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ABSTRACT

While agricultural activities, such as the application of manure on arable land and animal grazing on pastures, provide economic and environmental benefits, they may also pose microbial risks to water sources. The aim of this paper was to study the microbial fate and transport in an agricultural catchment and recipient water source through further development of the hydrological model HYPE. Hydrological modelling was combined with hydrodynamic modelling to simulate the fate and transport of *Salmonella* spp., verotoxin-producing *Escherichia coli* O157:H7 (VTEC) and *Cryptosporidium parvum* in an agricultural catchment of a drinking water source, Lake Vombsjön, in Sweden. This approach was useful to study the influence of different processes on the pathogen fate and transport, and to interpret the relative changes in the simulated concentrations. Sensitivity analysis indicated that the largest uncertainties in the model were associated with the estimation of pathogen loads, parameterisation of the pathogen processes, and simulation of partitioning between surface runoff and infiltration. The proposed modelling approach is valuable for assessing the relative effect of different risk-reducing interventions.

Key words | *C. parvum*, hydrodynamic modelling, hydrological modelling, pathogens, salmonella, VTEC

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INTRODUCTION

Agricultural activities, such as application of manure on arable land and animal grazing on pastures, provide economic and environmental benefits, but may pose microbial risks to water sources used for drinking water supply and recreation. Animal manure may be regarded both as waste and a valuable fertiliser, in particular for organic farming, and forms an important part of the agricultural ecosystem. Grazing animals are needed for maintaining certain nature reserves and promoting biodiversity. Thus, it is important to be able to appropriately assess the risk, avoiding both underestimation, in order not to compromise human health, and overestimation, as it would prevent the associated benefits. In agricultural catchments, there are often multiple faecal sources, but to guide decision-making, their relative impacts on the water source need to be assessed.

The impacts of the different faecal sources can be assessed by simulating the fate and transport of microbial pollutants in agricultural catchments using water quality modelling (Oliver *et al.* 2016). Hydrological (also called catchment/watershed-scale) models, for example, HSPF (e.g., Fonseca *et al.* 2017; Qiu *et al.* 2018) and SWAT (e.g., Bai *et al.* 2016, 2017; Cho *et al.* 2016a; Bergion *et al.* 2017; Kim *et al.* 2017), have been widely applied to estimate the impacts of particularly diffuse faecal sources in agricultural catchments worldwide (see reviews by Jamieson *et al.*

(2004), Bradford *et al.* (2013) and Cho *et al.* (2016b)). Hydrodynamic models have also been applied to estimate the impacts of particularly point faecal sources on water bodies (e.g., lakes, rivers, estuaries, and coastal zones) used for drinking water production, recreation and shellfish growing in different countries (see a review by De Brauwere *et al.* (2014b)). Hydrological models simulate the processes within the catchment, while hydrodynamic models provide a detailed description of the processes within the water source. The output of the hydrological model can be used as input for the hydrodynamic model, in order to provide a detailed description of the processes both within the catchment and the water source (Bougeard *et al.* 2010, 2011; De Brauwere *et al.* 2014a); however, to the best of our knowledge, such examples are scarce. Water quality models can be used to understand the importance of factors influencing the pollutant fate and transport, make predictions regarding the effects of climate and land use changes, and thus inform mitigation, management and regulations (Coffey *et al.* 2014; De Brauwere *et al.* 2014b).

Modelling microbial pollutants is challenging due to the limited evidence base on their behaviour in the environment and scarcity of the necessary data, especially in comparison to other agricultural pollutants, such as nutrients (Oliver *et al.* 2016). There are, however, opportunities to learn from nutrient models (Vermeulen *et al.* 2015). In Sweden, water and nutrient flows in the entire country are simulated using the semi-distributed process-based hydrological model HYPE (Hydrological Predictions for the Environment); this model can be further developed to include microbial pollutants.

The aim of this study was to adapt and combine hydrological and hydrodynamic models to describe microbial fate and transport in an agricultural catchment of a drinking water source. We chose to restrict the study to include *Salmonella* spp. (salmonella), verotoxin-producing *Escherichia coli* O157:H7 (VTEC) and *Cryptosporidium parvum* (*C. parvum*) in cattle. All these waterborne zoonotic pathogens (World Health Organization 2011) are known to be present in the Swedish cattle population, at different levels of prevalence (Eriksson *et al.* 2005; Björkman *et al.* 2015; Ågren *et al.* 2016). The objectives of this study were:

- to further develop the hydrological model HYPE to describe microbial fate and transport;
- to combine hydrological modelling (using the HYPE model) with hydrodynamic modelling (using MIKE 3 FM software) in an agricultural catchment of a drinking water source, Lake Vombsjön, located in southern Sweden;
- to determine which factors and processes influence the microbial fate and transport in the catchment and in the lake;
- to assess the relative impact of these factors and identify potential points for intervention;
- to evaluate the advantages and limitations of this modelling approach.

METHODS

Study area Lake Vombsjön

Lake Vombsjön is a lake situated in the southern part of Sweden (Figure S1, available with the online version of this paper). The lake provides 330,000 consumers with drinking water. Water from the lake is extracted and artificially infiltrated into the aquifer consisting of heterogeneous glaciofluvial sediments; after transport in the aquifer, the water is pumped and treated by rapid sand filtration and chlorination before being distributed to consumers. The surface area of the lake is 12 km^2 and the total catchment area is 447 km^2. The land use is dominated by arable land (62%) followed by forest (22.5%), pasture (10%), surface water (3%) and urban areas (2.5%). Soil types are dominated by till and glaciofluvial deposits. The mean precipitation and temperature in the study area were about 750 mm y^{-1} and +7 °C, respectively (1961–1990). The three major tributaries to the lake are the streams Borstbäcken, Torpsbäcken and Björkaån (Figure S1) draining 26, 42 and 340 km^2 and with average discharges 0.24, 0.39 and 4.56 m^3/s, respectively. There are many potential sources of faecal pollution in the catchment of the lake, such as manure application on arable land, grazing cattle on pastures, numerous on-site sewer systems, a wastewater treatment plant, and wild animals.

Scenarios: manure on arable land and grazing animals on pasture

Pollution from infected animals was simulated through two pathways: application of manure on arable land ('Fert') and manure from grazing animals on pasture ('Graz'). The amounts of the pathogens salmonella, VTEC and *C. parvum* on arable land and pastures were estimated based on calculations of theoretical pathogen concentration in the faeces from infected animals, herd prevalence and within-herd prevalence (see Tables S1–S3 in Supporting information for details, available online). As detailed data could not be obtained, the concentrations in faeces were estimated by expert judgement based on published data (Besser *et al.* 2001; Silverlås *et al.* 2009, 2010; Silverlås & Blanco-Penedo 2013); low, medium and high excretion levels and the proportions of infected animals excreting at these levels were assumed (Table S1). Herd prevalence was set to a worst-case scenario of 17% for salmonella, 25% for VTEC and 100% for *C. parvum*. The within-herd prevalence figures were based on published results assuming worst-case scenarios of medium and high prevalence (Laegreid *et al.* 1999; Callaway *et al.* 2005; Schouten *et al.* 2005; Cummings *et al.* 2010; Nielsen *et al.* 2011; Ågren 2012; Björkman *et al.* 2015) (Table S2).

In scenario 'Fert', contaminated manure was applied on all arable land upstream Lake Vombsjön. In the simulation, it was assumed that the estimated amount of pathogens in manure (Table S3) was spread on the arable land on 8 May 2012, prior to an event with high observed rainfall on 10 May 2012. It was assumed that:

- half of the maximum allowed yearly amount of manure was applied on 1 day (according to the Swedish regulations (Swedish Board of Agriculture 2004) 1.5 kg m^{-2} per year can be applied);
- 90% of the manure originated from cattle;
- no reduction in pathogen content occurred during manure storage before the application;
- 95% of the manure was ploughed into the soil prior to the rainfall, with the rest remaining on the soil surface.

In scenario 'Graz', contaminated manure was applied on all pasture upstream Lake Vombsjön. In the simulation, it was assumed that the estimated amount of pathogens in manure from the grazing animals (Table S3) was spread evenly over the 14 days starting from 10 June 2012, prior to an event with high observed rainfall on 24 June 2012. It was assumed that:

- the manure was produced during 14 days by the maximum number of animals allowed on pasture;
- the maximum number of animals allowed on pasture was seven adult animals per hectare;
- all pasture was grazed by cattle, 50% from dairy herds and 50% from beef herds;
- the number of beef calves below two months of age was 0.5 per hectare on 50% of the area, since only beef calves graze on pasture.

The pathogens on and in the soil reached surface water either by surface runoff or by outflow from the groundwater zone.

Water flows and pathogen concentrations in the tributaries to Lake Vombsjön were simulated using hydrological modelling with HYPE. The internal circulation within Lake Vombsjön was simulated using hydrodynamic modelling with MIKE 3 FM (MIKE Powered by DHI) based on the simulated inflows and pathogen concentrations from HYPE. The combination of models was used to estimate the pathogen concentrations at the drinking water intake in the lake resulting from agricultural activities in the catchment.

Hydrological modelling

HYPE model development for pathogens

The HYPE model is a hydrological model for simulation of water and substances in soils, rivers and lakes. An early version of the model is described by Lindström *et al.* (2010), but model development is ongoing and the reader is referred to web sources (http://hypecode.smhi.se/) for the latest model version, open source code and documentation. Part of the model development has been the inclusion of routines (described below) for simulating the fate of pathogens in the environment.

The modelled domain is divided into subbasins, each with a unique distribution of hydrological response units (HRUs). These HRUs are typically a combination of specific

land uses and soil types. The soil profile of each HRU is divided into a maximum of three soil layers. Runoff of water and substances from all soil layers is calculated and summed for each HRU for each time step and then routed through the network of rivers and lakes in the model. Many parameters in the model are linked to either soil type (e.g., field capacity) or land use (e.g., evapotranspiration parameters), while others are general. The time step for most HYPE applications is 1 day, but there is a possibility to run the model with a shorter time step if forcing data (precipitation and temperature) with a higher temporal resolution are available.

HYPE considers several processes (Figure 1) affecting the fate of pathogens in soils and surface waters. These are: release from source, decay (the net effect of die-off and growth), adsorption, sedimentation and resuspension. The simulations for pathogens are very much affected by the hydrological simulations, especially by the partitioning between various flow paths and the turnover times in different model compartments.

Land-based sources of pathogens in the model are either application of livestock manure to the land or excrement from, e.g., grazing animals. Pathogens may also enter surface water directly through point sources. Pathogens in manure or excreta are applied to specific HRUs at a specific date or repeatedly on the same date each year. The total application can be spread in time over a user-defined number of days. Applied pathogens are added to a pool of pathogens on the soil surface. The user may specify ploughing dates, when incorporation of all or part of the pathogens into the top soil occurs. Usually the top soil layer in arable land in HYPE applications consists of the soil down to the ploughing depth.

In this paper, the symbol # is used to denote the number of pathogens.

Release of pathogens from the source occurs during days with rainfall or snowmelt (Equation (1)). The number of released pathogens (F_{rel}, #) during a time step (Δt, d) is a function of the number of pathogens in the source (N_{source}, #), rainfall and/or snowmelt during a time step (V_{rel}, mm) and a release parameter (p_{rel}, mm^{-1}).

$$F_{rel} = N_{source} \cdot \left(1 - e^{-V_{rel} \cdot p_{rel}}\right) \qquad (1)$$

Pathogens released from the source either infiltrate into the top soil or enter the stream network directly through surface runoff, depending on the partitioning between the simulated flow pathways during the time step. Pathogens infiltrating into the soil may, to various degrees, sorb to soil particles. The number of pathogens adsorbing or desorbing is driven by the difference between the concentration in soil water and an equilibrium concentration (Equation (2)). The equilibrium concentration is calculated for each soil layer using a linear adsorption
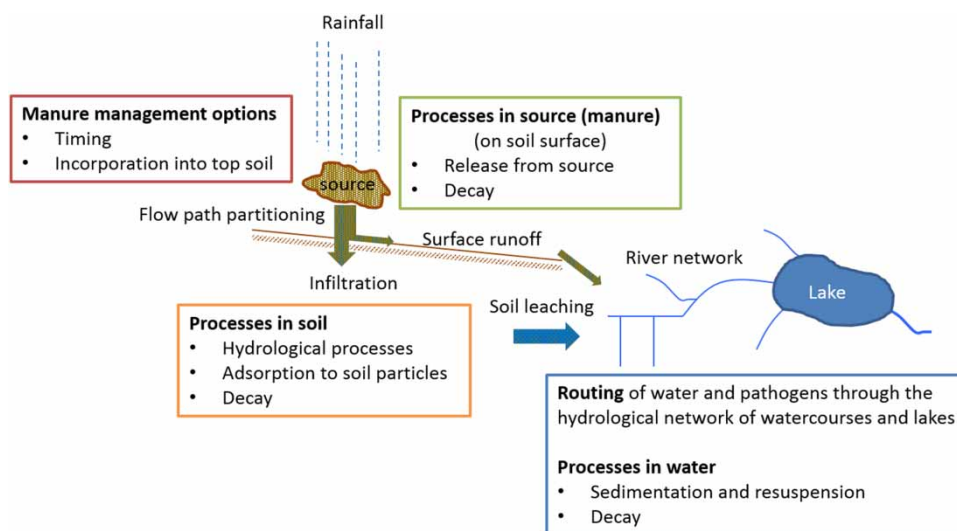

Figure 1 | Schematic representation of pathogen modelling in the HYPE model.

isotherm (Equation (3)). The equilibrium concentration is assumed to be reached during the time step. Pachepsky *et al.* (2006) suggest, in a review of process formulations for modelling manure-borne pathogens, that instantaneous adsorption may be more practical than kinetic adsorption for coarser scale applications, such as those intended for the HYPE model.

$$F_{sorb} = V_{soil} \cdot (C_{soil} - C_{eq}) \tag{2}$$

where F_{sorb} is the number of pathogens adsorbed or desorbed each time step (# km^{-2}), V_{soil} is the water content of the soil layer (mm), C_{soil} (μ# L^{-1}) is the concentration in the soil water (before the process) and C_{eq} (μ# L^{-1}) is the equilibrium concentration.

$$C_{eq} = \frac{N_{tot}}{V_{soil} + p_{ads} \cdot \rho_{bulk} \cdot d} \tag{3}$$

where N_{tot} (# km^{-2}) is the sum of pathogens in the soil layer either adsorbed to soil particles or in the soil water, p_{ads} is the partitioning coefficient (a model parameter, (# kg $soil^{-1}$)/(# L^{-1})), ρ_{bulk} is the bulk density (kg soil m^{-3}) and d is the thickness of the soil layer (m).

Pathogens may sediment in lakes and are then considered to be removed entirely from the system (Equation (4)). The amount of settled pathogens during a time step ($F_{sed,lake}$, #) depends on the pathogen concentration in the lake (C_{lake}, # m^{-3}), the lake surface area (A_{lake}, m^2) and the settling velocity, a model parameter (p_{sed}, m d^{-1}).

$$F_{sed,lake} = A_{lake} \cdot C_{lake} \cdot p_{sed} \cdot \Delta t \tag{4}$$

Sedimentation is also simulated in rivers, but here the pathogens sediment to a storage pool from where they may be resuspended to the water column at a later stage. The implemented process formulation is the same that was developed for particulate phosphorus by Rosberg (2003). The amount of sedimentation and resuspension is dependent on the flow in the rivers in relation to the bank full flow (calculated as the second highest simulated flow during a 1-year period) (Equations (5a) and (5b)). At

high flows, resuspension dominates, and at the bank full flow (or above), all previously settled pathogens are resuspended. With flow at half the bank full flow, the two processes are balanced, and no sedimentation or resuspension occurs during the time step. At lower flows, sedimentation dominates, and at zero flow, all pathogens in the water settle.

$$F_{sed,river} = a_{sres} \cdot C_{river} \cdot V_{river}, \ a_{sres} > 0 \tag{5a}$$

$$F_{resusp,river} = -a_{sres} \cdot P_{sed}, \ a_{sres} < 0 \tag{5b}$$

where $F_{sed,river}$ and $F_{resusp,river}$ are net sedimentation and resuspension during a time step (#), C_{river} is the concentration of pathogens in suspension in the river (# m^{-3}), V_{river} is the river volume (m^3), P_{sed} (#) is the pathogens settled to the river bottom and a_{sres} is the fraction engaged during a time step (Equation (6)):

$$a_{sres} = MAX\left(-1, MIN\left(1, \left(\frac{Q_{bank} - Q}{Q_{bank}}\right)^{p_{sres}} - \left(\frac{Q}{Q_{bank}}\right)^{p_{sres}}\right)\right) \tag{6}$$

where Q (m^3 s^{-1}) is the stream flow at the current day, Q_{bank} (m^3 s^{-1}) is the bank full flow and p_{sres} is a dimensionless model parameter.

Decay of pathogens is simulated in all model compartments, i.e., in the source, soil (both adsorbed and in the soil solute), lakes, rivers and river sediments. Decay is simulated as an exponential decay as suggested by Chick (1908) (Equation (7)):

$$F_{decay} = N_0 \cdot (1 - e^{-\mu \cdot \Delta t}) \tag{7}$$

where F_{decay} (#) is the number of deceased pathogens during a time step (Δt, d), N_0 (#) is the number of pathogens in the pool before the process is calculated, and μ is the decay constant (d^{-1}). μ is calculated (Equation (8)) from the model parameter $p_{halflife}$ (d).

$$\mu = \frac{\ln(2)}{p_{halflife}} \tag{8}$$

Pathogens from point sources may be added to the surface water system. They can be either constant during the simulation period or limited to a shorter period.

Model set-up for the catchment of Lake Vombsjön

The HYPE model for the catchment of Lake Vombsjön was extracted from the national set-up of HYPE for Sweden, called S-HYPE. The original version of S-HYPE was described by Strömqvist *et al.* (2012), but the model is being developed continuously. The catchment of Lake Vombsjön consists of 17 subbasins, with an average subbasin size of 26 km^2.

The parameter values for decay were estimated as the median of the values found in the literature for pathogen decay in water (Table S4, available online). The partitioning coefficient for sorption/adsorption varies greatly in the literature. The value for the partitioning coefficient was chosen based on a relatively low clay content (Pachepsky *et al.* 2006) in order not to underestimate the risks; the value was doubled for *Cryptosporidium* since oocysts to a high degree adsorb to soil (Petersen *et al.* 2012). The parameter for release from source was estimated from Shelton *et al.*'s (2003) data on manure-borne coliform bacteria; this is probably an overestimation for *Cryptosporidium* oocysts because of their higher sorption. The bacteria salmonella and VTEC were found to have similar decay rates and were assumed to have similar behaviour, thus the same parameter values were applied. The following values were used: the decay parameter $p_{halflife}$ (days) was assumed 3 for bacteria and 25 for *Cryptosporidium*; the partitioning coefficient p_{ads} (# kg soil^{-1})/(# L^{-1}) was assumed 5,000 for bacteria and 10,000 for *Cryptosporidium*; and the release parameter p_{rel} (mm^{-1}) was assumed 0.005 for all pathogens. Sedimentation and resuspension of pathogens were not included in the hydrological simulations, i.e., the parameter values were set to zero.

The S-HYPE model had previously been calibrated using the discharge observations from all of Sweden for the period 1999–2008. The performance was here validated using the observations from the only station within the study area (Eggelstad located in Björkaån) for the period 1981–2015. The Nash–Sutcliffe efficiency (NSE), which can range from $-\infty$ to 1, with 1 representing a perfect match, was 0.858 and 0.836 for calibration and validation using daily discharge, respectively.

Sensitivity analysis of the model for the catchment of Lake Vombsjön

Sensitivity analysis was performed for a selection of parameters and factors that were considered to have the largest impact on the simulated pathogen concentrations. The effect of the soil type was investigated by assuming that all agricultural land was located on either clay soils or coarse soils. The values for the following parameters and factors were changed one at a time by ±30% from their reference value:

- amount of applied pathogens;
- half-time for decay (HYPE parameter $p_{halflife}$);
- parameter for adsorption in soil (HYPE parameter p_{ads});
- parameter for release from manure due to rainfall (HYPE parameter p_{rel});
- precipitation (during the full simulation period);
- mixing volume in rivers (HYPE parameters *deadl* and *deadm*);
- surface runoff fraction due to intense rainfall (HYPE parameter *srrate*);
- surface runoff rate due to saturated soil conditions (HYPE parameter *srrcs*).

The peak concentration (# L^{-1}) and the total amount of pathogens (#) in the tributary Björkaån were compared to the reference results for each change.

Hydrodynamic modelling

Model set-up for Lake Vombsjön

To simulate the water circulation in Lake Vombsjön, a three-dimensional time-dependent hydrodynamic model MIKE 3 FM (MIKE Powered by DHI, https://www.mikepowered-bydhi.com/products/mike-3) was used. The MIKE 3 FM model is based on the numerical solution of three-dimensional incompressible Reynolds averaged Navier–Stokes equations using Boussinesq and hydrostatic assumptions. The model consists of continuity, momentum, temperature,

salinity and density equations, and is closed using a turbulent closure scheme.

The modelling domain was approximated with prisms (triangles in the horizontal plane) using a flexible mesh approach (Figure S2, available online). The mesh consisted of 817 nodes and 1,515 elements. The length of the triangles' sides varied from approximately 75 to 190 m, and was adjusted to describe the coastline and bathymetry. Vertically, the lake was approximated by layers. The thickness of the two uppermost layers can vary depending on the water level in the lake; in an undisturbed state, the thickness of these layers is 0.5 m each. The other layers have a fixed thickness of 1 m.

The model was set up to simulate the period January–December 2012. The following input data were used: inflow from the tributaries Björkaån, Torpsbäcken and Borstbäcken (output from the HYPE model), outflow from the lake, water extraction for drinking water production, precipitation on the lake surface, wind speed and direction, air temperature, cloudiness (clearness coefficient), relative humidity. The initial test conditions in the lake were defined by the constant surface elevation and the flow velocity was set to zero. The model was set up to account for the hydro-meteorological conditions (wind and precipitation on the lake surface), and to simulate the heat exchange between the atmosphere and the lake. The water density was formulated as a function of temperature. The bed resistance was described by a constant roughness height of 0.05 m. The horizontal eddy viscosity was simulated using the Smagorinsky formulation. The vertical eddy viscosity was simulated using the k-epsilon formulation. The model was run with default parameterisation.

In order to simulate the pathogen fate and transport in Lake Vombsjön, the microbial water quality model MIKE ECO Lab (MIKE Powered by DHI, https://www.mikepoweredbydhi.com/products/mike-eco-lab) was coupled to the hydrodynamic model of the lake. MIKE ECO Lab used flow fields from the hydrodynamic model to calculate the pathogen concentrations in the lake. The pathogen decay in the lake was described in the same way as in the HYPE model. Sedimentation of *C. parvum* oocysts in the lake was taken into account. It was conservatively assumed that the oocysts released into the lake were not attached to particles, thus the sedimentation velocity was specified as

0.03 m d^{-1}, which is the value suggested for free oocysts (Medema *et al.* 1998). It was assumed that resuspension does not occur.

The performance of the model was validated using the daily observations of the water level in the lake for the studied period May–August 2012; the NSE was 0.895.

Sensitivity analysis of the model for Lake Vombsjön

Sensitivity analysis was performed to study the effect of decay and sedimentation in the lake on the simulated pathogen concentrations. The following simulations were performed for scenario 'FertHigh':

- the pathogens do not decay and do not sediment in the lake – the pathogens were simulated as a conservative substance;
- the pathogens decay in the lake (the pathogen decay is described in the same way as in the HYPE model);
- *C. parvum* oocysts decay and sediment in the lake.

The results were compared in terms of the time-series of salmonella (also representing VTEC) and *C. parvum* concentrations at the water intake as a result of inflow from the tributary Björkaån.

RESULTS

The simulated concentrations resulting from manure application and cattle grazing (Table 1 and Figure 2) reflected the differences between the tributaries in terms of soil composition, land use, pathogen load and water flow. The highest pathogen concentrations were simulated in Torpsbäcken, with the exception of *C. parvum* in scenario 'Graz', when the highest concentration was simulated in Björkaån (Table 1). The tributary that was simulated to cause the highest pathogen concentrations at the water intake was Björkaån (Table 1 and Figure 2); Björkaån has the highest water flow and the largest catchment area among the tributaries.

The concentrations of salmonella and VTEC exhibited peaks after the first rain event, while the concentrations of *C. parvum* exhibited peaks after several rain events (Figure 2). Also, the concentrations of *C. parvum* at the

Table 1 | Simulated hypothetical maximum concentrations in (A) the tributaries to Lake Vombsjön and (B) at the water intake in Lake Vombsjön as a result of inflows from the tributaries

Pathogen/Tributary	(A) Concentrations in the tributaries[a]			(B) Concentrations at the water intake[b]		
	Björkaån	Torpsbäcken	Borstbäcken	Björkaån	Torpsbäcken	Borstbäcken
Salmonella (# L^{-1})						
FertMed	0.06	0.19	0.15	0.000084	0.000024	0.0000094
FertHigh	0.14	0.45	0.36	0.000200	0.000055	0.0000220
GrazMed	0.08	0.22	0.20	0.000077	0.000014	0.0000073
GrazHigh	0.18	0.52	0.46	0.000180	0.000032	0.0000170
VTEC (# L^{-1})						
FertMed	83	261	209	0.11	0.032	0.013
FertHigh	147	460	369	0.20	0.056	0.022
GrazMed	107	300	266	0.10	0.019	0.010
GrazHigh	188	529	470	0.18	0.033	0.018
C. parvum (# L^{-1})						
FertMed	60	75	60	0.28	0.028	0.010
FertHigh	120	148	119	0.54	0.055	0.020
GrazMed	122	108	96	0.96	0.058	0.021
GrazHigh	241	213	190	1.91	0.114	0.041

'FertMed'/'GrazMed': medium within-herd prevalence, 'FertHigh'/'GrazHigh': high within-herd prevalence.
[a]The water flows and pathogen concentrations in the tributaries to Lake Vombsjön were simulated using hydrological modelling with HYPE.
[b]The water circulation within Lake Vombsjön and pathogen concentrations at the water intake were simulated using hydrodynamic modelling with MIKE 3 FM based on the water flows and pathogen concentrations in the tributaries simulated using hydrological modelling with HYPE.

water intake decreased much slower in comparison to salmonella and VTEC (Figure S3, available with the online version of this paper). The bacteria salmonella and VTEC exhibited similar patterns since they were described in the models in a similar way. The differences between the simulated concentrations of bacteria and *C. parvum* can be explained by much slower decay of *C. parvum*. The simulated concentrations of salmonella and VTEC for scenarios 'Fert' and 'Graz' were similar, while the simulated concentrations of *C. parvum* for scenario 'Graz' were higher than for scenario 'Fert' (Figure 2). This is the result of the assumptions regarding the pathogen load, namely, the proportion of calf faeces (that contain the high pathogen concentrations) being larger in faeces on pasture than in the large volumes of manure. The simulated concentrations in the lake were increased for longer periods of time than in the tributaries, due to a longer residence time in the lake.

For the hydrological model, the sensitivity analysis showed that the results were sensitive to soil type; the simulated concentrations were considerably higher for clay soils and very much lower for coarse soils, compared with the soils in the study area. The soil type determined the flow path partitioning into surface runoff and infiltration. The pathogens that were infiltrated into the soil did not appear in the discharge, due to adsorption to soil particles and decay. Thus, transport of pathogens was dominated by surface runoff. Therefore, the results were also sensitive to the parameters and factors that influenced the surface runoff (Figure 3), e.g., the precipitation amount and the surface runoff parameter (*srrate*). The results were also sensitive to the decay parameter ($p_{halflife}$), particularly in the case of bacteria. The results were linearly dependent on the amount of applied pathogens. The range in the used literature values for decay of bacteria was larger than the range for *C. parvum*, in relative terms (Table S4). The uncertainty in the results for bacteria is thus presumably larger than the corresponding uncertainty for *C. parvum*. Changes in the adsorption parameter (p_{ads}) had almost no influence on the result, even when the parameter was changed by orders of magnitude, since the parameter settings still meant a very strong adsorption to the soil. In the sensitivity analysis, the changes in most
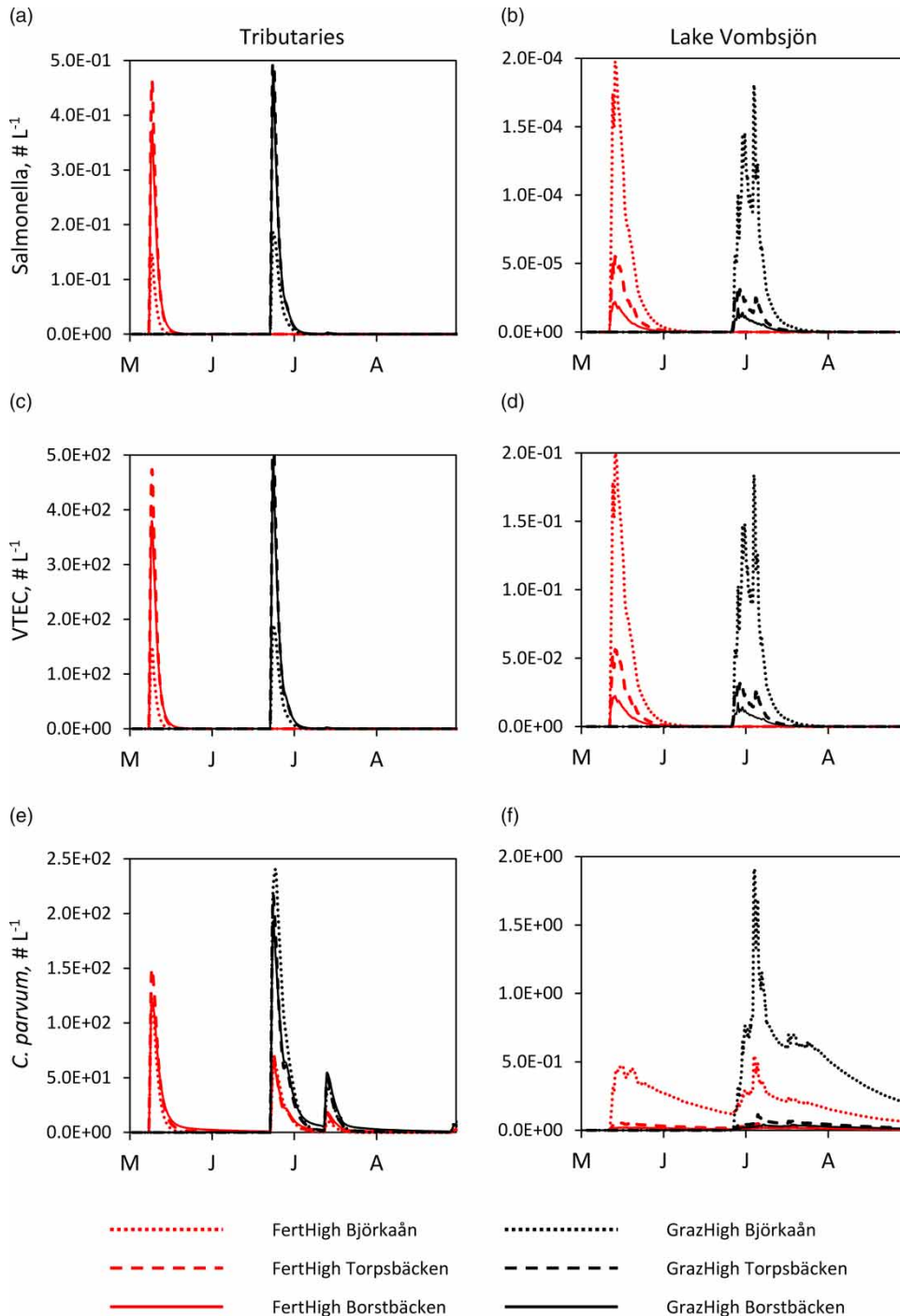
Figure 2 │ Simulated hypothetical concentrations (# L^{-1}) of salmonella (a and b), VTEC (c and d) and *C. parvum* (e and f) in May–August 2012 in the tributaries to Lake Vombsjön (a, c and e) and at the water intake in Lake Vombsjön as a result of inflows from the tributaries (b, d and f). The results for scenarios 'FertHigh' and 'GrazHigh' are shown in different shades. The tributaries Björkaån, Torpsbäcken and Borstbäcken are represented by dotted, dashed and continuous lines, respectively.

parameters and factors affected the peak concentration and the total amount of pathogens similarly (Figure 3). However, the change in precipitation affected the total

amount of pathogens more than the peak concentration, in particular for *C. parvum*, which decays slower than bacteria. Also, the change in the river mixing volume affected
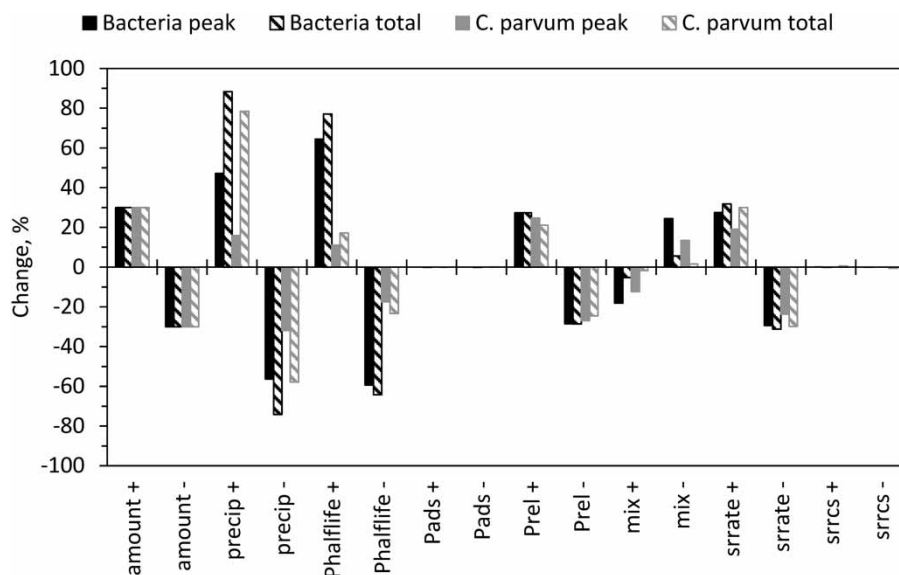
Figure 3 │ Sensitivity analysis of the HYPE model for the tributary Björkaån: the values for the parameters and factors were changed one at a time by ±30% from their reference value, and the simulated concentrations were compared to the reference results for each change. The results for bacteria (salmonella and VTEC) and *C. parvum* are represented by black and grey colours, respectively. The results for the peak pathogen concentration (# L^{-1}) and the total amount of pathogens (#) are represented by solid and striped fills, respectively. The parameters and factors are: 'amount' – amount of applied pathogens; 'precip' – precipitation; 'Phalflife' – half-time for decay; 'Pads' – parameter for adsorption in soil; 'Prel' – parameter for release from manure due to rainfall; 'mix' – mixing volume in rivers; 'srrate' – surface runoff fraction due to intense rainfall; 'srrcs' – surface runoff rate due to saturated soil conditions.

the peak concentration more than the total amount of pathogens.

For the hydrodynamic model, the sensitivity analysis (Figure S4, available online) showed that the assumptions about decay had a major impact on the simulated concentrations at the water intake, while the assumed sedimentation of *C. parvum* had only a minor impact. The importance of decay can be emphasised by the long residence time in the lake (about 190 days).

DISCUSSION

In this paper, the hydrological model HYPE was further developed to simulate the fate and transport of pathogens. The hydrological model was combined with the hydrodynamic model of the water source to simulate the pathogen fate and transport from the diffuse sources in the catchment to the water intake. Using the combination of the models, the relative impact of manure application on arable land and of cattle grazing on pastures in the catchment of Lake Vombsjön was assessed. This modelling approach proved useful to understand the effect of different processes and

to interpret the relative changes in the simulated concentrations. However, the actual figures per se are not very useful and should not be taken *ad notam*, due to the uncertainties outlined below.

In order to formulate and simulate the scenarios, assumptions were made implying uncertainties and limitations. The performance of the models in terms of simulating the hydrological processes in the catchment and the water circulation in the lake was good, as shown by the high NSE values. However, as adequate data regarding the pathogen load and the concentrations in water sources cannot be obtained, scenarios had to be used. The simulated pathogen concentrations in sources as well as recipients cannot be validated, because the required detail in temporal and spatial prevalence/concentration is impossible to fulfil by sampling. Based on the results of the sensitivity analysis and the studied literature data, we believe that the largest uncertainties in the model are associated with the estimation of pathogen loads, followed by parameterisation of the pathogen processes, and simulation of flow path partitioning in the HYPE model.

To estimate pathogen loads in the scenarios, assumptions had to be made about prevalence of infected herds,

prevalence of infected animals in an infected herd, and excretion from individual animals. Data on these aspects are scarce and largely unvalidated. Prevalence data may be obtained by intensified (and costly) screening studies, but there will always be uncertainties regarding the temporal and spatial variation. The formulated scenarios were regarded as worst-case in the Swedish context, as the prevalence of some of the pathogens (particularly salmonella) is lower in Swedish livestock than in most parts of the world. However, the most critical aspect that influences the total pathogen load in an area is the estimated excretion from infected animals. The available data are often from experimental infections, and little is known about excretion (amount and temporal pattern) from naturally infected animals, including individual and temporal variation. Such detailed data would be very difficult to obtain, and hence we rely on estimates, usually worst-case assumptions.

The modelling results showed that the pathogens mainly reached the tributaries via surface runoff. The pathogens that entered the soil due to infiltration and ploughing did not reach the tributaries because of adsorption to soil particles and decay. The modelling results were sensitive to the parameters and factors that influenced the amount of surface runoff. A realistic simulation of flow paths is thus important. The flow path partitioning in the HYPE model was evaluated by Tonderski *et al.* (2017), using the stable isotope ^{18}O in a small agricultural catchment in southern Sweden; overall, the results were promising, but with room for further improvement. In addition, the literature data on some of the parameters to which the results were sensitive, e.g., pathogen decay and release from manure due to rainfall, were scarce and/or reported in big ranges. This is consistent with the challenges reported in the literature on microbial water quality modelling (De Brauwere *et al.* 2014b; Vermeulen *et al.* 2015; Oliver *et al.* 2016).

CONCLUSIONS

The presented modelling approach is highly valuable for assessing the relative effect of different risk-reducing interventions. For Lake Vombsjön, the potential mitigation measures should be focused on the catchment of Björkaån, since it was the tributary that contributed the most to the

concentrations at the water intake. Also, the results demonstrated that incorporating the manure into the soil by ploughing directly after the application reduces the risk of pathogens reaching the surface waters. Furthermore, the simulated scenarios of manure application and grazing on pastures yielded the results in the same order of magnitude, with the exception of *C. parvum*, for which the grazing scenario yielded higher concentrations in the lake, simply due to the assumption of a higher proportion of highly excreting animals in this scenario. Also, the effects of these activities on the microbial water quality in the lake may persist during several weeks, particularly in case of *C. parvum*.

The future research should focus on improving the presented modelling approach by addressing the uncertainties regarding pathogen parameterisation and simulation of flow path partitioning. Moreover, application of different interventions should be part of further modelling work, to identify feasible strategies for risk reduction. The hydrological HYPE model is set up in great detail for all of Sweden and is at present being set up for the whole world. Thus, the HYPE model could be used to explore the influence of geographical, meteorological and hydrological factors on the variations in microbial concentrations in time and in space.

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