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Published in:
Journal of Environmental Management

DOI (link to publication from Publisher):
10.1016/j.jenvman.2023.119483

Publication date:
2024

Document Version
Publisher's PDF, also known as Version of record

Citation for published version (APA):
Thorndahl, S., Nielsen, J. M., & Rasmussen, M. R. (2024). Model-based prediction of bathing water quality in a lake polluted by fecal coliform bacteria from combined sewer overflows. *Journal of Environmental Management*, *349*, Article 119483. https://doi.org/10.1016/j.jenvman.2023.119483

Journal of Environmental Management 349 (2024) 119483

Contents lists available at ScienceDirect

Journal of Environmental Management

journal homepage: www.elsevier.com/locate/jenvman

Research article

Model-based prediction of bathing water quality in a lake polluted by fecal coliform bacteria from combined sewer overflows

Søren Thorndahl *, Janni Mosekær Nielsen, Michael R. Rasmussen

Aalborg University, Department of the Built Environment, Aalborg, Denmark

ARTICLE INFO

Keywords:
Combined sewer overflow
E. coli
Real-time prediction
Bathing water quality
Lake
Bathing water directive

ABSTRACT

In the European Union, recreational water quality is regulated by the bathing water directive, which requires authorities to regularly take water samples to identify fecal bacterial pollution, which can compromise the bathing water quality at designated recreational bathing water areas. Using a case study from Lake Knudsøin Denmark, this paper shows that the bathing water quality occasionally is compromised by overflows from combined sewer systems. Due to the randomness in the frequency of overflow occurrences, the entailing decrease in bathing water quality is not normally detected by the regulatory sampling campaigns. By dedicated sampling campaigns conducted in this project in the proximity of outlets and recreational bathing areas and by hydrodynamical transport modeling, it is shown that the transport patterns of pollutants are crucially and rapidly dependent on dynamic conditions. The occasional short-term pollution by fecal bacteria and consequent decrease in bathing water quality are, therefore, challenging to capture (both spatially and temporally) by regular water sampling. Rather than increasing the frequency of water sampling, an online model-based warning system for fecal bacteria contamination in bathing areas is proposed. This warning system framework includes: (1) dynamical modeling of combined sewer overflow based on rainfall over a catchment area, (2) a hydrodynamical model that simulates current fields in multiple vertical layers based on wind forcing and water fluxes, and (3) a particle dispersion model which provides an estimate of pollutant concentrations. The output from the model has shown potential to issue bathing prohibition if there is a risk of fecal bacteria concentrations below the criteria for good bathing water quality.

1. Introduction

With an aim to protect public health by ensuring the quality of recreational waters, the World Health Organization has published guidelines on recreational water quality for both coastal and fresh waters (World Health Organization, 2021). In the European Union, recreational bathing water quality is regulated by the EU Bathing Water Directive 2006/7/EC (EU, 2006). It requires the national authorities to identify bathing waters annually and to define the length of bathing water seasons. For identified dedicated recreational bathing waters, "bathing water quality assessments" should be carried out by monitoring the bathing water quality based on microbiological contamination of fecal bacteria. For inland (fresh) bathing waters, the bathing water quality should be identified as "poor", "sufficient", "good" or "excellent" according to the criteria of Intestinal enterococci and Escherichia coli as specified in Table 1. Coliform fecal bacteria, including Intestinal enterococci and Escherichia coli (hereinafter referred to as enterococci and E. coli, respectively), are commonly used as indicators of the presence of pathogenic microorganisms (e.g. as exemplified by de Brauwere et al. (2014), North et al. (2014), Tiwari et al. (2021))

The criteria in Table 1 should comply with a predefined number of regulatory samples (minimum four samples) during the bathing season. When the bathing water quality is identified as poor, a prohibition or advice against bathing should be alerted. However, samples taken during short-term pollution may, according to the bathing water directive, be disregarded and replaced by samples taken seven days after the end of the short-term pollution. If the replacement sample shows a satisfied criteria, the bathing water quality is not identified as "poor".

Bathing waters can be classified as "sufficient", "good", and "excellent" if the criteria in Table 1 is complied, and if the bathing water is subject to short-term pollution on the condition that (EU, 2006, Annex II): *"adequate management measures are being taken, including surveillance, early warning systems and monitoring, with a view to preventing bathers' exposure, by means of a warning or, where necessary, a bathing prohibition"*.

It is clear that bathing water may be subject to short-term pollution if wastewater or diluted wastewater from combined sewer overflow (CSO) structures is discharged in close proximity to the bathing area.

* Corresponding author.
E-mail addresses: st@build.aau.dk (S. Thorndahl), jmn@build.aau.dk (J.M. Nielsen), mr@build.aau.dk (M.R. Rasmussen).

https://doi.org/10.1016/j.jenvman.2023.119483
Received 9 August 2023; Received in revised form 25 September 2023; Accepted 18 October 2023
Available online 29 October 2023

Table 1
Fresh water bathing water quality criteria (maximum permitted value) based on microbiological contamination. (*)Based upon a 95-percentile. (**)Based upon a 90-percentile. (EU Bathing Water Directive (EU, 2006), Annex I).

Parameter	Excellent quality	Good quality	Sufficient
Intestinal enterococci (cfu/100 ml)	200(*)	400(*)	330(**)
Escherichia coli (cfu/100 ml)	500(*)	1000(*)	900(**)

As frequent sampling, such as daily or weekly, can be costly, time-consuming, and involve a significant latency period in test results (typically 24–72 h, including sampling, transport, and laboratory analysis), it is often not feasible to conduct more frequent sampling in order to ensure the safety of the bathing water quality (Seifert-Dähnn et al., 2021; Quilliam et al., 2019). Furthermore, proxy measurements, such as overflow discharge or turbidity might not provide accurate results in determining actual concentrations of coliform bacteria (Nevers and Whitman, 2005).

In light of this, it is possible to develop model-based warning systems that can prevent bathers' exposure to polluted water in the event of short-term pollution from fecal coliform bacteria. Therefore, we have used the provisions outlined in *Annex II* of the *EU Bathing Water Directive* (EU, 2006) as a foundation for creating a framework for predicting bathing water quality in a lake occasionally contaminated by fecal coliform bacteria from CSOs.

Model prediction of potential exposure of bathers to fecal pollution requires insights into the transport, kinetics and fate of pollutants from source to potential risk to bathers' health. The obvious source of fecal contamination in case of overflow spills is from municipal wastewater and the resuspension of sewer sediments in sewers transporting wastewater (Jalliffier-Verne et al., 2016). There might also be other sources of coliform bacteria, e.g., from stormwater systems with cross connections between waste- and stormwater systems or sources from animal feces on urban surfaces or in open stormwater ponds (McCarthy et al., 2012). Here, we focus solely on the contribution from CSO spills (hence, municipal wastewater and resuspension of sewer sediments), but acknowledge the fact that there might also be internal sources of fecal bacteria in bathing waters, e.g., in the lake from and in bottom sediments resuspended by recreational use. An et al. (2002). The magnitude of pollution with fecal bacteria depends significantly on the hydraulic characteristics of sewer catchment, sewer system, and overflow structure layout as well as the system's ability for self-cleansing, and thus resuspension or first flush effects (Bertrand-Krajewski et al., 1998). A dependence on both antecedent dry weather periods, as well as rain intensity, is therefore expected to affect coliform bacteria concentrations in CSO effluents (Madoux-Humery et al., 2013).

CSO volumes, or time series of overflow discharges, can be monitored in real time or simulated by commercial urban drainage models such as DHI (2019a). Simulation of CSO volumes required a good representation of overflow structures (Ahm et al., 2016) as well as model calibration to ensure a correct volume balance (e.g. Thorndahl and Willems, 2008). Short-term forecasting of overflow volumes might also be a possibility if rainfall forecasts are available (Thorndahl et al., 2013; Thorndahl and Rasmussen, 2013).

Assuming that CSO spill volumes and bacterial concentrations are estimated correctly, the next step in predicting the transport of fecal bacteria is to focus on the dilution and transport in the receiving water body. The main forces of transport in the receiving water body are determinants for the choice of modeling approach. If the receiving water transport mainly is forced by gravity (fluxes) or if affected by windshear might determine whether simple dilution models based on volume balance are sufficient or whether more complex hydrodynamic models are needed. One-directional models might be sufficient if there is one main flow direction as e.g. shown by Wilkinson et al. (1995), de Brauwere et al. (2014), and Servais et al. (2007); whereas two or three-dimensional models are needed if flow patterns are more complex or even driven by differences in density (Björklund et al., 2018; Hong et al., 2021). Other than the advective transport of pollutants, the potential growth and decay of fecal bacteria depending on temperature, available substrates and oxygen, sunlight exposure, water transparency, pH, etc. should be included if dominating the survival of fecal bacteria in the receiving water (Šolić and Krstulović, 1992). In a successful and well-calibrated model setup, the concentrations of fecal bacteria in bathing areas can be predicted and alerts issued if bathing water quality is compromised.

Model prediction of bathing water quality has previously been presented by Mälzer et al. (2016), Džal et al. (2021), Crowther et al. (2001), Thoe et al. (2012), Nevers and Whitman (2005) using statistical approaches, regression models, or data-driven models such as artificial neural networks. A common requirement and thus a potential limitation in these approaches, is the need for a substantial number of observations to predict effectively. An alternative to approaches mainly based on past samples, is physically based approaches where numerical hydrodynamical models are used to predict both the transport of water and the potential exposure of bathers to fecal bacteria. Such approaches have been presented by Gao et al. (2015), Björklund et al. (2018) and Hong et al. (2021). These types of approaches require insights into the dominating processes of transport, dilution, and biological activity to be able to develop models, estimate model parameters, as well as observation data for model calibration and validation.

The exposure to bathers and the risk of compromised health issues related to swimming in polluted water is another issue. Here we follow and rely on the criteria given by the bathing water directive. Based on model simulations it is possible to issue warnings if thresholds of E. coli and enterococci exceed the "good" quality threshold specified in the bathing water directive. The actual issuing of warnings and communication of compromised health issues related to bathing in polluted water is indeed important in a warning system setup; however this is out of the scope of this paper to discuss further.

As previously discussed, numerous studies in the literature have examined individual processes involved in the transportation of fecal contamination from its source to the potential risk to the health of bathers. Nevertheless, there exists a need to further explore and develop integrated predictive models and to compare outcomes of this type of real-time prediction with the findings from regulatory sampling, as mandated by the bathing water directive.

1.1. *Study outline and motivation*

In this approach, a framework of model-based prediction of bathing water quality in a lake polluted by fecal coliform bacteria from combined sewer overflows is demonstrated through a case study of a popular bathing lake called Knudsøin Denmark.

In lake Knudsø, the Municipality of Skanderborg (Skanderborg Kommune) is the responsible authority for taking water samples at the predefined bathing water areas and for analyzing the samples according to the specifications given by the bathing water directive. The sample results are reported to The Danish Environmental Protection Agency (EPA) under the Ministry of Environment in Denmark. The data are publicly available at https://arealdata.miljoeportal.dk/ last access: Aug 5, 2023. The water utility service company of Skanderborg (Skanderborg Forsyning) is responsible for operating the sewer system within the Municipality of Skanderborg. The water utility company has installed several flow meters to monitor the sewer system and the discharge of diluted wastewater to Knudsøfrom the CSO structures. Fig. 1 shows the reported concentrations of E. coli. and enterococci in a period from 2016 to 2022 from one bathing area called Sdr. Ege Strand (beach) and the monthly accumulated combined sewer overflow volumes from a closely located CSO structure (see Fig. 2). The reported data correspond to 13 samples per year on average. The Municipality of Skanderborg has thus sampled more than four samples per year as required by the bathing water directive. Based on the data presented

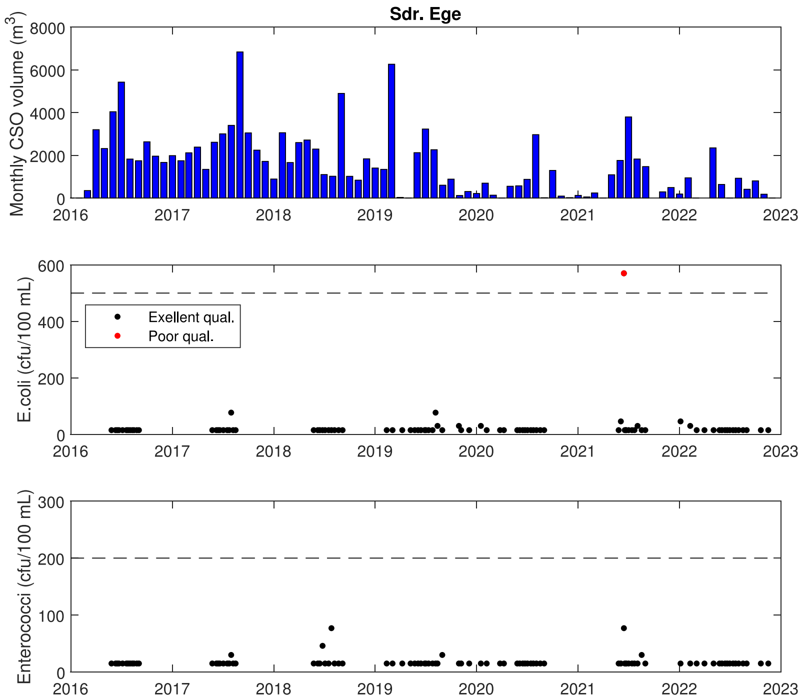

Fig. 1. Measurements from the Sdr. Ege Beach: Top: Measured combined sewer overflow (CSO) volumes. Middle: Reported concentrations of E. coli. Bottom: Reported concentrations of Enterococci. Dashed line shows the concentration threshold for excellent bathing water quality according to the bathing water directive.

in Fig. 1, it is clear that during the seven years of monitoring – despite an annual average discharge of diluted wastewater of 17,800 m^3 – the "excellent" bathing water quality criteria for E. coli (500 cfu/100 ml) is only exceeded on one occasion, and the criteria for enterococci is never exceeded at the bathing area of Sdr. Ege. Additionally, as far as the authors are aware, there are no official reports documenting health concerns associated with bathing in Knudsø. It is, however, possible that non-severe health issues may have occurred, but were not officially reported or documented.

The lack of a clear causal relationship between the overflow discharge and the concentration of fecal coliform bacteria in the water samples raises a number of questions about the sources and initial outlet concentrations of fecal bacteria as well as the mechanisms, transport, biological degradation, and survival of fecal bacteria in the lake. The potential effects of sampling frequency and the possibility of replaced (and not reported) samples due to short-term pollution events are also worth considering. These factors may contribute to the disconnect between combined sewer overflows and the unanticipated excellent bathing water quality. Therefore, this paper aims to examine specific events of combined sewer overflow and correlate them to the contamination of bathing areas and water quality through dedicated water sampling campaigns and modeling.

Based on the potential for early warning as outlined in the bathing water directive, this paper presents a proposed framework for a model-based warning system for bathing water quality. The proposed model consists of three components: 1) an overflow model that estimates overflow volumes based on wastewater and stormwater loads from the catchment area, 2) a hydrodynamic model that simulates flow and currents in the lake, and (3) a particle dispersion model used to estimate fecal bacteria concentrations. The effectiveness of the warning system framework is assessed through validation against measurements of overflow discharge, lake currents, and fecal bacteria concentrations from sampling campaigns. The model aims to understand better the mechanisms of transport, degradation, and survival of fecal bacteria in the lake and to use this understanding to improve the prediction of bathing water quality.

The paper is structured as follows: The case study area, input data for modeling, and observed sampled data are presented in Section 2. Methods for the three modeling parts of the warnings system framework are presented in Section 3. Analysis of single events with combined sewer overflow where we have conducted water sampling is presented in Section 4 along with the pollution dispersion modeling. Uncertainties in the modeling setup and representative water sampling are discussed in Section 5. Conclusions are provided in Section 6.

2. Case study area and data

2.1. Project site: Lake Knudsø

The case study site is located in the Lake Knudsøin Skanderborg Municipality, Denmark. There are three designated bathing areas at Knudsø: Birkhede Camping Beach, Knudhule Beach, and Sønder Ege Strand (Sdr. Ege Beach), which can be seen in Fig. 2. The bathing areas at Sdr. Ege Stand and Knudhule have been assigned the Blue Flag by the non-profit organization Foundation for Environmental Education (FEE). The Blue Flag ensures standards for water quality, safety, facilities, environmental education, and information.

Lake Knudsøis part of the Gudenå network (the longest river system in Denmark). It covers a surface area of approximately 2 km^2 and an average depth of 13.4 m. The lake's maximum depth is measured at 29 m, making it one of Denmark's deepest lakes. Lake Knudsøis located to the north of the town of Ry, which has a population of around 7,000 people. As shown in Fig. 2, three CSO structures are discharging into the lake. One of these structures, U5, is located at the wastewater treatment plant in Ry and combines discharge from treated wastewater with occasional CSO spills. This outlet releases the treated wastewater and overflow water into the bottom of the lake, where it is subject to dilution, sedimentation, and degradation processes. The buoyancy of diluted wastewater, influenced by factors such as stratification and seasonal variations in water density, is not anticipated to have a significant impact on the dispersion of coliforms in the lake, although this aspect has not been thoroughly investigated. All in all, U5 is not considered a notable contribution to the distribution

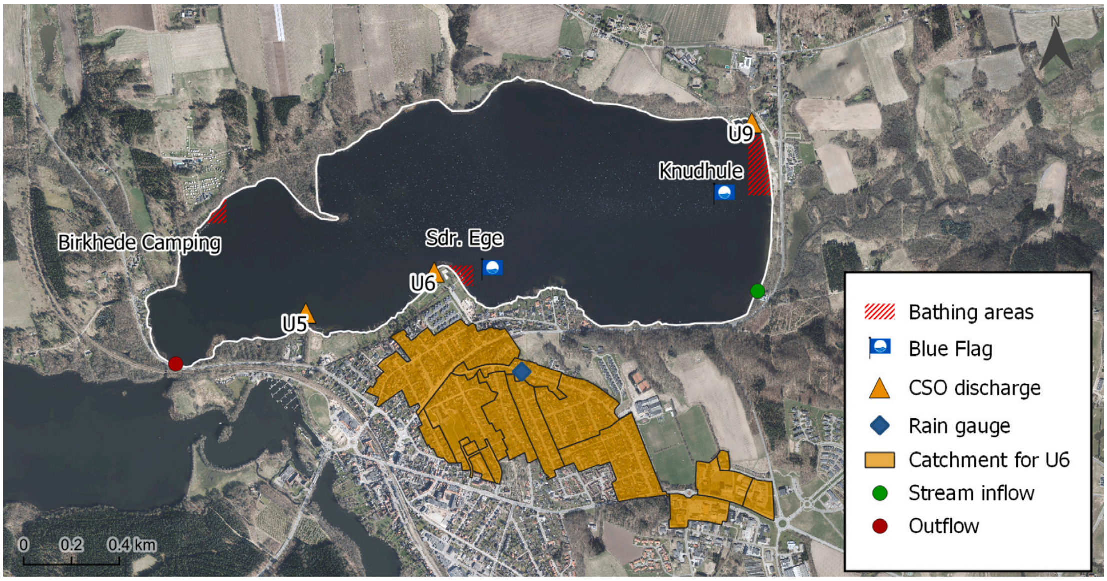

Fig. 2. Knudsøwith bathing areas and outlets from combined sewer overflow structures.

of fecal bacteria in the lake and is thus not included in the warning system framework.

U9 is a minor CSO outlet (emergency overflow from a pumping station) that discharges very infrequently, so it is not included in the warning system framework. The primary source of diluted wastewater is the U6 outlet, which serves an urban catchment area of 0.6 km^2. Fig. 1 reports the measured overflow discharges. Given its proximity (250 m) to the bathing area at Sdr. Ege Beach, the U6 outlet is the primary focus when predicting the bathing water quality in this study.

The main foundation of this paper is a project on bathing water quality in lake Knudsø: *Safe Recreational Lake Waters II* funded by the *Danish Environmental Protection Agency* (2020–2022) (Miljøstyrelsen, 2023). The project focuses on a warning system for poor bathing water quality due to fecal bacteria contamination and cyanobacteria (often referred to as blue–green algae). However, it is out of this paper's scope to describe detection, modeling, and warnings of cyanobacteria blooms further.

2.2. Overflow and precipitation measurements

Overflow discharges, as presented in Figs. 1 and 3 are recorded by a doppler flow gauge installed in the outlet pipe from the CSO structure upstream U6.

A tipping bucket rain gauge records the precipitation at the project site (see Fig. 2 for location). Data are logged every minute on both sensors and immediately available online.

2.3. Fecal coliform bacteria samples

In addition to the required regulatory testing of bathing water quality, we have conducted an additional water sampling campaign for this project during the bathing season 2021. This campaign included manual surveillance of the overflow discharge on days with forecasted rain. A total of four manual water sampling campaigns were conducted during the 2021 bathing season: May 5, May 25, June 20, and July 5–6. Manual water samples were collected at outlet U6 (Table 2) and the bathing area (from the pier) at Sdr. Ege (Table 3) both during and after overflow events and occasionally after overflow events at the bathing areas of Knudhule and Birkhede.

Samples were taken according to ISO 19458:2006 - "Water Quality - Sampling For Microbiological Analysis" and analyzed by membrane filtration, incubation on a chromogenic coliform agar medium, and

Table 2
Sampled and analyzed concentrations of E. coli and Enterococci at the outlet U6.

Sample time	E. coli (cfu/100 mL)	Enterococci (cfu/100 mL)
05-May-2021 12:25	144 000	81 000
05-May-2021 12:27	87 000	95 000
05-May-2021 12:56	103 000	93 000
05-May-2021 12:59	96 000	110 000
25-May-2021 07:27	59 000	163 000
20-Jun-2021 10:36	380 000	680 000
20-Jun-2021 10:42	1 020 000	770 000
20-Jun-2021 10:48	310 000	1170000
20-Jun-2021 10:54	60 000	350 000
20-Jun-2021 11:02	50 000	280 000
20-Jun-2021 11:41	59 000	92 000
20-Jun-2021 11:46	140 000	200 000
20-Jun-2021 12:39	34 000	93 000
05-Jul-2021 13:53	730 000	800 000
05-Jul-2021 14:26	55 000	61 000
05-Jul-2021 14:40	90 000	102 000
05-Jul-2021 14:57	49 000	106 000
05-Jul-2021 15:17	54 000	84 000
05-Jul-2021 15:47	71 000	72 000
05-Jul-2021 16:46	102 000	24 100
05-Jul-2021 18:45	47 000	16 300
05-Jul-2021 22:46	30 000	19 000
06-Jul-2021 06:48	0	200

subsequent coliform plate counting based on ISO 9308-1:2014 for E. coli and ISO 7899-2:2000 Enterococci. The Danish Technological Institute performed the analyses.

Fig. 3 and Tables 2 and 3 demonstrate that collecting dedicated samples during overflow events reveals high fecal coliform bacteria concentrations that significantly exceed the bathing water criteria. As expected, the outlet typically has high concentrations, and some samples at the bathing area of Sdr. Ege also surpasses the bathing water quality standards. These findings will be discussed in further detail in the results Section 4".

2.4. Lake specific data

The lake bathymetry is presented in Section 3.2 based on the reporting of Skaarup and Wahlberg (2019).

Wind data are applied as input to the hydrodynamical model. Wind speeds and directions for both historical periods (for setup and

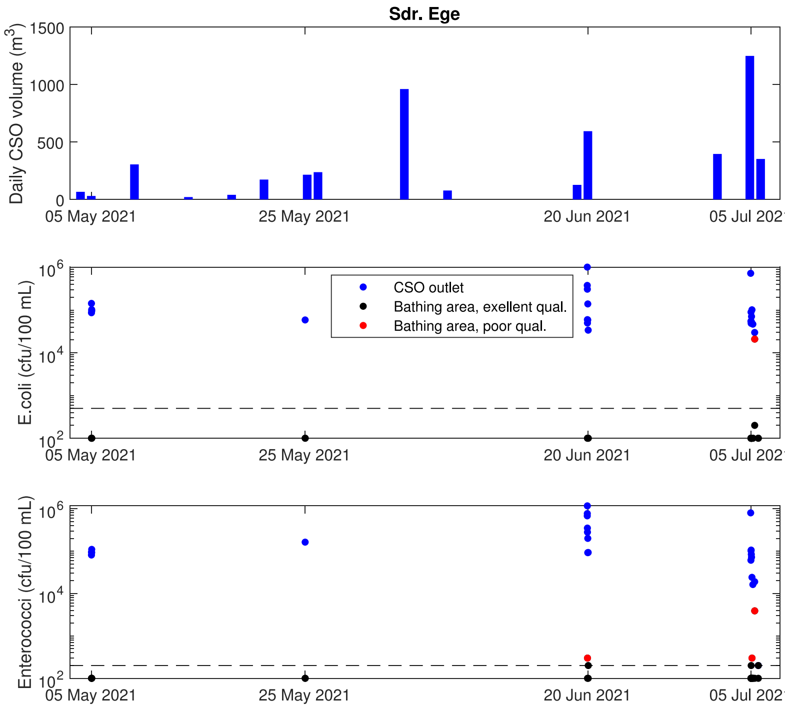

Fig. 3. Observed daily combined sewer overflow volumes and sampled concentrations of E. coli and Enterococci, May to July 2021 at Sdr. Ege. Miljøstyrelsen (2023).

Table 3
Sampled and analyzed concentrations of E. coli and Enterococci at the bathing area of Sdr. Ege Beach (pier).

Sample time	E. coli (cfu/100 mL)	Enterococci (cfu/100 mL)
05-May-2021 12:29	0	0
05-May-2021 12:33	0	0
05-May-2021 13:02	0	0
05-May-2021 13:06	0	0
25-May-2021 07:30	0	0
25-May-2021 07:34	0	0
20-Jun-2021 11:07	0	600
20-Jun-2021 11:07	0	300
20-Jun-2021 12:44	0	400
20-Jun-2021 12:49	0	200
05-Jul-2021 14:28	100	0
05-Jul-2021 14:32	0	0
05-Jul-2021 14:42	0	0
05-Jul-2021 14:45	0	0
05-Jul-2021 14:58	100	200
05-Jul-2021 15:03	100	0
05-Jul-2021 15:19	0	0
05-Jul-2021 15:22	0	0
05-Jul-2021 15:49	0	0
05-Jul-2021 15:53	0	0
05-Jul-2021 16:47	100	0
05-Jul-2021 16:51	0	300
05-Jul-2021 18:46	0	0
05-Jul-2021 18:50	100	0
05-Jul-2021 22:47	200	100
05-Jul-2021 22:51	21 000	3900
06-Jul-2021 06:49	100	200
06-Jul-2021 06:54	0	0

calibration) and real-time (for warning system) are obtained from the Danish Meteorological Institute (https://www.dmi.dk/frie-data/ last access: Aug, 5 2023) at a station in Skanderborg, located approximately 10 km from the project site. This meteorological station is the closest to the project site; however, the main wind speed and direction are not expected to vary significantly over the distance.

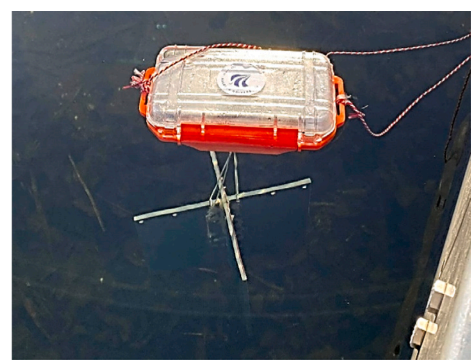

Fig. 4. Photo of drifter with drouge.

To study the currents in the lake Knudsøfour field experiments are conducted using a lagrangian drifter (Subbaraya et al., 2016). The drifter consists of a water-tight box that floats on the surface of the lake, with an X-shaped drogue attached to it by a 40 cm line (Fig. 4). Inside the box is a smartphone equipped with GPS, which, in minute intervals, logs the position of the drifter and sends this information to an online server. By releasing the drifter at various locations in the lake under different weather conditions, the resulting trajectories can be used to understand the near-surface currents in the lake and help to validate the hydrodynamical model (Fig. 9). The experiments are described in detail in Skaarup and Wahlberg (2019) and Nielsen and Fastrup (2020).

3. Methods

This study's warning system for detecting fecal coliform bacteria contamination in Lake Knudsøconsists of three interconnected models as outlined in the flowchart in Fig. 5. The first is a linear reservoir model that predicts the discharge of combined sewer overflow discharge into the lake based on the size of the catchment area (Section 3.1). The second is a hydrodynamic flow model that predicts

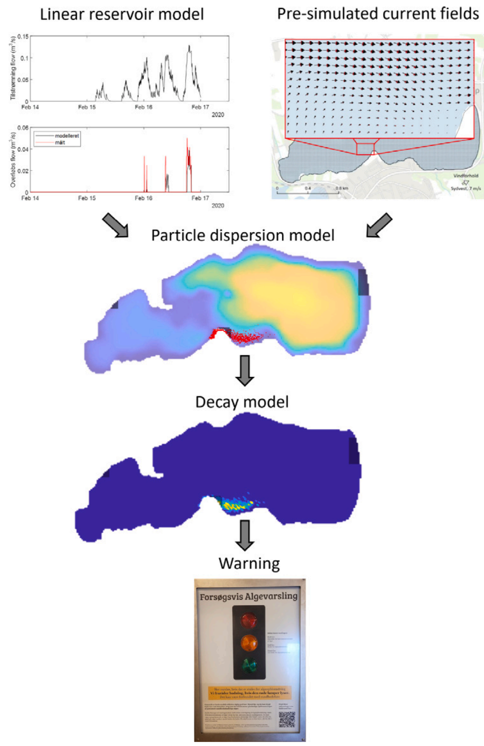

Fig. 5. Flow diagram of model setup and warning system.

flow patterns within the lake (Section 3.2). Due to the extensive computational time of the hydrodynamical model, a catalogue of pre-simulations of multiple forcing conditions under steady-state assumptions is used in real time operation. The third is a particle dispersion model that simulates fecal bacteria's transport, dispersion, and decay (Section 3.3). Together, these models provide a comprehensive approach for real-time predicting and mitigating the risks of poor bathing water quality at the designated bathing areas.

3.1. Combined sewer overflow model

There exist commercial hydraulic models, such as Mike Urban (DHI, 2019a), that can simulate the dynamic flow of storm- and wastewater in drainage systems, calculate overflow discharge volumes, and predict water levels in individual pipes (e.g., Thorndahl, 2009; Schaarup-Jensen et al., 2009). However, for the purposes of this project, we are only interested in the total volume of water discharged into Lake Knudsø, rather than the flow in individual pipes. Therefore, we have chosen to build a simple linear reservoir model, which considers the intensity of rainfall over the catchment, the size of the catchment, a catchment-dependent time constant, and the capacity of the intercepting pipe leading to the wastewater treatment plant. When the runoff from the catchment area exceeds the capacity of the intercepting pipe, the excess flow is discharged as overflow. The catchment runoff and the CSO discharge are calculated as:

$$Q_t = Q_{t-1} + \frac{dt}{t_{lag}}(i_{t-2}F_r - Q_{t-1}) \tag{1}$$

$$Q_{CSO,t} = Q_t - Q_{intercept} \tag{2}$$

In which Q_t is the runoff flow from the catchment at time t, t_{lag} is the reservoir lag time, dt is the time step, i_t is the rain intensity at time t, F_r is the contributing catchment area, $Q_{intercept}$ is the capacity of the intercepting pipe, and Q_{CSO} is the combined sewer overflow discharge.

The model parameters are known beforehand except for the reservoir lag time, t_{lag}. This parameter is determined through calibration, where measured overflow volumes are compared to calculated overflow volumes for a number of events. The aim of the calibration is to find a value of the reservoir lag time that results in an average match between the measured and calculated overflow volumes (see Section 4.1).

3.2. Hydrodynamic model

The hydrodynamical model is based on a commercial three-dimensional MIKE 3 setup by DHI (DHI, 2019b). In our setup, the model simulates the current fields in multiple vertical layers based on wind forcing and boundary conditions of the lake in and outflow. The windshear is the dominant force in determining the currents in the lake, compared to the inflow (green dot on Fig. 6) and outflow (red dot on Fig. 6) from the stream (Knudå). We disregard any contributions of changes in flow patterns due to flow in CSO outlets since these are considered minor contributions to the currents.

In MIKE 3, we use a finite difference scheme to solve the three-dimensional Navier–Stokes equations. To optimize the trade-off between accuracy and computational efficiency, the hydrodynamic model is implemented using a structured cartesian grid with dimensions of 14 m by 12 m (see Fig. 6). The vertical grid consists of a hybrid sigma-z level structure, comprising three sigma layers with a maximum thickness of 0.5 m and 69 z-level layers with a thickness of 0.4 m. This configuration results in a total of 376,271 elements in the model.

Two hydrodynamic model setups are created, one with and one without thermal stratification. These two setups are used as initial conditions for the model depending on the time of year of the initialization. Based on analyses of temperature measurements (Fig. 7), it is determined that a stable stratification exists in Knudsøfrom mid-June to the end of September at a depth of approximately 11.5 m from the water surface (Skaarup and Wahlberg, 2019; Temponeras, 2019; Nielsen and Fastrup, 2020). As a result, the prediction model is initialized with pre-simulated flow patterns modeled with stratification within this period, while simulations without stratification are used to initialize the model for the remainder of the year. In the results presented in Section 4, we do however only apply the model setup initialized with stratification, since we focus on the primary bathing season during summer in Denmark. Depending on the forcing of the model, the thermocline can be broken down and reestablished.

To ensure comprehensive coverage, we initially conduct pre-simulations for four different wind speeds (1, 3, 7, and 12 m/s) and eight different wind directions (0, 45, 90, 135, 180, 225, 270, and 315 degrees) in both the model with and without stratification, resulting in a total of 64 full hydrodynamical pre-simulation runs. The maximum wind speed simulated is 12 m/s, as higher wind speeds are rare in the area. We run all simulations until steady-state conditions are achieved, which takes approx. two days of simulation time for wind speeds of 3, 7, and 12 m/s and 2.5 days for wind speed of 1 m/s (on a standard desktop computer). To obtain pre-simulated current fields for wind speeds at 1 m/s intervals and wind directions at 5 degree intervals, interpolation is performed between the pre-simulations, resulting in 1,728 simulated current fields. The interpolation is conducted using linear interpolation for each cell by dividing flow velocities and eddy viscosities into their respective three-dimensional components.

The considerable simulation time required for the full hydrodynamic simulations necessitates using pre-simulations of currents under various wind forcing conditions. In real time applications, we can select the pre-simulation that most closely represents the current weather situation and utilize it to further simulate pollutant dispersion without compromising the time delay of the warning system due to computation time.

Despite the fact that we run the model in steady conditions, we allow continuous and real-time simulations for the wind forcing to change for every model initiation. The setup can thus be considered as a semi-dynamic approach separated into steady-state time blocks.

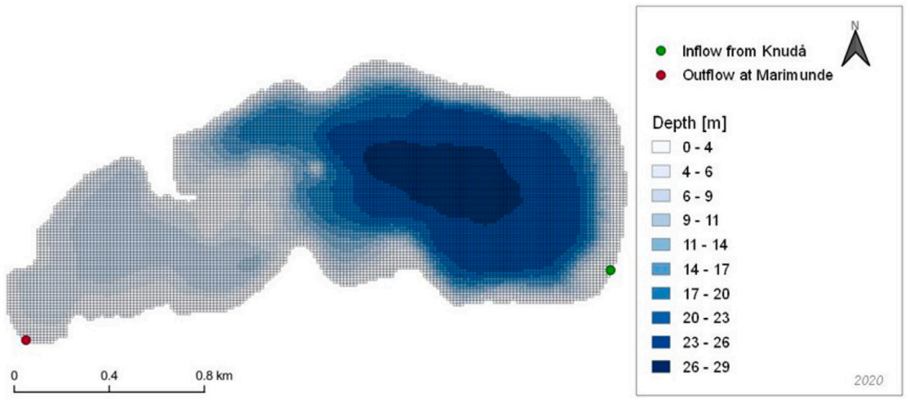

Fig. 6. Bathymetry and hydrodynamical model discretization of Lake Knudsø.

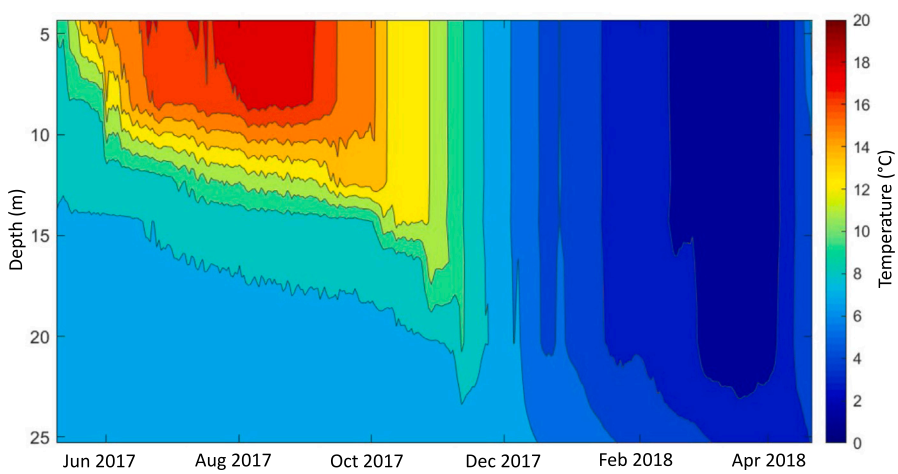

Fig. 7. Temperature profile from Lake Knudsø during 2017 and 2018 (Skaarup and Wahlberg, 2019; Temponeras, 2019).

As opposed to running the hydrodynamical model continuously, running pre-simulated scenarios might result in a loss of dynamics and abrupt changes in flow patterns in the transition from one pre-simulation to another. Currently, it would be impossible to simulate a full hydrodynamical model with the same spatial and temporal resolution in real time, and thus some simplification is required for real-time operation. In this case, the pre-simulations have a clear advantage since the model resolution is not compromised.

3.3. Particle dispersion model

The developed particle dispersion and decay model is designed to simulate the transport and decay of fecal bacteria in Knudsø. It is implemented on top of the interpolated current fields to operate fast in real time. This is why it is chosen over the commercial options offered by DHI MIKE 3, such as the Particle Tracking Module (DHI, 2019d) or the Advection-Dispersion module (DHI, 2019c).

The model uses a random walk model to simulate particles' horizontal and vertical transport, taking into account advection and dispersion. This is achieved by drawing random numbers from a standard normal distribution. Random walk models are preferred for particle transport modeling because they are simple and do not introduce numerical dispersion (Dunsbergen and Stalling, 1970).

Particles are released at the discharge point in the model based on the overflow volume modeled by the linear reservoir model. The transport of these particles is then calculated using the following expressions (Larsen, 1983):

$$x_i = x_{i-1} + v_x \cdot \Delta t + Z_1 \sqrt{2 \cdot v_h \cdot \Delta t} \quad (3)$$

$$y_i = y_{i-1} + v_y \cdot \Delta t + Z_2 \sqrt{2 \cdot v_h \cdot \Delta t} \quad (4)$$

$$z_i = z_{i-1} + v_z \cdot \Delta t + Z_3 \sqrt{2 \cdot v_v \cdot \Delta t} \quad (5)$$

Where x, y and z are the particle positions, i is the temporal index, v is the flow velocity in the x, y and z directions, respectively, Δt is the time step, Z is a random number from the standard normal distribution, and v is the horizontal and vertical eddy viscosity, respectively. Velocities and eddy viscosities are fixed based on the pre-simulations.

In the particle tracking model, we assume the same density of particles as the water and do thus not allow for sedimentation processes of particles nor buoyancy of diluted wastewater in the model setup. This is indeed a crucial assumption which sometime in the future could be investigated further.

The decay in concentrations of E. coli and enterococci over time due to sunlight exposure is modeled by a first-order decay model that accounts for factors such as water temperature, solar irradiation, and visibility depth (secchi depth) (Sagarduy et al., 2019; Šolić and Krstulović, 1992). This model allows us to predict the rate at which these fecal bacteria will decay over time and, therefore, the concentration likely to be present in a given water body:

$$C = C_0 \cdot exp(-k \cdot dt) \quad (6)$$

Where C is the concentration of coliform bacteria, C_0 is the initial concentration of coliform bacteria, dt is the time step and k is a decay constant that depends on the water temperature, solar irradiation (secchi (transparency) depth, and sunlight exposure). We use climatological averages of solar irradiation, water temperature, and secchi depth since sensitivity analyses of decay rates in Skaarup and Wahlberg (2019) have shown minor importance of inter-annual variability. The details of obtaining a time-varying k can be found in Skaarup and Wahlberg (2019), Erichsen et al. (2006), Sagarduy et al. (2019).

The initial concentrations of E. coli. and enterococci in CSO spills are fixed to $2.4{\cdot}10^6$ cfu/100 ml and $9.2{\cdot}10^5$ cfu/100 ml, respectively. This is based on a weighted average of literature values from raw wastewater and stormwater from Erichsen et al. (2006), who, based on Danish conditions, report an average concentration of E. coli. and enterococci of $4.5{\cdot}10^7$ cfu/100 ml and $3.4{\cdot}10^6$ cfu/100 ml in raw wastewater as well as $2.0{\cdot}10^4$ cfu/100 ml and $8.0{\cdot}10^3$ cfu/100 ml in runoff from impervious urban surfaces. By estimating the average ratio between waste and stormwater in the CSO discharge, we estimate the aforementioned values, acknowledging that these are indeed uncertain.

These estimated weighted initial concentrations are in the upper end of the sampled concentration intervals from the U6 outlet (Table 2). However, in the conducted samples, some initial dilution is to be expected since samples are taken in the lake just outside the U6 outlet and therefore the initial bacterial concentrations from the CSO are expected to be larger than the average of the conducted samples in the outlet. For this reason, we consider the weighted average of both E. coli and enterococci to be applicable to initiate the model. We recognize that these parameter values exhibit a significant correlation with factors such as antecedent dry weather periods or the occurrence of first flush phenomena. As a result, their time-fixed values are subject to uncertainty in the integrated model setup. This is discussed further in Section 5.

In the particle tracking model, the overflow concentrations are implemented by releasing 100 particles for every 1 m^3 of overflow.

3.4. Warning system

The warning system framework combining Section 3.1, 3.2, and 3.3 is set up in a MATLAB environment to operate in a hindcast mode (for analysis of historical events) or in a nowcast mode (for real time operation). The flow chart of Fig. 5 shows how the individual parts of the model are connected: The linear reservoir model forced by a rain series input provides a boundary condition time series of fecal bacteria concentrations proportional to the modeled CSO discharge. This time series is applied as boundary conditions to the particle dispersion model. By interpolating the hydrodynamical pre-simulations, which cover the present wind speed and wind direction, a current field is implemented in the particle model for the present time step. The particle dispersion model simulates the transport and dilution of fecal bacteria, and the decay model decreases the fecal bacteria concentrations by a transient decay term. In the integrated warning system framework, the model chain is executed every 30 min and thus updated with new boundary conditions for every model run using the final number of particles and their individual position from the former simulation as an initial condition for the new run.

If in any of the simulation runs, the pollution plume from the CSO structure reaches the designated bathing area, and the fecal bacteria concentrations are exceeded by 500 cfu/100 ml for E. coli and 200 cfu/100 ml for enterococci, the model will activate an electronic warning sign at the beach. This measure ensures that bathers are promptly and directly notified of any potential hazards to their health resulting from poor water quality. The warning is canceled when the concentration is simulated below the threshold for at least 30 min.

In the current available sampling campaign and modeling framework we do not have enough data to fully calibrate the sub models individually nor to estimate the confidence in every parameter value. We, therefore, use the following Section 4 to justify choices of parameter values in the modeling framework, however acknowledging that there is indeed subjectivity related to the choice of parameter values. This is also discussed further in Section 5.

4. Results

4.1. Combined sewer overflow model

The linear reservoir model is calibrated to estimate average overflow volumes in accordance with recorded accumulated overflow discharges for the year 2021 (Fig. 8, left). The calibration procedure is executed by manually adjusting the reservoir lag time, t_{lag} minimizing the absolute error between modeled and observed daily over flow volumes for the year 2021. Fig. 8 (right) shows an example of modeled and observed time series of overflow discharge from the event June 20, 2021. Here we show the results for both observed and modeled overflow. It is, however, intended that, in practice, the overflow should be calculated in real-time using only rainfall data as input (Fig. 8 top, right). The calibration, therefore, provides the foundation for real-time estimation of overflow discharges, which is used as an input to the hydrodynamical model.

4.2. Hydrodynamical modeling

To validate the hydrodynamical model, simulated flows are compared to drifter trajectories as described in Section 2.4. The drifter trajectories are observed in winter and spring periods and consequently represent periods without expected thermal stratification in the lake. The comparisons are therefore solely based on the model setup initialized without stratification. While the drifter experiments are conducted over a short time frame and in a specific region of the lake and may not fully represent all possible forcing conditions, the model-derived trajectories shown in Fig. 9 still show good agreement with the observed trajectories. Based on these results, it is estimated that the hydrodynamic model can effectively predict the currents and pollution dispersion in the lake. However, ideally, a full calibration of the hydrodynamical model would have been executed if more trajectory data were available both during different periods of the year or in locations of the lake with varying bathymetry. Moreover, drifter experiments with a drouge positioned in different depths could help to obtain a full understanding of the influence of thermocline, windshear, etc. on the three-dimensional current field.

4.3. Pollutant transport modeling

Simulations of the four events (May 5, May 25, June 20, and July 5–6) are conducted using the particle dispersion model. Despite the extremely high levels of E. coli and enterococci present in the CSO outlet (Fig. 3 and Table 2), the measured concentrations did not surpass the bathing water criteria during the first three events at the bathing area of Sdr. Ege (Table 3). However, the criteria is significantly exceeded during the July 5–6 event. The following sections provide a detailed analysis of each of the four events:

Event May 5: The overflow event on May 5, 2021 results in a modeled overflow volume of 60 m^3 (41 m^3 observed) and is thus a rather small event compared to the other. Although none of the water samples taken at the bathing area show fecal bacteria concentrations above the bathing water criteria, the simulations show that the criteria are still compromised during the event. Fig. 10 illustrates the simulated pollution plume at four 30-minute intervals starting on May 5, 14:00. From the figure, it is clear that due to a west-northwest wind, the pollution spreads from the outlet to the bathing area, resulting in simulated concentrations of up to 1,000,000 cfu/100 ml of E. coli at the Sdr. Ege beach (Fig. 11). The overflow occurs at 12:06, and samples are taken in the period between 12:30 and 13:00. Therefore, the water samples are collected before the pollution plume reaches the bathing area Sdr. Ege at approx. 13:30. In retrospect, it would have provided more insight into the event to conduct more water samples in a period of time following the overflow occurrence.

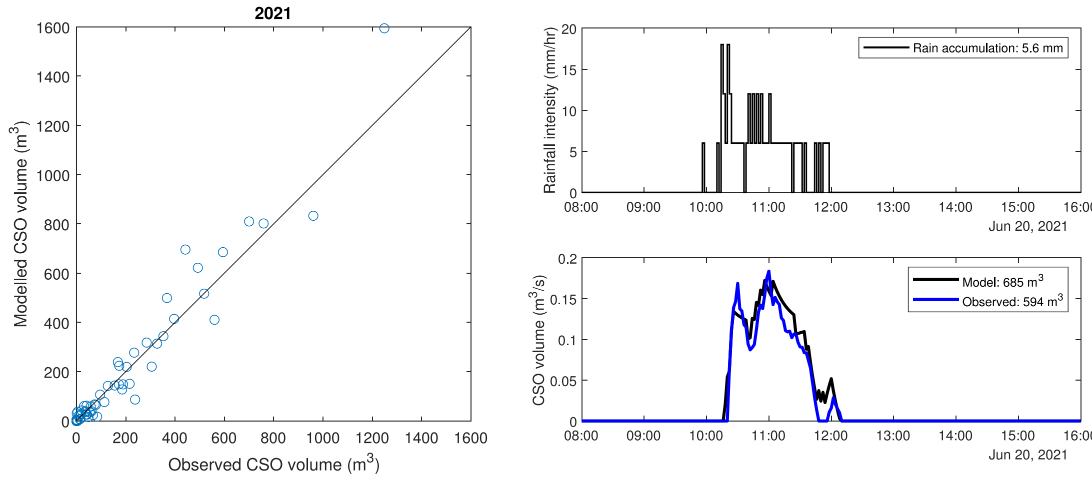

Fig. 8. Left: Modeled and observed daily overflow volumes for the whole year 2021. There are 52 overflow events in total in 2021 and the observed and modeled data is correlated by a $R^2 = 0.96$. Right: Example of rainfall input as well as observed and modeled time series of CSO from the event June 20, 2021.

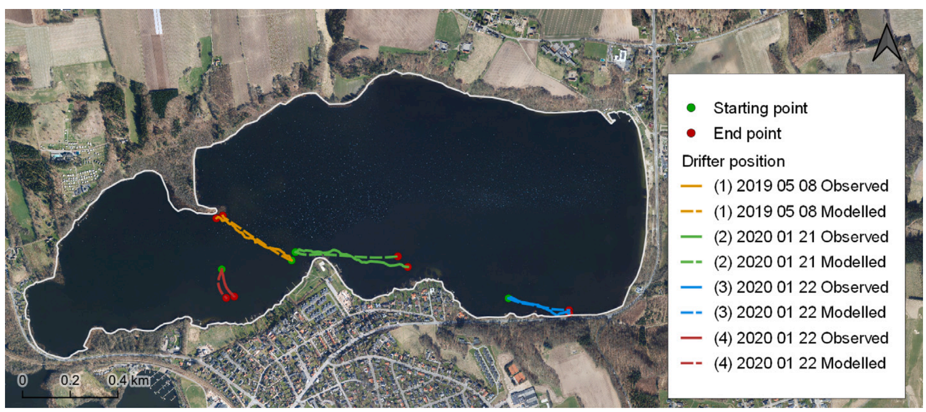

Fig. 9. Observed and modeled drifter trajectories in Knudsø.

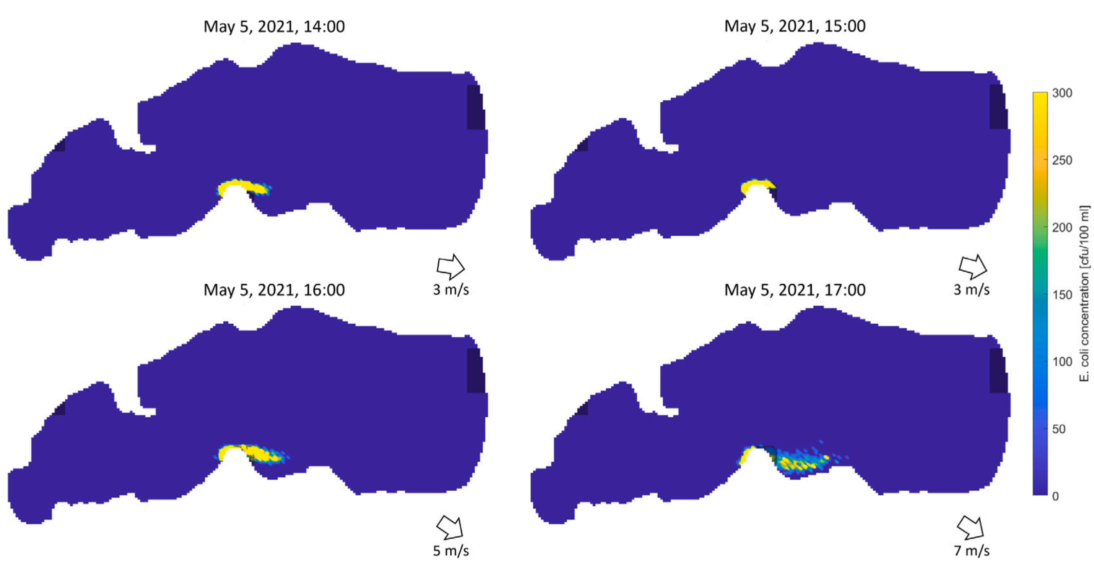

Fig. 10. Simulated spatial distribution of E. coli concentrations at hourly time steps succeeding the overflow event on May 5, 2021.

Since the data collected for the event were sampled before the pollution plume arrived at the bathing areas, we studied the sensitivity of the model framework in terms of arrival time of the plume. This is conducted by increasing the initial concentration of fecal bacteria as well as decreasing the decay constant. The arrival time of the plume is however not affected by the initial concentration and since the transport time from the U6 outlet to the bathing area of Sdr. Ege, in this event is very short, there is not any significant decrease in concentrations due to decay. In this case, the independence of model parameters contributes to a heightened level of reliability in the model.

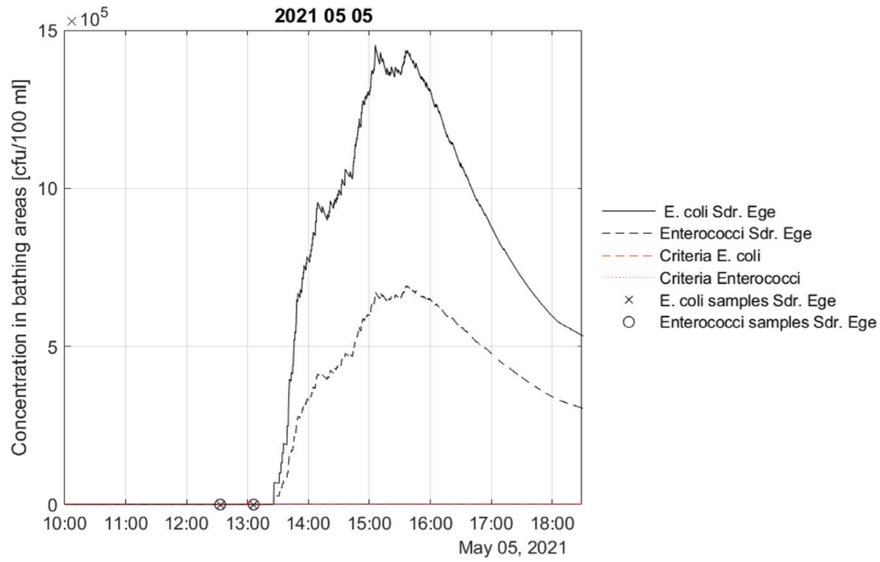

Fig. 11. Simulated og sampled concentrations of E. coli and enterococci at the bathing area at Sdr. Ege Beach on May 05, 2021.

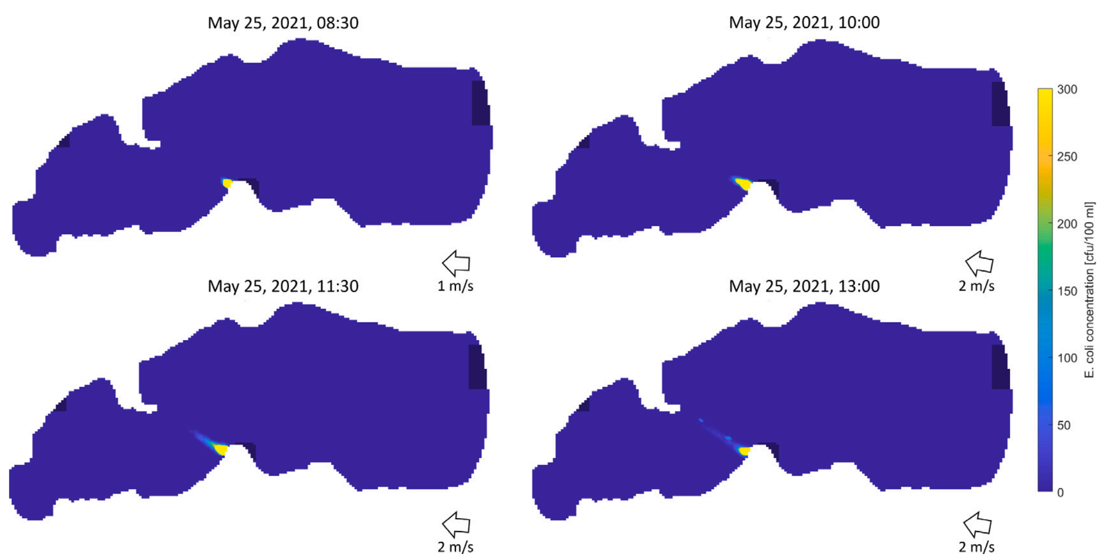

Fig. 12. Simulated spatial distribution of E. coli concentrations at 4-h time steps succeeding the overflow event on May 25, 2021.

Event May 25: The overflow event on May 25, 2021 yields a modeled overflow volume of 150 m^3 (215 m^3 observed). A sample taken from the CSO outlet revealed high levels of E. coli (59,000 cfu/100 ml) and enterococci (163,000 cfu/100 ml). The primarily eastward wind carries the pollutants away from the Sdr. Ege beach area towards the northwest, as shown in Fig. 12. This advection of the pollution plume is further supported by the fact that no fecal bacteria pollution is sampled at the bathing area of Sdr. Ege (Fig. 3).

Event June 20: The overflow event on June 20, 2021 has led to a modeled overflow volume of 685 m^3 (594 m^3 observed). The event is similar to the one on May 25, with high concentrations of E. coli (1,020,000 cfu/100 ml) and enterococci (1,170,000 cfu/100 ml) being sampled in the CSO outlet during and shortly after an overflow event. However, due to the eastern and southeasterly wind directions, the pollution is transported away from the bathing area in Sdr. Ege as shown on the maps in Fig. 13. The enterococci levels at the bathing area are sampled to be slightly higher than the criteria for excellent water quality, measuring at 300 cfu/100 ml (Table 1). Given that the pollution plume is moving northwest, it is believed that the sampled increased level of enterococci is due to an overflow event that occurred on June 19 since the concentration of enterococci is observed to decrease from the maximum of 300 cfu/100 ml to 0 cfu/100 ml over the course of the June 20 event.

Event July 5–6: The overflow event on July 5, 2021 results in a modeled overflow volume of 1,300 m^3 (1,600 m^3 observed). Nine water samples are taken at Sdr. Ege Beach following the event (Table 3). No fecal bacteria are detected at the beach in the first 5.5 h after the overflow. However, a sample taken around 9.5 h after the event shows significantly higher concentrations of E. coli and enterococci than bathing water criteria (Fig. 15). A sample taken the following day at the bathing area, 18 h after the overflow event, shows no contamination with fecal bacteria, indicating rapid changes in fecal bacteria concentration in the upper water column (see Fig. 14).

The concentrations in the bathing areas – as measured and modeled – are displayed in Fig. 15. The measurements and model results are in good agreement during the period when no fecal bacteria are detected in the bathing area. The measurement taken around 23:00, which shows high concentrations, is consistent with the concentration levels of the model. Both measurements and model results suggest that a warning should be issued for the bathing area. Additionally, the correlations between E. coli and enterococci are similar in both measurements

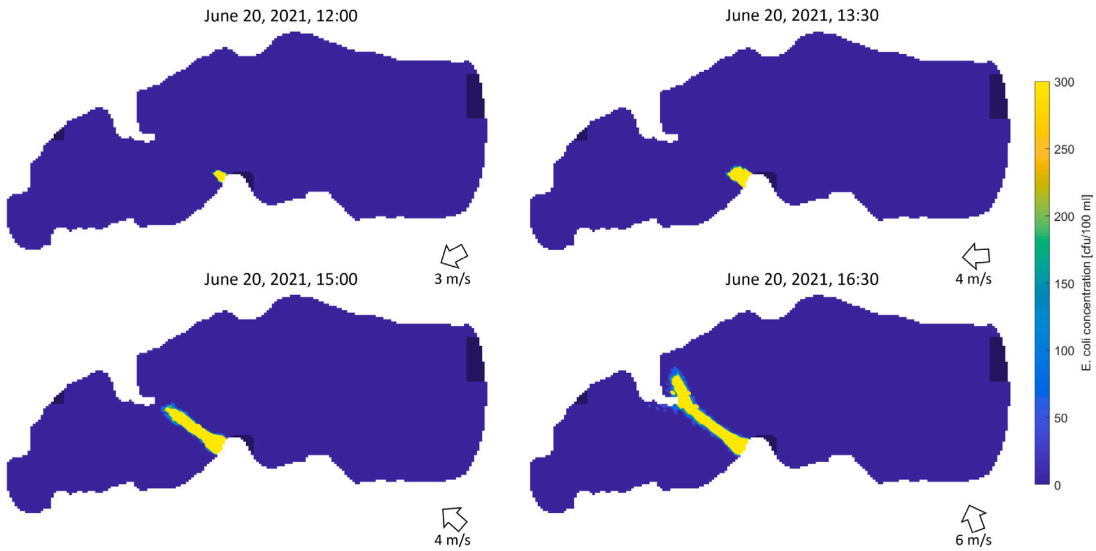

Fig. 13. Simulated spatial distribution of E. coli concentrations at 4-h time steps succeeding the overflow event on June 20, 2021.

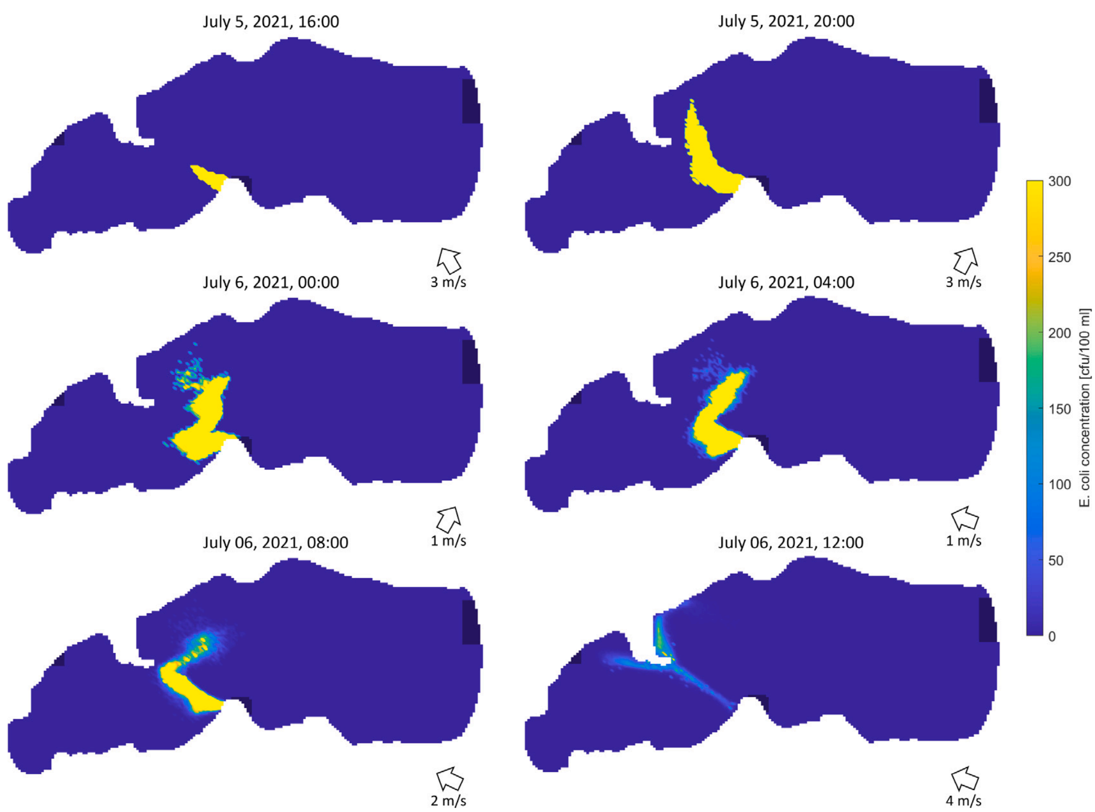

Fig. 14. Simulated spatial distribution of E. coli concentrations at 4-h time steps succeeding the overflow event on July 5 and 6, 2021.

and model simulations. Minor discrepancies in concentrations may be explained by factors such as pollutant dispersion, estimation of concentrations in the overflow discharge, biological decay, or sampling location. Furthermore, the model predicts high concentrations at around 07:00 the following day; however, measurements taken at that time do not show increased fecal bacteria concentration. This discrepancy suggests that the modeled decay rate may be lower than the actual decay rate. However, there are insufficient data to adjust the decay term based on this. Nevertheless, it is clear that the samples taken during the event indicate poor bathing water quality at Sdr. Ege Beach and this conclusion is supported by the dispersion model as well. Consequently, it is evaluated that the dispersion model provides reliable results. If more calibration data becomes available in the future, such discrepancies might be reduced or explained in more detail for other events.

4.4. The combined warning system

In earlier sections, we have presented simulation results for fecal contamination during four events. These simulations are conducted retrospectively, meaning the warning system did not operate in real time. However, there are no technical obstacles in implementing a real-time system using the current setup. A warning for poor water bathing quality can be issued using an electronic panel, as illustrated in Fig. 5.

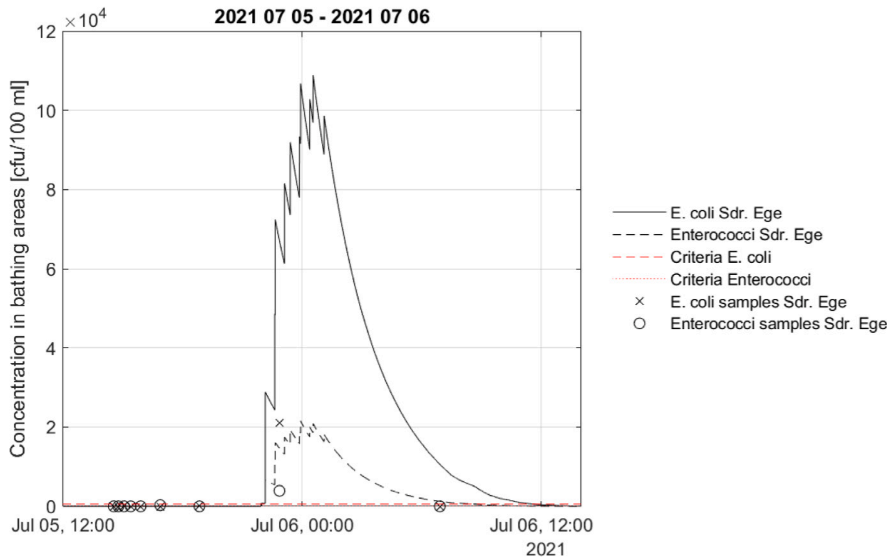

Fig. 15. Simulated og sampled concentrations of E. coli and enterococci at the bathing area at Sdr. Ege Beach on July 5–6, 2021.

5. Discussion

It is evident that there are significant uncertainties in the presented framework regarding sampling and modeling. Some of these uncertainties need further investigation before real-time setup implementation. The presented current setup is basically based on a qualified adjustment of the model parameters related to pollutant concentrations rather than a proper calibration procedure (except for the linear reservoir model). Hence, some uncertainties or current discrepancies between observations and models might be quantified and reduced by further calibration. In the following, we describe the main uncertainties and discuss the challenges and impacts of each part of the model and water sampling in terms of model calibration and general improvement of the warning model framework.

The combined sewer overflow model generally provides reliable outputs to the modeling framework due to calibration of the linear reservoir model against flow observations. Uncertainties in rainfall input and catchment descriptions are of minor magnitudes compared to other modeling uncertainties. One could argue that if permanent flow monitoring were installed in outlets from CSO's, the linear reservoir model could be omitted and the input to the particle dispersion model could be based on directly on observations instead of model simulations.

The hydrodynamical model and the resulting current fields are difficult to calibrate/validate and represent during multiple forcing situations, and, in this study, it has only been possible to validate the currents by drifter trajectories under a few forcing conditions. Furthermore, the thermocline's stratification and dynamics can be challenging to model and validate. In Lake Knudsø, it is primarily the windshear that causes the currents in the lake and, therefore, the windshear, along with the seasonal temperature changes, that causes the stratification to break. Since we focus on the summer months, we assume a strong stratification as measured prior to this study. A proper calibration would require drifter experiments under multiple forcing conditions in different seasons of the year in order to e.g., adjust the turbulence model, or wind friction factors in the hydrodynamical model. The fact that we do not simulate the full hydrodynamical model transient in real time, but rely on interpolations of pre-simulations under stationary conditions might entail a loss of some dynamics in the model. As argued earlier, we simulate with an initial stratification in the summer period which in some situations might be wrong.

The particle dispersion model depends on valid dispersion coefficients (derived from eddy viscosities). In this case, we rely on the eddy viscosities simulated by the hydrodynamical model. Furthermore, the initial concentrations are associated with significant uncertainties. As shown in the water samples from outlet U6 (Table 2), the concentrations of fecal bacteria vary over decades under the course of an event. A calibration of initial concentrations is therefore difficult to generalize for multiple conditions. In this case, rather than using fixed values for the initial concentrations of E. Coli and enterococci in the CSO water, simulations with a span of likely concentrations might help to estimate the uncertainties related to the crucial parameters describing initial concentrations, and thereby propagate uncertainties related to predicting critical bacteria concentrations at bathing areas.

We assume the fecal bacteria to be transported in the upper water column; however, some density differences between diluted wastewater and the upper water column in the lake might affect the vertical transportation of diluted wastewater and the fecal bacteria. The decay and decomposition of the fecal bacteria are dependent on temperature and concentration levels. In Lake Knudsø, these processes are poorly understood, and consequently, crude assumptions are made in the model setup.

Despite our knowledge of significant uncertainties in the transport modeling of pollution plumes as well as the decomposition processes of coliform bacteria, we still believe that we can capture the most predominant processes and thereby quantify the risk of bathing water contamination. In the events with sample observations of significantly exceeded bathing water quality criteria, the model can capture the situation where no pollution is transported to the designated bathing area and the situation where pollution is transported directly to the bathing area. Even though the specific concentration levels might be subject to some uncertainty, the setup proves a causal and explainable relationship between observations and the model.

As also shown, representative water sampling can be complicated and change orders of magnitude within minutes. Accordingly, taking a representative water sample and using this as the infallible truth for that specific point and time is unrealistic and complicates model validation. Furthermore, other sources of fecal bacteria, e.g., from animal feces or bacterial growth in sediments, might also contribute to increased bacterial activity. This is not included in the modeling framework. In order to estimate uncertainties and possibly improve the data quantity for calibration, increasing the number of samples during and after rain events could be a possibility in order to further improve the warning system framework. Another possibility could be to monitor other parameters (e.g., turbidity, nutrient concentrations, etc.), which are easier and cheaper to monitor in real time (North et al., 2014). A correlation between these additional parameters and the presence of E. coli and enterococci might help to further improve model predictions and uncertainties in model predictions. Potentially, this could lead to data assimilation of parameter values or adjustments of the model to, in real time, adapt the model to the present conditions.

6. Conclusion

This paper presents data from the regulatory sampling at a bathing area in Lake Knudsø, Denmark. The sampling required by the EU bathing water directive shows no sign of fecal bacteria pollution at the bathing area of Sdr. Ege. However, the subsequent classification of the location having excellent bathing water quality at all times is questionable. The fact that a combined sewer overflow outlet is located close to the designated bathing water area raises several questions on the transport and fate of fecal bacteria in the lake. It is shown that the overflow frequently spills diluted wastewater into the lake and that the fecal bacterial concentration of this diluted wastewater occasionally is very high. By modeling four events where an intensive sampling campaign has been executed, it is shown that during some forcing conditions, the pollution plume is transported away from the bathing area and therefore does not propose a risk of polluting the bathing water. During other wind-forcing conditions, however, the fecal bacteria are transported directly to the designated bathing area, causing exceeded criteria for bathing water quality.

The main conclusion of this paper is, therefore, that the sampling for excellent bathing quality is very dependent on location and time in order to measure poor water quality. The required four samples each year, as specified by the EU bathing water directive, are insufficient to estimate the risk of having temporarily impaired bathing water quality during a bathing season. Sampling and modeling results show that the bathing water quality can be significantly compromised during single events with spills of diluted wastewater. Hence, the regulations specified by the bathing water directive are probably better for identifying poor bathing water quality due to constant or frequent discharge of wastewater or high background concentrations in local areas.

The proposed warning system is a feasible alternative to frequent water sampling to identify poor bathing water quality. The setup is able to simulate the risk of poor water quality continuously. Bathing prohibition can be issued based on model simulations. Moreover, the model framework can also be used to initiate targeted sampling of water quality in order to map the fate and transport of pollutants further.

It is however important to emphasize that in the existing configuration, there is a degree of subjectivity involved in setup of the individual parts of the model, the assessment of model parameter values, and choice of initial conditions. These aspects can introduce uncertainty into the model's predictions. There is, if implemented in a real-time warning system, potential to continuously increase the reliability of the model predictions by including more samples of fecal bacteria in outlets, bathing areas, and other parts of the lake, as well as more experiments studying the flow currents in the lake.

CRediT authorship contribution statement

Søren Thorndahl: Writing – original draft, Revision, Formal analysis. **Janni Mosekær Nielsen:** Reviewing, Editing, Figures and modelling. **Michael R. Rasmussen:** Reviewing, Funding, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Soren Thorndahl reports financial support was provided by Danish Environmental Protection Agency (MST).

Data availability

The authors do not have permission to share data.

Acknowledgments

The authors would like to acknowledge the partners in the project *Safe Recreational Lake Waters II* for their contributions to project management, water sampling, analysis, and ideas: Rikke Markfoged (Danish Technological Institute), Stig Jonassen (Skanderborg Forsyning), and Sara Elsborg Starcke (Niras). Furthermore, the authors would like to acknowledge the Danish Environmental Protection Agency (Danish EPA) for funding under the MUDP program (The Danish Eco-Innovation Program, https://ecoinnovation.dk/english/).

The authors acknowledge the students at Aalborg University who have used this project as a case for their master's theses (Steffen Skaarup and Pernille Wahlberg in 2019, Janni Mosekær Nielsen and Claus Fastrup in 2020, and Tobias Sandegaard Aarsnes and Mikkel Ledet Nielsen in 2022) and bachelor thesis (Lise Ditte Nielsen in 2022).

Finally, the authors acknowledge the use of temperature data provided by Maria Temponeras from Skoleskibet Ry (Temponeras, 2019).

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