sand anisotropy ratio A_{sand} . In addition, the groundwater levels were sensitive to the parameters of the drained peatlands (hydraulic conductivity $K_{XY_drained}$ and anisotropy ratio $A_{drained}$) and pristine mires ($A_{high_K_peat}$, $\alpha_{high_K_peat}$, $K_{XY_low_K_peat}$, $\beta_{high_K_peat}$) surrounding the unconfined Kälväsvaara groundwater aquifer. In our model representation, the properties of the top pristine peat (the anisotropy ratio $A_{high_K_peat}$ and van Genuchten parameter $\alpha_{high_K_peat}$) and the hydraulic conductivity K_{XY_till} and anisotropy ratio A_{till} of till were also found to be among the five most sensitive parameters.

The five most influential parameters varied spatially (**Fig. 6**). The drained peatland parameterisation was found to play an important role mainly in the parts of the aquifer located close to extensively drained areas, but the effect of drainage was not limited to the locations at the esker margins, but extended farther towards the esker centre. The groundwater levels were also sensitive to the parameterisation of highly permeable top peat layers at observation points situated on the margins of pristine mires and in parts of the aquifer relatively close to pristine areas. The parameterisation of glacial till was found to be influential mainly in zones situated on the borders of the esker, whereas the parameterisation of bottom peat layers

influenced only a small area located in the eastern part of the Kälväsvaara aquifer, in the headwater areas of the Leväoja and Heteoja streams.

Fig. 6.

Lake levels showed the highest sensitivity to sand hydraulic conductivity $K_{XY_{sand}}$, sand anisotropy ratio A_{sand} , hydraulic conductivity of glacial till $K_{XY_{till}}$ and van Genuchten parameter $\alpha_{high_K_{peat}}$ of top peat layers. The levels of the lakes Leililampi and Lummelampi, located in more peat-dominated landscape, showed high sensitivity to the hydraulic conductivity of the top pristine peat $K_{XY_{high_K_{peat}}}$, whereas the level of the kettle hole lake Ruunalampi was sensitive to hydraulic conductivity of the bottom peat. In contrast, the water levels of lake Pieni Kirkaslampi were mostly influenced by coupling length of the overland forest $l_{e_{forest}}$, anisotropy ratio and hydraulic conductivity of till A_{till} and $K_{XY_{till}}$ and the rill storage height of the forest $h_{RS_{forest}}$.

The fluxes between the Kälväsvaara aquifer and the surrounding mires were most sensitive to hydraulic conductivity of sand K_{xy_sand} and anisotropy ratio of sand A_{sand} . Other parameters that were ranked among the five most influential parameters were anisotropy ratio of till A_{till} , anisotropy ratio of the top peat layers of peat $A_{high_K_peat}$, anisotropy of drained areas $A_{drained}$ and hydraulic conductivity of the bottom peat $K_{XY_low_K_peat}$.

For the Olvassuo and Leväsuo mires, anisotropy ratio of drained peat $A_{drained}$ was the only influential parameter in common, beside esker properties. In terms of the other parameters analysed, the two mires differed from each other. In the Leväsuo mire, anisotropy ratio of till A_{till} and hydraulic conductivity of

the bottom peat $K_{XY_low_K_peat}$ were among the most dominant parameters, whereas in the Olvassuo mire effective rainfall P_{eff} and hydraulic conductivity of drained areas $K_{XYdrained}$ were found to be among the five most sensitive parameters.

Discharge at springs showed the highest sensitivity to anisotropy ratio of glacial till A_{till} and top layers in pristine mires and $A_{high_K_peat}$, hydraulic conductivity of till $K_{XY_{till}}$ and overland flow properties of rill storage and obstruction storage height of pristine peatlands h_{RS_NP} and h_{OS_NP} . Discharge at monitoring sites and predefined reaches was most influenced by hydraulic conductivity of glacial till K_{XY_till} , anisotropy ratio of top layers of pristine mire peat $A_{high_K_peat}$ and till A_{till} , hydraulic conductivity of sand K_{XY_sand} and bottom peat layers $K_{XY_low_K_peat}$ and coupling length of channels $l_{e_channel}$. In addition, numerous other parameters (see Table 3) were found to be among the five most influential parameters.

The parameter sensitivity analysis for saturation output of the top peat layers focused on wetland areas, where volumetric water content was of high importance for the state of the mire. The most important parameters were related to van Genuchten parameters of pressure head-saturation-hydraulic conductivity relations in pristine peatlands $S_{r_high_K_peat}$, $\beta_{high_K_peat}$, $\alpha_{high_K_peat}$ and in drained peatlands $S_{r_drained}$, $\beta_{drained}$, $\alpha_{drained}$ and hydraulic conductivities and anisotropy ratios of top layers of pristine peatlands $K_{XY_high_K_peat}$ and $A_{high_K_peat}$ and ditched areas $K_{drained}$ and $A_{drained}$. At two observation points, the hydraulic conductivity of till K_{XY_till} was classified as one of the most influential parameters.

4. Discussion

4.1 Implications for modelling of boreal esker-mire systems

Fully-integrated models are gradually becoming a promising method to study groundwater-surface water interactions at larger scale. Boreal aapa mires are valuable ecosystems that substantially depend on the groundwater inputs. There is little knowledge to date on how the hydrology of these systems and their connection to groundwater aquifers should be modelled and the most important parameters. This work demonstrated that fully-integrated models are suitable tools to simulate hydrological connections between an esker and surrounding aapa mires. Despite simplifications made in the model (steady state and simple zonation scheme), this study yielded valuable insights into modelling complex boreal eskermire systems by disclosing the most important parameters and present the first step to generate understanding of temporal GW-SW dynamics in boreal aapa mire-esker systems. Overall, the parameters found to be most influential are in good agreement with previous studies confirming the current conceptual understanding of processes. While professional reasoning could yield similar results, the GSA method provided a systematic framework to test model ability to represent our conceptual understanding, which is needed to advance hydrological modelling.

Overall, the sensitivity analysis showed that different types of outputs were sensitive to a variety of parameters and highlighted the existence of strong hydrological connections and feedback between the aquifer and groundwater-dependent peatlands in terms of interdependence of outputs to the same parameters. The groundwater levels in the esker aquifer were sensitive to the hydraulic properties of surrounding peatlands, while the hydrological state of the mires defined by flux between esker and peatlands was sensitive to the properties of both systems. This feedback and the sensitivity of various model outputs are discussed in more detail below.

The variety of influential parameters identified indicates that it is critical to gather diverse datasets for model building and calibration of complex systems. This is an important aspect when creating integrated

models for management purposes. The modelling of GW-SW interactions can be highly important at sites for which these data requirements cannot be fulfilled, either due to high cost or due to remoteness of the site. For this reason, it would be plausible to present modelling in terms of ensembles of models capturing the uncertainty of some outputs to the most influential parameters identified with the GSA.

4.2 The most influential parameters for modelling esker-aapa mire systems

Groundwater levels were most sensitive to the hydraulic properties of the aguifer, supporting earlier findings in other groundwater-surface water modelling studies (Bonton et al., 2012; von Gunten et al., 2014). This implies that the dominant effect on groundwater levels is exerted by the hydrological properties of the aquifer itself, with aquifer hydraulic conductivity having the largest impact. However, the complex pattern of the most significant parameters (Fig. 6) shows that the groundwater levels in esker aguifers not only depend on mineral soil hydraulic properties, but are also affected by the spatially varying properties of the surroundings pristine mires and drained peatlands. This indicates that groundwater models of esker aquifers should include an adequate representation of surrounding peatlands. A similar conclusion was reached by Rossi et al. (2014) in respect of drained area management and mire conservation. Thus, determination of the spatial variability of peat hydraulic characteristics is essential in order to properly represent groundwater levels in various parts of the esker. This is challenging in practice, as peatland characteristics are spatially highly variable (Holden and Burt, 2003; Päivänen, 1973). Another issue is that parameters of various zones most likely interact and compensate for errors related to parameterisation of models. Despite these difficulties, these findings demonstrate that large-scale modelling is needed to accurately model boreal glaciofluvial formations.

In addition, the elementary effects (Morris) method pinpointed the potential importance of the van Genuchten parameter of top pristine peat $\alpha_{high\ K\ peat}$ on groundwater levels. Previously, the parameter

was thought to have minor significance for modelling saturated peatlands (Ala-aho et al., 2017) and usually was kept constant in the calibration process (Ala-aho et al., 2015a; Hwang et al., 2012; Thompson et al., 2015). As aapa mires are environments that are nearly saturated throughout the year (Laitinen et al., 2007), the parameter was also not anticipated to be important in this case. However, the randomly generated parameter sets of elementary effects analysis do not ensure full saturation of the top peat layers. Different shapes of water retention curves may produce different hydrological responses to the overall changes in groundwater levels and affect the overall water content of top peat over long time scales. To conclude, our results indicate that van Genuchten parameter α of top peat may be crucial for modelling esker-mire systems and should be carefully chosen. This is especially important when analysing the effects of exceptionally dry climate conditions or the effects of aquifer exploitation, e.g. abstraction of groundwater, on wetland ecosystems.

In general, lake water levels showed the highest sensitivity to the same parameters that controlled groundwater levels. This finding is in good agreement with the recent finding by Isokangas et al. (2015) that most kettle lakes within another esker aquifer are strongly groundwater-dependent. An exception was Pieni Kirkaslampi, the level of which was most sensitive to parameters of little physical relevance, such as coupling length of the overland forest l_{e_forest} . Further investigation revealed that none of the sets tested was able to reproduce the observed lake level with sufficient precision and the elementary effects were two orders of magnitude lower than for other lakes. The lake is known to be located at a local perched aquifer, a representation of which was not included in the model due to lack of data on its extent. This exception illustrates the importance of a conceptual understanding of groundwater systems in order to correctly interpret the outcome from GSA. It also illustrates that unexpected results in terms

of most influential/insensitive parameters may provide new information about model dynamics or help to identify problems in the model structure.

The fluxes between the Kälväsvaara aquifer and the surrounding mires were also found to be controlled by the esker hydraulic properties ($K_{xy,sand}$ and A_{sand}). In addition, the fluxes were sensitive to a wide range of hydraulic properties of surroundings: pristine mires, drained peatlands and underlying glacial till. The overall magnitude of the total flux was defined by the value of effective rainfall, when the combination of other parameters was responsible for the partitioning of the total flux between various peatland parts (see Fig. S11 in Supplementary Materials). The importance of the hydraulic properties of the esker and the properties of peatland zones highlight the close hydrological connection between the esker and the surrounding wetlands. There is a parametric interdependence of these systems, i.e. the hydrological state of each depends on the properties of others and the fluxes to each mire are defined by the combination of the esker and peatland hydrological properties. This interdependence of parameters also indicates the existence of hydrological feedback between esker and surrounding mires, which is still poorly understood. This shows that management actions affecting peat hydrological properties, e.g. drainage (Päivänen, 1973; Silins and Rothwell, 1998), in the long term also affect groundwater levels in the aquifer and control the exchange flux. This is a critical finding for groundwater resources management and conservation activities in boreal eskers that has not been well studied and described previously.

The most sensitive parameters for spring discharge were partly in contradiction with spring formation mechanisms. In particular, the sensitivity to overland flow properties was unexpected. It well known that overland flow parameters are responsible for partitioning and strongly affect the magnitude of surface

runoff (Frei and Fleckenstein, 2014; Panday and Huyakorn, 2004). However, caution is required when interpreting these results, as further investigation of modelled spring discharge revealed that the median flow at defined spring locations was approximately 0 m³s⁻¹. This means that most of the randomly generated parameter sets failed to reproduce springs, which highlights the importance of mesh size in large-scale models as small-scale spring systems are essential features in the hydrological system studied here. The spring formation mechanisms within the area were found to be very diverse and our simplified zonation was unlikely to reflect local geological features, which need to be included in models in most cases to simulate spring flows adequately.

Discharge at other observation points was sensitive to a variety of parameters, indicating that various run-off mechanisms dominate in various parts of the model, but in most cases the stream discharge at a given point was influenced by underlying soil properties, i.e. properties that directly control the connection between groundwater and streams (Conant et al., 2004; Kalbus et al., 2009; Woessner, 2000) and affect partition of precipitation into surface runoff and recharge. The high influence of $l_{e_channel}$ was, however, unexpected. Coupling length l_e controls the conductance term which in term defines exchange flux between subsurface and surface domains in the dual-node coupling approach (for more detail concerning coupling see the manual Aquanty (2015)). The sensitivity of discharge to coupling length implies that this parameter should be chosen with care, as suggested by Liggett et al. (2012). The relationship between streamflow at various observation locations and channel coupling length $l_{e_channel}$ (see **Fig. S12** in Supplementary Materials) did not show any trend. In contrast, the channel coupling length $l_{e_channel}$ varying at four p-levels produced a wide response range and numerous outliers, indicating that this parameter does not dominate streamflow response but the interactions with other parameters and/or other non-linear behaviour contribute to the stream discharge response. The model

sensitivity to coupling length may be influenced by such factors as topography, surface flow, surface ponding and hydraulic gradients (Liggett et al., 2012). In addition, the high importance of channel coupling length $l_{e_channel}$ might be due to separate heterogenous streambed representation as the conductance at a river-aquifer interface depends on both, coupling length and vertical hydraulic conductivity. The interactions of these two parameters might indeed be expected. The characterization of streambed heterogeneity was found to be one of the most important factors for modelling simultaneously hydraulic head, streamflow and GW-SW exchange between aquifer and river (Mattle et al., 2001; Schilling et al., 2017; Tang et al., 2018, 2017).

As anticipated, saturation of the top peat layer was most sensitive to the van Genuchten parameters of pressure head-saturation-hydraulic conductivity relations. Overall, the results were in good agreement with the mathematical description in the model and our process understanding. The Morris plots (see Supplementary Materials **Fig. S13**) demonstrated that for each observation point, there were 3-7 parameters to which the model was clearly sensitive. In practice, this may correspond to weak identifiability of the parameters due to a high degree of freedom. It may be possible to improve identification if the available data describe a wide range of system states from very dry to extremely wet. However, in the case of aapa mires this requirement may be not sufficient, as the mire surface may fluctuate with water levels and maintain the water content (Roulet, 1991), a process known as 'mire breathing' (Ingram, 1983).

4.3 Uncertainty and limitations of the applied method

This work considered one aspect of uncertainty involved in fully-coupled physically-based modelling of boreal esker-aapa mire systems. Moreover, the zonation scheme used did not represent fully the

complexity of the system in terms of either the complex stratigraphy of the esker or the mosaics of peatlands occurring within the model domain. Despite this gross simplification of the system, the results produced overall good agreement with measured data and thus good model feasibility.

The elementary effects approach with small sample size is a qualitative method allowing only the relative importance of parameters to be estimated. In this work, we decided to focus on the five most sensitive parameters, i.e. parameters that produced the highest elementary effects. However, the importance of the particular values of μ^* and σ is context-dependent (Morris, 1991). Thus, this systematic way of choosing the most sensitive parameters may lead in some cases to omitting some parameters that may be of importance, or including parameters of lower significance. Choosing classification threshold on sensitivity may be difficult. **Fig. 7** shows Morris plots for fluxes between the esker and Leväsuo and Olvassuo mires. A category of parameters with a rank lower than five is located in the vicinity of parameters ranked as significant and decreases steadily towards zero. Values of μ_i^* that are overall similar in magnitude suggest that the relative importance of the parameters may be not well resolved for the 20 trajectories analysed. In addition, more parameters than the five defined (see **Table 3**) may influence the magnitude of GW-SW interactions, but it can be challenging to differentiate between them (Morris, 1991).

Fig. 7

The overall results of the GSA may be dependent to some degree on the choice of sampled parameter ranges, as discussed by Shin et al. (2013). In the present study, the precise definition of feasible parameter ranges was challenging and thus not all ranges may have been fully suitable to represent processes in the

esker-wetlands landscape. There are multiple reasons behind this: (a) parameter values were sometimes not available in the literature or represent sites with significantly different climatological/geological conditions, (b) limited information was available on some site-specific characteristics, (c) the properties derived from literature/measured records may not be appropriate to the scale of model and the conceptualisation of some small-scale processes, and (d) the effect of some features (e.g. drainage ditches) on parameter values may not be possible to evaluate without appropriate data. Finally, it must be borne in mind that some ranges, e.g. parameters of water retention functions for the bottom peat, were defined using only a few samples and they may not have accurately represented natural variability. Moreover, the values obtained may be prone to errors and inaccuracies in the measurement records and shortcomings in the fitting procedure. Furthermore, the parameter ranges used for the GSA analysis may have been outside the effective parameter ranges required to model key processes.

Saturated-unsaturated soil processes are highly important in shallow groundwater systems, so model sensitivity to parameterisation of these unsaturated soil hydraulic properties should be further tested. In the present modelling study, we used van Genuchten-Mualem equations to describe pressure head-saturation-hydraulic conductivity relations. A significant problem in this stems from the random sampling of the parameters of the van Genuchten-Mualem equations that define unsaturated flow processes. The water retention curves formed by random sampling of the predefined ranges of the van Genuchten equations do not necessarily have any physical meaning. This issue is illustrated in **Fig. 8a**, where it is clear that many of the randomly sampled curves for sand are physically not realistic for this type of porous medium. Similar problems emerged for other soil types. The problem stems from the non-physical relevance of the fitting parameters α and β (Dendrou and Dendrou, 1999) and it is further pronounced when the parameters of Van Genuchten relations are weakly constrained due to lack of information on the site-specific variability of the soil hydraulic properties. As **Fig. 8b** shows, if we had

lowered the parameter variability to one-quarter of the original range, the random sampling would have produced physically realistic curves.

Fig. 8

The issue is even more evident for peat soil, in which high variability in hydraulic parameters results from the typical high soil heterogeneity and is associated with challenges in measurement of peat properties (Baird et al., 2004; Beckwith et al., 2003; Surridge et al., 2005). The inclusion of non-physical pressure-saturation-relative conductivity relations may produce model outputs of little physical relevance. This problem undermines the applicability of formal sensitivity and uncertainty methods based on random sampling for models that use a van Genuchten (or similar) description of pressure head-saturation-hydraulic conductivity relations and when the parameter ranges are wide. The formal methods admittedly show model numerical sensitivity to these parameters, but may not always provide physically valid results, masking the sensitivity of some parameters in favour of others. This issue can be addressed by discarding randomly generated physically unrealistic curves through additional constraints, but this requires good prior knowledge about the likely shape of these.

For the 66 sets tested out of a total of 1180, the model solution did not converge within the execution time limited to three days. Further investigation of these sets revealed that convergence problems were not related to physical plausibility of the van Genuchten parameters. We did not find any particular pattern that would explain this phenomenon. Thus, we believe the problems in convergence were caused mainly by certain combinations of parameter values and initial conditions.

The number of trajectories analysed (r = 20) was relatively low with respect to the model complexity. Previous studies have demonstrated that this number is usually adequate to obtain qualitative importance measures (Campolongo et al., 2007, 1999; Campolongo and Saltelli, 1997; Herman et al., 2013). Despite this, it is possible that the amount of runs performed in this study was not sufficient to obtain full coverage of the parameter space and may have led to instability in the rankings (Ruano et al., 2012). To examine this issue, a corresponding GSA with a higher amount of trajectories could be conducted. On the other hand, the reasonably physically sound results demonstrate that a similar outcome would most likely be produced even with more trajectories inspected.

Finally, it is obvious that the steady-state results do not reveal fully the dynamics of GW-SW interactions and cannot disclose all most significant parameters for modelling transient processes occurring in eskermire systems. Instead, the steady-state simulations show artificial time-averaged responses of the system and associated parameter sensitivity. The steady-state results, thus, may not be relevant for depicting the spatial dynamics of the actual system and does not provide any information on the temporal variability of GW-SW interactions, which can fluctuate significantly during various seasons of the year (Ala-aho et al., 2015a). Especially, winter and spring discharges might be strongly biased as winter processes, such as snow accumulation, snowmelt and soil freezing and thawing, were not included in this model despite winter conditions can prevail over 6 months of the year in the Kälväsvaara area and are of great importance in northern locations (Cochand et al., 2019; Schilling et al., 2019). This means that, winter and spring discharges may be sensitive to parametrization of winter processes, but these effects were beyond the scope of this study. A second major simplification of these steady-state simulations is lack of spatial and temporal variability in representation of evapotranspiration, which consequently could conceal the importance of some evapotranspiration parameters that may affect summer response of the

Olvassuo-Kälväsvaara site. Despite these limitations, steady-state models can be still useful tools to solve different practical problems (e.g. long-term effects of pumping) when data availability is low and serves as a starting point for producing transient state simulations that should be consider in further studies.

5. Conclusions

This study examined the effect of parameterisation of a large-scale boreal esker-aapa mire system. The elementary effects (Morris) method for global sensitivity analysis was applied to a 3D steady-state model of the Kälväsvaara groundwater aquifer and Olvassuo groundwater-dependent aapa mire, built with the fully-integrated physically-based code HydroGeoSphere. Global sensitivity analysis identified the most important parameters for modelling various outputs of esker-mire systems, a novel finding. The results in terms of the most influential parameters were in good agreement with the current process understanding of these systems. The hydraulic conductivity and anisotropy ratios of the esker and its surroundings were dominant, but numerous other parameters were also found to variably influence the various models outputs, including parameters describing pressure head-saturation-hydraulic conductivity relations and overland flow properties. These results imply that a wide variety of hydrological data is required to correctly calibrate integrated models focusing on GW-SW interactions in groundwaterdependent ecosystems. In particular, parameterisation of peat plays an important role, since groundwater levels in boreal unconfined esker aquifers are not only dependent on soil hydraulic properties, but are also affected by the properties of the surrounding peatlands. Similarly, the esker-mire flux is not only affected by peat hydraulic properties, but is also sensitive to the properties of the aquifer media. This feedback implies that surrounding peatland ecosystems should be included in models evaluating changes in the aquifer and that hydrological mire models should include a proper representation of surrounding mineral deposits. The results also indicate that the van Genuchten parameters describing pressure head-

saturation-hydraulic conductivity relations in upper parts of peatland may be crucial for modelling eskermire systems, particularly in cases where the groundwater level is expected to decline markedly.

Overall, the elementary effects approach was found to be a suitable and easily applicable tool for studying the parameter sensitivity of large-scale fully-integrated models. However, the method and other formal global sensitivity techniques may not be the most appropriate means to evaluate fully the parameter sensitivity of van Genuchten pressure head-saturation-hydraulic conductivity relations. When there is high uncertainty/variability present in the van Genuchten parameter ranges, randomly generated van Genuchten curves may not result in physically meaningful outputs, leading to overestimation of the sensitivity effects of these parameters and masking the importance of others. On the other hand, the importance of van Genuchten parameters identified here implies that these parameters should be carefully chosen, as they may affect the results. Previous fully-integrated modelling studies of peatlands have assumed that these parameters do not play any significant role and have kept their values constant, but the effect demonstrated here means that these parameters require further study.

Finally, this study provides evidence that, due to the growing availability of computational resources, global sensitivity analysis of large-scale fully-integrated physically-based models is becoming feasible in terms of computing power. Thus, we are reaching the point at which availability of input and calibration data, rather than computational resources and issues of model convergence, are limiting factors. Despite this limitation, the present study shows the power of fully-integrated physical-based hydrological models to represent sensitive GW-SW ecosystems and they should be applied more widely for management purposes (e.g. groundwater abstraction).

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Figures with captions

Fig. 1. Location of the study site (upper right corner) and map of the model domain showing the monitoring network and type of land use.

- Fig. 2. Conceptual cross-section A-B (see map of the Kälväsvaara aquifer and adjacent wetlands in Fig. 1). The soil under peatlands is composed of glacial till, while the esker soil consists of interspersed layers of sand, gravel, boulders, glacial till and silt, which were represented in the model as a homogeneous layer (esker soil). The outstretching sand aquifer deposits were represented by increasing the extent of the esker media under peatlands by 500 m. For visualisation purposes, peat layers were exaggerated vertically.
- **Fig. 3**. Properties of the study area: (a) bedrock surface elevation model; (b) 10 m x10 m digital elevation model (DEM); (c) zonation of subsurface domain and (d) zonation of surface flow domain with the triangular element mesh.
- **Fig. 4.** Simulated and measured hydraulic head at the lakes and groundwater monitoring locations in the Olvassuo-Kälväsvaara study area.
- **Fig. 5.** Results of the calibrated model: (a) exchange flux; (b) groundwater level elevation; (c) degree of saturation. Note positive values for exchange flux represent groundwater discharge.
- **Fig. 6.** Parameters most influencing groundwater levels within the esker aquifer, grouped according to the porous media zone type (at least one influential parameter occurred within the specified zone; sand excluded).
- **Fig. 7.** Morris plots for the exchange fluxes between the Kälväsvaara esker aquifer and (a) the Leväsuo mire and (b) the Olvassuo mire. The five most influential parameters are marked in black. Parameters in blue indicate other parameters with rank higher than 5 that may also be influential.

Fig. 8.	a) Water retention curves for sand formed by sampling the pre-determined ranges sampled in the	1e
	four-level grid. The bold lines show examples of curves which are physically irrelevant for sar	ıd
	soils; (b) water retention curves generated for 25-50 percentiles using same sampling interva-	ls
	(p=4) as in the global sensitivity analysis (GSA); these smaller intervals produced physical	ly
	sound curves.	

Declaration of interests

ould have appeared to influence the work reported in this paper.	
The authors declare the following financial interests/personal relationships which may be considered as	
otential competing interests:	

☑ The authors declare that they have no known competing financial interests or personal relationships that

