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Dynamic modelling of bathing water quality with biodegradation of Escherichia coli in TELEMAC-3D

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Abstract

Bathing water is of great concern as almost all bodies of water in Sweden today are affected by human activities. Usage of models for bathing water quality may give the possibility to assess and evaluate short-term contamination. The main objective of this thesis was to develop and evaluate a script for degradation of the faecal indicator bacteria Escherichia coli, E. coli, in an aquatic environment. This to deeper understand, predict and identify spreading and degradation of E. coli in bathing water in the future. A literature study focusing on how bathing water quality is classed and how E. coli is degraded in aquatic environments was performed. The literature study formed the basis for an implementation of an exponential first-order degradation model of E.coli in TELEMAC-3D and a performed sensitivity analysis of the used degradation model of E.coli. It has been concluded that the developed script for degradation of E. coli in TELEMAC-3D is operating in accordance with the used exponential first-order degradation model of E.coli. However, there is limited information found of how E.coli is degraded and described mathematically. It was found that the major factors controlling the degradation of E. coli are light intensity at the surface and water temperature. A simplified case with the set-up of an experiment in a form of a simple geometry was modelled. For the simplified case, the results from calculations by hand, a simulation in TELEMAC-3D and the experiment were compared. It could be concluded that the calculations by hand and the simulation in TELEMAC-3D are best correlating with each other, while the experiment differs from the analytical calculations by hand and simulation in TELEMAC-3D. A reason for this might be that information concerning how the experiment was conducted were limited. On the other hand, that the calculations by hand and the simulation in TELEMAC-3D was correlating shows that the developed script is working in accordance with the used exponential first-order degradation model of E. coli. Overall, it can be said that empirics and research of how E. coli are degraded is restricted and further research is needed to gain a deeper knowledge of bathing water quality.

Contents

Abbreviations

CFUs: Colony Forming Units

CSO: Combined sewer overflows

E. coli: Escherichia coli

IE: Intestinal Enterococci

SPM: Suspended Particle Material

Definitions

TRACER: A substance introduced into a biological organism or other system so that its subsequent distribution may be readily followed from its colour, radioactivity, or other distinctive property.

T90-value: The persistence of a fecal indicator can be described by the time for a 90% reduction of fecal indicator concentrations (T90-value).

1 Introduction

In this section, some background information on bathing water quality is first presented followed by a presentation of the project aim and objectives. The method used to research the objectives are then presented. At last, the limitations of the thesis are presented.

1.1 Background

Bathing water quality is important for many people. It affects the planning for the vacation and our recreational activities. The needs and requirements for deeper knowledge of bacteria and other microorganisms from urban areas, and how these may affect its recipients, has increased since the Bathing Water Quality Directive (2006/7/EG) was introduced in 2006 by the European Union. Especially important questions to highlight are how contamination of bacteria can affect the bathing water quality. The Bathing Water Quality Directive (2006/7/EG) is an initiative that aims to give the public an opportunity to choose a good bathing site. (Havs- och vattenmyndigheten, 2016b)

To estimate the microbial water quality the water is often collected and evaluated with analytical methods. However, in recent time the interests of understanding and evaluating the bathing water quality further through different hydrodynamic models has increased. For example simulations in computer models can be performed to describe the hydrodynamic situation in a water body and take the decay of microorganisms in the environment into account. This is preferable as a complement to the analytical testing of water. Moreover, with help of hydrodynamic modelling, the spatial and temporal variability of microbial concentrations can be described. The influence of different faecal sources from e.g. stormwater and overflow from sewage pipes can also be studied with hydrodynamic modelling. Several scenarios and situations can be simulated and thus be used for predictions and forecasts. (Sokolova, 2013a)

The long-term climate predictions indicate that the intensity of precipitation events will increase, which increases the load on the sewage systems. However, taking in mind the current capacity of the sewer system it is likely that more frequent sewer overflow events will occur giving a higher risk of contamination in water bodies. In this context, hydrodynamic modelling constitute a suitable tool to represent and forecast the impact of these extreme weather events on the bathing water quality. Furthermore, it gives opportunities to provide short-term forecasts on bathing water quality and more specifically in this case Escherichia coli, E. coli. (Sokolova et al., 2013b)

Moreover, as the risk of unhealthy bathing water increases, the demand for predictions of bathing water quality will also increase. This also increases the demand on that the models are verified with empirical data.

This Master Thesis was made in cooperation with *SWECO Environment*, *Kust och Vattendrag*, in Malmö. The group *Kust och Vattendrag* started to work with the open source software TELEMAC in order to develop their own applications and to decrease the costs put on software as well as the transparency of the mathematical calculations that the software offers. This has led to that this Master Thesis took form and that TELEMAC-3D was used to develop a script describing the biodegradation of E. coli for predictions of bathing water quality. TELEMAC-3D is a set of modelling tools allowing to treat every aspect of natural free surface hydraulics: waves, currents, transport of tracers and sedimentology. The code in TELEMAC-3D solves three-dimensional equations such as the transport-diffusion equations of intrinsic quantities (salinity, temperature, concentration) and the free surface flow equations. (EDF R&D. 2016)

1.2 Project aim and objectives

The overall aim of this master thesis is to develop and evaluate a script for biodegradation of the faecal indicator bacteria E. coli in a marine environment. This to be able in the future to deeper understand, predict and identify spreading and degradation of bacteria in the bathing water.

The following sub-objectives will form the basis for the degree project:

- To investigate how biodegradation of E. coli occurs in aquatic environments through a literature study.
- To interpret and assess how biodegradation of E. coli can be mathematically described in aquatic environments through a literature study.
- Develop and evaluate a TELEMAC-3D script for biodegradation of E. Coli.

1.3 Method

In the following section, the method used to accomplish the objectives is described. The method consists of four parts that are presented below: Literature study, Theory and modelling of TELEMAC-MASCARET, a Sensitivity analysis and a Simplified case.

1.3.1 Literature study

A literature study has been conducted focusing on highlighting how bathing water quality is classified and how the faecal indicator E. coli is theoretically degraded in a marine environment. The literature study forms the basis for the design of the bathing water quality script.

1.3.2 Theory and modelling of TELEMAC-MASCARET

Theory and information of TELEMAC-MASCARET are first presented followed by a description of the developed script for biodegradation of E. coli in TELEMAC-MASCARET.

1.3.3 Sensitivity analysis

A sensitivity analysis was done in Python 3.6 of the used equation for degradation of E. coli. The analysis was done in order to analyse which parameters and variables that are most important for the degradation of E.coli according to the used equations.

1.3.4 Simplified case

A simplified case with the set up of an experiment in the form of a simple geometry (a tank) was modelled. The simplified case was performed in order to compare the developed script with the results of the experiment and with calculations of the equation by hand in Excel.

1.4 Limitations

The main limitations of the study are that no input data to the model is available and that during the study it was found that there were little empirical data that the developed script could be validated against. The reasons for this is that it is a new way of studying bathing water quality and that municipalities have not yet started to take analytical samples applied to models like this one. Important to notice is that there are also other causes of poor bathing water quality, such as algae bloom or other types of pollutants such as Intestinal Enterococci (IE). Both "algal bloom" and IE are sometimes included as a parameter when judging the bathing water quality. However, these parameters have not been covered in this project more than that IE has been shortly mentioned in the literature study. Furthermore, another limitation is that there is limited information of how E. coli is degraded and how this is described mathematically. Making the uncertainty of the developed script high as background information of the implemented first-order degradation model for E. coli is limited.

2 Literature study

In this section, it is first described what bathing water quality is along with the implementation of the Bathing Water Directive (2006/7/EC) followed by information of the current situation of Bathing water quality today. Secondly, information is presented concerning what a microbial indicator-bacteria is and how it can be used when studying bathing water quality. At last, factors affecting the degradation of E. coli and how it is described mathematically is presented.

2.1 Legislation of bathing water quality

In Sweden, today almost all bodies of water are affected by human activities. To secure the future use and quality of our water resources the European Union (EU) introduced the EU - Water Framework Directive (2000/60/EU) in 2000 that was implemented into the Swedish legislation. The main objective was that in 2015 have "Good ecological status" in our surface water and "Good chemical status" in the groundwater. In 2006 the European Union introduced new environmental goals through the Bathing Water Directive (2006/7/EG) with the aim to improve the bathing water quality at official bathing sites so-called EU baths in the member states. The Bathing Water Directive is transposed into Swedish legislation through the Badvattenförordningen (2008:218) with support in chapter 5 and 9 in the code Miljöbalken that is a part of the Swedish law concerning environmental issues as well as the regulations and general advice in (HVMFS 2012:14) and (HVMFS 2016:16) through the Swedish Water Authority, Havs- och vattenmyndigheten, in cooperation with the Swedish Public Health Authority, Folkhälsomyndigheten. (Svenskt Vatten AB, 2011a)

2.1.1 The Bathing Water Directive (2006/7/EC)

The Bathing Water Directive, 2006/7/EC, is an EU directive that was stated in order to protect people's health. Its main purpose is to ensure that the public is informed about the bathing water quality. The Directive regulates what is considered to be acceptable water quality at seaside resorts that have over 200 visitors per day during the bathing season. For the bathing areas that have fewer visitors, it is voluntary to register and control as EU baths. In order to be able to reach the directive, water samples at bathing sites are collected, tested and inspected regularly by the municipality to detect possible contaminants by studying faecal indicators such as the bacteria E. coli and Intestinal Enterococci (IE). By detecting these organisms, the water quality can also be improved as well as gaining a deeper understanding of the variations, and movement of water quality in different areas. Leading to that the bathing water quality can be improved in areas where it is required. (Risinger, 2015)

The need and requirements for better knowledge of bacteria and other types of microorganisms that are present in the urban environment and how they may affect nearby recipients have during the last years increased as the new Water Quality Directive has been implemented. Especially important issues that are highlighted are how the emissions of bacteria can affect the bathing water quality. (Svenskt Vatten AB, 2011a)

2.1.2 Bathing sites not covered by the Bathing Water Directive (2006/7/EC)

Bathing sites that have less than 200 visitors per day, during the bathing season, are not covered by the Bathing Water Directive (2006/7/EC), (Risinger 2015). For these sites, the Swedish Water Authority (Havs- och vattenmyndigheten) recommend that the municipalities should follow the same routines as for the so-called EU-bathing sites even though it is not obligatory. A classification concerning water quality of the bathing sites may then be done likewise the EU-bathing sites, which may give a better water quality across the country. Even though these sites are not covered by the Bathing Water Directive (2006/7/EC) they are under supervision and follows chapter 26 in the code Miljöbalken and is practised by the municipality's regulatory authority. Furthermore, the municipality shall pay special attention to bathing facilities and bathing sites. This responsibility is reflected in Section 45, paragraph 5, of Regulation (1998: 899) on environmentally hazardous activities and health protection. (Havs- och vattenmyndigheten, 2016b)

2.1.3 The current situation and development of bathing water quality in Sweden

According to Havs - och vattenmyndigheten (2017), the clear majority of the EU baths in Sweden are today having a good water quality. Prior to the 2017 bathing season, the bathing water quality is classified as "excellent", "good" or "satisfactory" for 400 of Sweden's 444 EU bathing sites, equivalent to 90.1%. This is an increase compared with previous years and the number of sites that have been properly tested has also increased. These results are based on four to six water samples per year, where the analyze takes a couple of days. The water samples, therefore show a long-term result of the water quality at the bathing sites due to that during this time the bacteria have already been degraded or transported from the sampling site. Five Swedish EU bathing sites (1.1%) have been rated "bad" bathing water quality, four fewer than last year. For these sites, investigations about sources of pollution and possible measures are needed. (Havs- och vattenmyndigheten, 2017)

Even though, most bathing sites according to Havs- och vattenmyndigheten show good water quality, bathing sites are most likely affected by faecal contamination and other bacteria from nearby urban communities or other sources of emissions. Pollutants from municipal sewage treatment plants and stormwater are distributed through waste-water pipes directly or indirectly to nearby recipients and a bacterial impact on coastal sites can therefore not be ruled out. At the same time, there is an increased interest in having bathing sites in or close to urban areas. (Svenskt Vatten AB, 2011a)

Until the nineties, stormwater was only discussed through the aspect of flow and load. However, during the end of the nineties, the composition of the stormwater gained more focus. This led to that wetlands and dams being built on a large scale across the country. The aim was to separate the pollution from the water. Unfortunately, most of these constructions were introduced without knowledge of specific pollutants or how recipients are affected by the discharge of stormwater and treated wastewater to recipients. (Svenskt Vatten AB, 2011a)

During the last decades, a changed system thinking has been seen. Today the water is delayed and collected into fewer and more concentrated overflow pipes. At high-flow situations, a part of the wastewater can be diverted past the wastewater treatment plant. Storage tanks and improved control functions have been added, reducing the risk of unnecessary overflow of untreated wastewater. Stormwater is being separated to an increasing extent, and the wastewater treatment plants are thus less stressed. Furthermore, stormwater is more often led to open ponds before it is finally released to the recipient. (Svenskt Vatten AB, 2011a)

A need to develop simple methods to be able to evaluate the pollution of different types of bacteria (indicator bacteria) and other microorganisms from urban areas and how these can influence recipients and bathing sites has during the last years been identified. (Svenskt Vatten AB, 2011a)

With the use of modelling bathing water quality, it may be possible to assess and evaluate short-term contamination. This may lead to that in the near future it can be possible to introduce a form of bathing water alert for areas affected by short-term pollution. These form of bathing water alerts have already been implemented in big parts of the Danish coast and in some parts of the Swedish coast. Furthermore, with help of models concentrations that are to low to detect by standard analytical methods can be viewed and detected. However, it is depending on how good the input is and if the model can be calibrated. The model also gives the opportunity to study the spreading of a contamination in a recipient, with transport to and from bathing water and dilution during the transport. If such a bathing water alert is introduced it may, on one hand, ensure that the bathing site is closed when there is a risk to the bathers' health due to the presence of pathogenic bacteria. On the other hand, it does not close unnecessarily as unnecessary closures may have a direct impact on the local revenue. (Erichsen et al., 2006) This Master Thesis is a step towards introducing assessment and evaluation of short-term contamination of faecal indicators at bathing water sites by implementing and modelling the degradation of E. coli in TELEMAC-3D.

2.2 Microbial Indicator Bacteria

To be able to analyse and make model calculations that represent how faecal bacteria can affect the bathing water quality, so-called indicator organisms can be used. Faecal indicators are generally used to detect the presence of faecal contamination in water. Indicator organisms normally occur in the intestine of both humans and warm-blooded animals and do not usually cause outbreaks of disease. However, if these bacteria are present in the water it is an indication that the water contains faeces or sewage and therefore also so-called faecal contaminants. Under normal conditions, these indicators do not grow outside the host organism. The indicators are relatively unproblematic from the point of view of infection. They are simple, can rapidly be analysed and can provide important information about possible effects of faecal contamination in, for example, bathing water. The main reason to use indicators instead of testing water for pathogens is due to the costs and complexity of pathogens. Two examples of bacteria that can be used as indicators are E. coli and IE. (Svenskt Vatten AB, 2011a)

Faecal indicator bacteria can come from a number of other faecal and non-faecal sources including sands, wrack, sediments, and submerged vegetation and not only from humans. However, according to Wang et al. (2013), the faecal bacteria from humans is expected to be the greatest risk to other humans, while exposure to other types of faeces is usually of a lower risk. (Wang et al., 2013)

According to Sokolova (2013a), the criteria for faecal indicators are that they should not be pathogens themselves. Furthermore, they should be universally present in faeces of humans and animals in large numbers, persist in water in a similar manner to faecal pathogens, not multiply in natural waters and be present in higher numbers than faecal pathogens. Sokolova continues to state that the indicator should respond to treatment processes in a similar way to faecal pathogens and be readily detected by simple, inexpensive methods. (Sokolova, 2013a)

Important to stress is that concentrations of faecal indicator bacteria e.g. E. coli are not directly related to the concentrations of pathogens in the environment. Some reasons for this is that indicator bacteria and pathogens have a different fate in the environment and that pathogens are only excreted by infected individuals as they are not a part of the normal faecal microbiota. Even so, indicators such as E. coli provide information about the degree of faecal contamination in a water source. Additionally, it can be said that if faecal contamination is present then pathogens are most likely also present. (Sokolova et al., 2013c)

The requirements for sampling of bathing water quality tests are specified in HVMFS 2012:1 and follows the international standard SS-EN ISO 19458:2006 in order to ensure a certain standard. Shortly described the sampling location, should be the place in the bathing water where most people are expected to swim or where the greatest risk of contamination is expected in the bathing water profile. The depth of water at the sampling location should, if possible, be at least one metre and the sample should be taken at 30 centimetres depth. The sample container should be transparent and of uncoloured material with a minimum volume of 250 ml and sterile at the time of sampling. Sampling shall be carried out with aseptic technique to prevent accidental contamination. The sample container should be labelled with a waterproof pen and noted with waterproof pen in the protocol. The sample should be protected from light and stored at a temperature of 4 °C ($\pm$ 3 °C) during storage and transport to the laboratory. The time between sampling and analysis should be as short as possible and the analysis should take place on the same day. If this is not possible, the analysis should begin within 24 hours from the sampling date. It is an advantage if the laboratory can quickly report the results of the analysis, especially if the sample is deemed "unfit" or "Valid with a remark". The test results should be reported to the website *Badplatsen* as soon as possible and no later than 10 working days after the sampling. The analyzes that are to be performed in accordance with HVMFS 2012:14 for each individual test are E. coli (CFU/100 ml) and IE (CFU/100 ml). (Havs- och vattenmyndigheten, 2013)

Colony Forming Units (CFU) refers to individual colonies of bacteria, mold or yeast. A colony is a mass of individual cells of the same organism that are growing together. It is used in order to determine the number of viable bacterial cells in a sample per ml or g that is how many capable-of-living microbes that are present in a certain measurement. By doing so it is possible to see the degree of contamination in a sample of e.g. marine water. To get the total number of colony forming units [CFU], the resulted colony forming unit per unit [CFU/ml] is multiplied by the total volume [ml]. (Goldman et al., 2008)

Limit values of individual analytical tests for the two indicator bacteria E. coli and IE for Sweden has been set through the Water Quality Directive 1976/160/EEG. New guidelines for the assessment of individual tests have not been made since then. Bathing water directive and the assessments limit values can be seen in table 2.1. (Havs- och vattenmyndigheten, 2013)

Table 2.1: Assessment for single samples. (Havs- och vattenmyndigheten, 2013)

Parameter	**Valid**	**Valid with remark**	**Unagreeable/ Unfit**
E. coli (CFU/100 ml)	≤ 100	100-1000	$\geq$1000
IE (CFU/100 ml)	≤ 100	100-300	≥ 300

Studying table 2.1, it can be seen that the test is valid if the content of E. coli and IE is not more than 100 CFU/100 ml. A valid assessment means that the content of bacteria is so low that it does not indicate a health risk. If the content exceeds 100 CFU/100 ml for E. coli and/or IE, the sample will be given a valid with remark assessment. This result means that the content of bacteria is enhanced, however, it does not indicate a health risk. The municipality does not need advise from bathing. In cases where E. coli exceeds 1000 CFU/100 ml, the sample is considered unfit as the content of bacteria could be a health risk. For IE, the sample is deemed unsuitable if the content exceeds 300 CFU/100 ml. In the case that the assessment is unfit, a re-examination should be made to monitor the extent and duration of the contamination. In this case, it should be advised against bathing in the water. (Havs- och vattenmyndigheten, 2013)

From the bathing season in 2010, the long-term evaluation by the European Union is based on the estimation of percentile from the four consecutive seasons seen in table 2.2 and 2.3. In the two tables, (*) is based on a 95-percentile assessment and (**) and is based on a 90-percentile assessment. (Havs- och vattenmyndigheten, 2016a)

Table 2.2: Limit values for inland water (Havs- och vattenmyndigheten, 2016a)

Parameter	**Excellent Quality**	**Good Quality**	**Satisfying Quality**
Escherichia coli (CFU/100 ml)	500 (*)	1 000 (*)	900 (**)
Intestinal Enterococci (CFU/100 ml)	200 (*)	400 (*)	330 (**)

Table 2.3: Limit values for coastal waters and water in the transition zone (Havs- och vattenmyndigheten, 2016a)

Parameter	**Excellent Quality**	**Good Quality**	**Satisfying Quality**
Escherichia coli (CFU/100 ml)	250 (*)	500(*)	500 (**)
Intestinal Enterococci (CFU/100 ml)	100 (*)	200 (*)	185 (**)

2.2.1 Escherichia coli

Escherichia coli (E. coli) is considered the most suitable indicator of faecal contamination by WHO (2011). Furthermore, according to Chan et al. (2013), E. coli is commonly used as the main indicator for bathing water quality due to its high correlation with swimming-associated illnesses. The gram-negative rod-shaped bacteria, E. coli, are about 1 μm long and are necessary for the digestion as E. coli constitute a large proportion of the intestinal flora. According to Svenskt Vatten AB (2011), human faeces contain 108-1010 CFU E. coli per gram of faeces and about one-tenth of lower enterococcal content. The cell wall consists of lipopolysaccharides. E. coli is not directly injurious to health. However, there are varieties of E. coli that can form toxins and cause serious diseases as for example Haemolytic-uremic syndrome, which may affect the kidney function in humans. (Svenskt Vatten AB, 2011a)

In more detail, E. coli is a genus of the total coliform bacteria and belongs to the thermotolerant coliforms due to its ability to ferment lactose at 44-45°C. It differentiates from the other thermotolerant coliforms as it can produce the enzyme β-glucuronidase and due to its production of indole from tryptophan. E. coli are typically present in high numbers in human and animal faeces, sewage and water recently affected by faecal pollution. Remarkably, the bacteria are rarely found in the absence of faecal pollution even though some indications for growth in tropical soils and persistence in external environments e.g. watersheds exists. (WHO, 2011)

Analysing, the persistence of E. coli in external environments more specifically no good understanding is known. According to Donnenberg (2013), it is said that E. coli must have evolved mechanisms to cope with both living in external environments and in a host. Additionally, the phenotypic response of a cell when it moves from the external environment to a host and vice versa is also still quite unidentified. It is further discussed that E. coli may have originally been host dependent but with time evolved to be persistent in the external environment of which these environments may have little to do with faecal input. (Donnenberg, 2013)

Moreover, during most situations of water quality monitoring when studying the population of thermotolerant coliforms it predominantly consists of E. coli. This has led to that E. coli has become the first choice of organisms in monitoring programmes for verification, including supervision of e.g. drinking-water quality. (WHO, 2011) Furthermore, when E. coli is used as an indicator it represents the total faecal contamination from all warm-blooded animals (humans, livestock, domestic pets, wild animals) and birds (Sokolova et al., 2012). For this thesis E. coli has therefore been chosen as the indicator bacteria for analysis and model calculations that represent how bacteria can affect the bathing water quality.

2.3 Degradation of E. coli

In this section, previous research or reports that have studied the effect on the degradation of E. coli will first be presented. This is followed by information concerning how degradation of E. coli can be mathematically described by a first-order degradation model and how the specific decay rate coefficient can be described. The mathematical formula used to develop the script is presented together with two other methods of how the decay rate coefficient can be described.

2.3.1 Factors that affect degradation of E. coli

According to *Some environmental factors affecting survival of fecal pathogens and indicator organisms in seawater* by El-Sharkawi et al. (1989), the exposure to sunlight is the most important factor for self-purification of water polluted due to sewage outfalls. Survival times were shorter when the organism was exposed to sunlight than in the dark for both fresh and seawater, being from several hours up to 24 hours compared to several days in the dark. Furthermore, it was found that E. coli survived longer in freshwater than in seawater at a temperature range of 30-35 °C. For the temperature parameter, it was found that E. coli survived from 1-5 days at 40 °C and 2-7 days at 25-35 °C, in other words, the bacteria died off more rapidly at 40 °C. (El-Sharkawi et al., 1989)

Furthermore, in the article *Comparative studies on the survival of indicator organisms and pathogens in fresh and sea water* by Evison (1988), it was also found that the effect of light is important. The study showed that the lethal effect of light increased with increasing intensity at a temperature of 15 °C. Additionally, it was also found that the faecal organisms, e.g. E. coli, survived twice as long in freshwater compared to seawater at a temperature of 15 °C. (Evison, 1988)

According to Krstulovic' et al. (2007) in the article *Effect of Solar Radiation and Temperature on Survival of Faecal Coliforms in Seawater* they found that the major factor controlling the survival of faecal coliforms in seawater was the presence of sunlight. In the report, it is stressed that the effect of solar radiation contributes to a more rapid inactivation of coliform bacteria compared to temperature. However, it is also discussed that the effect of temperature on the survival of faecal coliforms are greater when it is combined with sunlight, which suggests that sunlight and temperature act synergistically. The effect of temperature was obscured by the effect of sunlight up to a depth of 30 m. Nevertheless, below a depth of 30 m temperature becomes more important as a factor controlling the number of faecal coliforms. Krstulovic' et al. (2007) summarises by stating that it, therefore, is apparent that solar radiation and temperature interact to produce the greatest part of the observed decline of faecal coliforms in seawater. Additionally, Krstulovic' et al. (2007) concludes that temperature affects the survival of E. coli in the study more than dissolved oxygen and salinity. (Krstulovic' et al., 2007)

In the article *Hydrodynamic modelling of microbial water quality in drinking water sources* by Sokolova E. (2013a), the main factors affecting degradation are hydrodynamic processes, exposure to sunlight and the water temperature, with a higher temperature it has been seen that the degradation is faster. It was also seen that if a vertical temperature stratification occurred it affected the decay. If a clear thermocline, which separates the hypolimnion and the epilimnion, occurred the contamination would stay above the thermocline, in the epilimnion. This phenomenon most often occurs during the summer season. On the other hand, during autumn a lake would be well mixed from bottom to top. Last, during the winter season, the stratification is weak and therefore unlikely to have a major influence on the transport processes of E. coli. To summarise, it can according to Sokolova (2013) generally be said that the decay of faecal indicators is expected to be site-specific and that it depends on environmental conditions, such as the exposure to sunlight, the physical and chemical water properties, the water temperature and the presence of indigenous microorganisms. (Sokolova, 2013)

Moreover, in the article *Simulation tools to support bathing water quality management: Escherichia coli bacteria in a Baltic lagoon* by Schernewski et al. (2012) the degradation of E. coli was investigated and modelled in a three-dimensional flow model. In the article, it was concluded that the abundance of E. coli is positively correlated with turbidity and inversely correlated with salinity. It was also concluded that high organic carbon content and small particle size in coastal sediments were found to improve the survival of E. coli. The shading effect of reed standing close to beaches as well as frequent sediment resuspension processes was also found to be favourable for survival of E. coli. (Schernewski et al., 2012)

In the article *Real-time forecasting of Hong Kong beach water quality by 3D deterministic model* by Chan et al. (2003) the beach water quality in coastal areas in Hong Kong was modelled. The model was a 3D deterministic model with included degradation of E. coli. The equation for degradation was based on Mancini (1978) seen in section *2.3 Degradation of Escherichia coli (E. coli)*, however with specific constants developed on laboratory measurements of E.coli decay rates and validation of field studies in the area. In the study, the authors concluded that the two major factors affected the decay of E. coli were solar radiation and tidal levels. A clear correlation between higher solar radiation and increased decay was seen. Furthermore, it was concluded that tidal levels affected the E. coli levels. During flood and high tides, a high concentration of E. coli was seen and during the ebb and low tides levels of E. coli were usually low. It was also seen that a noticeable difference in the overall daily E. coli level was observed for diurnal tide and semi-diurnal tide conditions. During diurnal tides, the concentrations of E. coli were slightly lower in comparison with semi-diurnal tides were the concentrations were generally higher. The difference can be explained by the tidal current speed and travel time during different tidal conditions. In natural environments, the bacteria die-off is higher with longer time. (Chan et al., 2013)

The relationship between degradation of E. coli and suspended particle material, SPM, was studied in the article *Decay rates of faecal indicator bacteria from sewage and ovine faeces in brackish and freshwater microcosms with contrasting suspended particulate matter concentrations* by Perkins et al. (2016). In the study, it was found that SPM concentrations had none or a minimal influence on the decay rates of E. coli in freshwater. However, it was observed that the decay rates increased with an increased SPM concentration in brackish waters. Additionally, Perkins et al. (2016) also discussed the complexity of inactivation of coliform bacteria in aquatic systems and that further knowledge and research needs to be performed to assure the relationship between decay rates, SPM and salinity. (Perkins et al., 2016)

2.3.2 Mathematical model of degradation of E.coli

The mathematical formulations of decay processes for E. coli, in this case, used as the indicator bacteria, is described below. Biodegradation is according to Joutey et al.(2013) defined as the biologically catalysed reduction in complexity of chemical compounds. Furthermore, it is described as the process by which organic substances are broken down from larger to smaller compounds by microbial organisms. (Joutey et al. 2013)

The general degradation of faeces indicators such as E. coli is assumed to follow a general exponential first-order model, equation 1. (Chick & Martin, 1908)

$$C(t) = C(t = 0) * e^{(-k*t)} \tag{1}$$

Where, C is the concentration [organisms ml^{-1}], t is the time [d] or [h] and k is the decay rate coefficient at 20 °C. The degradation rate coefficient can be described in several different ways. Three different approaches to describing k will be presented below, where the third case is the method used to develop the script.

At first, the k can be described with help of a slight modification of a decay model that was proposed by Mancini (1978) to describe the decay of coliform bacteria in natural waters. The Mancini model describes the effect of light intensity, water temperature and the salinity, equation 2. (Svenskt Vatten AB, 2011b)

$$k = k_0 * \theta_s^{Sal} * \theta_I^{Int} * \theta_T^{(Temp-20)} \tag{2}$$

Where, k_0 [d^{-1}] is the degradation at 20°C and salinity 0 ‰ in darkness (no light available i.e. resembling the conditions at the bottom of e.g. the lake). Furthermore, θ_s is the salinity coefficient for the decay rate, ranging from 0-1 where 1 equals freshwater and 0 saltwater, Sal [‰] is the salinity. θ_I is the light coefficient, Int [$\mathrm{kW\,m^{-2}}$] is the light intensity over the water column with different depths, θ_T is the temperature coefficient for the decay rate and $Temp$ [°C] is the water temperature. (Svenskt Vatten AB, 2011b)

Secondly, k is described differently in the water quality module *D-Water Quality* by Deltares (2017b). The water quality module *D-Water Quality* is part of several modelling suites by Deltares. D-Water Quality allows for building of water quality models for saline, brackish and freshwater systems, on the basis of a pre-existing hydrodynamic model built with *Delft3D* or any other of Deltares hydrodynamic models. The water quality model can be used with a 1D, 2D or 3D hydrodynamic model. Furthermore, it can be used in a multi-compartment catchment modelling context as well as with the use of structured and unstructured grids. (Deltares, 2017b)

The empirical equations for the process used in the module are originally developed by Mancini (1978) described above in equation 2. The specific mortality rate of E.coli has been further developed by Deltares and is seen in equations 3 to 5. The degradation rate depends on the temperature, the intensity of UV radiation, salinity (chloride concentration) and the concentration of inorganic suspended matter. (Deltares, 2017b)

$$k = ((R_{C0} + (k_{Cl} * Cl)) * v^{T-20} + (Rc_{Rad} * DL * I * f_{UV} * \frac{1 - e^{-(Ext_{UV})*H}}{Ext_{UV} * H})) \quad (3)$$

Where, R_{C0} [d^{-1}] is the first-order mortality rate, k_{Cl} [$\mathrm{m}^3\,(\mathrm{g} * \mathrm{d})^{-1}$] is chloride related mortality constant, (Cl) [$\mathrm{g\,m}^{-3}$] is the chloride concentration and v [-] is the temperature coefficient of the mortality rate. Furthermore, T [°C] is the water temperature, Rc_{Rad} [$\mathrm{m}^2\,(\mathrm{W} * \mathrm{d})^{-1}$] is the radiation related mortality constant, DL [d] is day length, I [$\mathrm{W\,m}^{-2}$] is solar radiation at segment upper boundary and f_{UV} [-] is the fraction of UV-radiation in visible light. Furthermore, Ext_{UV} [m^{-1}] is the total extinction of UV-radiation and H [m] is the water depth.

$$Ext_{UV} = Ext_{Bak} + Ext_{IM1} * (IM1) \quad (4)$$

Where, Ext_{Bak} [$1\,\mathrm{m}^{-1}$] is the background extinction, Ext_{IM1} [$\mathrm{m}^2\,\mathrm{g}^{-1}$] is the extinction coefficient of inorganic suspended matter and $(IM1)$ [$\mathrm{g\,m}^{-3}$] is the concentration of inorganic suspended matter.

$$I = I_0 * e^{-Ext_{UV}*H} \quad (5)$$

Where, I_0 [$\mathrm{W\,m}^{-2}$] is the total radiation at the water surface.

Information concerning the parameters and editable variables within a range where the range can be seen in brackets, used in equation 3 to 5 are summarized in table 2.4.

Table 2.4: Parameters and editable variables within a range, seen in brackets, for calculations of degradation. (Deltares, 2017b)

Parameter/ Variable	**Description**	**Value**	**Unit**
f_{UV}	Fraction of UV-radiation in visible light	0.12	[-]
k_{Cl}	Chloride related mortality constant	$[1.1 * 10^{-5}]$	$[m^3\,(g * d)^{-1}]$
Rc_{Rad}	Radiation related mortality constant	0.086	$[m^2\,(W * d)^{-1}]$
v	Temperature coefficient of the mortality rate	1.07	[-]
DL	Day length	0.58 (Depends on latitude and season)	[d]
R_{C0}	First-order mortality rate	0.8 (0.8-5.0)	$[d^{-1}]$
T	Temperature	15 (Depends on local conditions)	[°C]
Ext_{Bak}	Background extinction	0.08 (0.08-1.0)	$[m^{-1}]$
Ext_{IM1}	Extinction coefficient of inorganic suspended matter	0.01 (0.01-0.05)	$[m^2\,g^{-1}]$
I_0	Total radiation at the water surface	160 (Depends on latitude and season)	$[W\,m^{-2}]$

The last described approach to express k is based on the Chick and Martin model (1908), equation 1. This method is used to develop the script for this thesis. The method for calculating k is based on information concerning water temperature, light intensity and salinity. In this case, an infinite oxygen supply is assumed. Information presented in equation 6 to 11, table 2.5 and 2.6 and in correlation with it is retrieved from *Implementation and description of different early warning systems for bathing water quality* (Erichsen et al, 2006). Information concerning how the equations and its parameters have been retrieved is not more specified in the study by Erichsen et al. (2006) than described in this section.

The decay parameter k $[h^{-1}]$ consists of decay contributions from light respectively dark conditions and is described in equation 6.

$$k = K_m + K_L * I_z \tag{6}$$

Where, K_m is the decay contribution when dark conditions $[h^{-1}]$, K_L is the decay contribution when light conditions $[m^2\,(W * h)^{-1}]$, I_z is the light intensity at depth z $[m^2\,W^{-1}]$. The decay contribution, K_m, when dark conditions, is calculated with equation 7.

$$K_M = a_T * T - k_{m0} \tag{7}$$

Where, a_T is the temperature dependency constant for dark reaction $[(°C * h)^{-1}]$, T is the actual water temperature [°C] and k_{m0} is the initial coliform decay rate constant for dark reaction $[h^{-1}]$. Equation 7 is only valid between 4 and 24 °C.

K_L, the decay contribution when light conditions, is calculated with help of equation 8. (Erichsen et al, 2006)

$$K_L = S_m * \frac{(b_T * T + K_{L0})}{(a * S_m - (\frac{1}{a}) * S)} \tag{8}$$

Where, T is the actual water temperature [°C], S is the actual salinity [psu], S_m is the reference salinity constant [psu], a is the correction for salinity constant [-], b_T is the temperature dependency constant for light reaction $[\mathrm{m}^2\,(\mathrm{W} * \mathrm{h} * {}^\circ\mathrm{C})^{-1}]$ and K_{L0} is the initial coliform decay rate for light reaction $[\mathrm{m}^2\,(\mathrm{W} * \mathrm{h})^{-1}]$. Equation 8 is only valid between 12 and 34 °C. (Erichsen et al, 2006)

In general, bathing water temperatures of equation 7 and 8 for the decay constants are covered. However, there is also a risk of bacterial contamination during winter bathing. According to Erichsen et al. (2006), there are no studies describing the decay in cold water. Erichsen et al. (2006) therefore proposes to use $K_M = K_M$ (4 °C) for $T < 4$ °C and $K_L = K_L$ (12 °C) for $T < 12$ °C, with the argument that light emitted during the same period is significantly less than in summer, the light contribution to the decay is simultaneously less and therefore it is considered that this does not give rise to major problems. (Erichsen et al, 2006) The light intensity at depth z, I_z $[\mathrm{W\,m^{-2}}]$, can be described by Lambert-Beer's law, equation 9.

$$I_z = I_0 * e^{-\mu * z} \tag{9}$$

Where, I_0 $[\mathrm{W\,m^{-2}}]$ is the light intensity at the water surface, μ is the extinction coefficient $[\mathrm{m^{-1}}]$ and z is the depth to the contamination [m]. The extinction coefficient can be decided from the secchi depth, SD [m], in equation 10. For the determination of μ, it is assumed that the secchi depth corresponds to the depth at which 15 % of the light radiation remains. This ratio may, however, range from about 10 % up to 25 % depending on the area. (Erichsen et al, 2006)

$$\mu = -ln(\frac{0.15}{SD}) \tag{10}$$

In a situation of contamination of faecal bacteria, it is likely that large amounts of dissolved organic matter are found in the water body. Soluble organic matter is not necessarily seen in the measured secchi depth however it has a large impact on I_z. Erichsen et al. (2006) therefore recommend that secchi depth measurements are used with caution and unless the light penetration is measured specifically at the contamination situation the measured water body's secchi depth during normal conditions should be reduced by 50 % when used in the model. (Erichsen et al, 2006)

To sum up, the degradation of E. coli can be described in a single equation according to equation 11.

$$C_{E.coli} = C_{E.coli_0} * e^{(-((a_T*T-k_{m0})+(S_m*\frac{(b_T*T+K_{L0})}{(a*S_m-(\frac{1}{a})*S)})*(I_0*e^{-(-ln(\frac{0.15}{SD}))*z}))*t)} \quad (11)$$

Information concerning the parameters used in equation 6 to 11 are summarized in table 2.5. No specific information of how the parameters have been developed and verified have been found.

Table 2.5: Parameters for calculations of degradation

Parameter	**Description**	**Value**	**Unit**
a_T	Temperature dependency constant, dark reaction	0.002425	$[(°C * h)^{-1}]$
k_{m0}	Initial coliform decay rate, dark reaction	0.00826	$[h^{-1}]$
S_m	Reference salinity	34.5	[psu]
a	Correction for salinity	1.54	[-]
b_T	Temperature dependency constant for light reaction	$0.133 * 10^{-3}$	$[m^2 (W * h * °C)^{-1}]$
K_{L0}	Initial coliform decay rate for light reaction	$2.124 * 10^{-3}$	$[m^2 (W * h)^{-1}]$.

Studying, equation 6 to 11 described in this section it can be observed that the equations for degradation of E. coli are only subject to decay, and the decay processes describing the variations of the bacteria in time and space are dependent on external factors such as salinity, light influx and water temperature. Additionally, the more background data available for analysis the more precisely can the bathing water quality be estimated to be. The prerequisite for making bathing water forecasts in the recipient is that the bacterial load is known and well described. Furthermore, it can be said that if there is no credible information on the magnitude of the contaminant, it is not meaningful to do advanced model calculations. (Erichsen et al., 2006)

If no information concerning initial concentrations of E. coli are found for calculations of $C_{E.coli}$, Erichsen et al. (2006) recommend initial concentrations, $C_{E.coli_0}$, that can be used for different types of sources in cases where no direct measurements are available, see table 2.6. For further information and explanations for the estimated values see Erichsen et al. (2006).

Table 2.6: Estimated standard values for initial concentrations of E. coli. (Erichsen et al. 2006)

Source	**E. coli per 100ml**
Untreated wastewater	$4.5 * 10^7$
Combined sewer overflows (CSO)	$9.0 * 10^6$
Purified sewage, after clarification	$3.0 * 10^5$
Purified sewage, after sandfiltration	$9.8 * 10^4$
Watercourses, dry weather	$5.0 * 10^3$
Watercourses, wet weather	$5.0 * 10^4$

These recommended concentrations, table 2.6, are conservative and based on the 95% percentile of the concentrations found in the literature. Erichsen et al. 2006 continue to state that as large variations in the initial concentrations may exist, better estimates of concentration levels in the sources are given if local measurements are performed. However, it is emphasized that it will be necessary to perform several series of measurements at the right times (i.e. in connection with the overflow itself, if the contamination comes from an overflow, etc.) to ensure that the measurements are representative of the individual sources.

3 Theory and modelling with TELEMAC-MASCARET

This section is divided into two parts. First, the computer software used is presented and explained. Secondly, how the mathematical model of degradation of E. coli is implemented into TELEMAC-3D through the developed script is described.

3.1 Computer software

In this section, the computer software used to develop and run the script are shortly presented and described.

3.1.1 TELEMAC-MASCARET

The open source software TELEMAC-MASCARET was first created by Laboratoire National d'Hydraulique et Environnement (LNHE) of the Research and Development Division of EDF (EDF-R&D). Today it is managed by the following organisations: Artelia (formerly Sogreah, France), BundesAnstalt für Wasserbau (BAW, Germany), Centre d'Etudes Techniques Maritimes et Fluviales (CETMEF, France), Daresbury Laboratory (United Kingdom), Electricité de France R&D (EDF, France), and HR Wallingford (United Kingdom). (TELEMAC, 2017a)

TELEMAC-MASCARET is a set of modelling tools allowing to treat every aspect of natural free surface hydraulics: waves, currents, transport of tracers and sedimentology. In TELEMAC-MASCARET all the data structures are gathered within Fortran files (further described in section *3.1.2 Fortran 90*), which are known as modules. These modules are all different with each having a distinct aim. Examples of modules are WAQTEL, Water Quality Module TELEMAC, describes different water quality processes in the modelling procedure. Furthermore, SISYPHE that describes sediment transport and bed evolution and TOMAWAC describing wave propagation in coastal areas. Additionally, TELEMAC-2D is a module describing 2D hydrodynamics and TELEMAC-3D is a module in the TELEMAC modelling system describing the 3D hydrodynamics. In this thesis, the module TELEMAC-3D is used.(TELEMAC, 2017a)

3.1.1.1 TELEMAC-3D

The code in TELEMAC-3D solves three-dimensional equations such as the transport-diffusion equations of intrinsic quantities (salinity, temperature, concentration) and the free surface flow equations. Its main properties are that the velocity is given in all three directions as well as the concentration of transported quantities plus that it takes in the water depth. The primary applications are found in free surface flow, both seas and rivers. It can take many processes into account as e.g current drift and diffusion of a tracer, with generation or disappearance terms and the influence of temperature and/or salinity on density. (EDF R&D. 2016)

More specifically, the three-dimensional hydrodynamic model and its equations describe the three-dimensional velocity field (U, V, W) and the water depth, h, as well as from the bottom depth, the free surface, S, at each time step. Furthermore, it solves the transport of "active" and "passive" tracers. The "active" tracers, e.g. salinity and temperature, changes the water density and acts on flow through gravity i.e. affects the hydrodynamics. On the other hand, the "passive" tracers do not affect the hydrodynamics and are only transported. (TELEMAC, 2017)

The 3D-hydrodynamic equations solved in TELEMAC 3D are based on the following assumptions (TELEMAC, 2017):

- Inconsequential variation of density in the conservation of mass equation incompressible fluid.
- A free surface changing in time is applied in the 3D Navier-Stokes equations.
- Hydrostatic pressure hypothesis (resulting in that the pressure at a given depth is the sum of the weight of the overlying water body plus the air pressure at the fluid surface.
- The variation in density is only taken into account as buoyant forces, i.e. Boussinesq approximation for the momentum.

The three-dimensional equations being solved due to the assumptions above are:

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = 0 \tag{12}$$

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} + W\frac{\partial U}{\partial z} = -g\frac{\partial Z_s}{\partial x} + \nu\Delta(U) + F_x \tag{13}$$

$$\frac{\partial V}{\partial t} + U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y} + W\frac{\partial V}{\partial z} = -g\frac{\partial Z_s}{\partial x} + \nu\Delta(V) + F_y \tag{14}$$

$$p = p_{atm} + \rho_0 g(Z_s - z) + \rho_0 g \int \frac{\Delta p}{\rho_0} \tag{15}$$

$$\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial x} + V\frac{\partial T}{\partial y} + W\frac{\partial T}{\partial z} = \nu\Delta(T) + Q \tag{16}$$

Information of the different terms in equation 12 to 16 are summarized in table 3.1.

Table 3.1: Terms for calculation of the three dimensional hydrodynamic. (TELEMAC,2017)

Term	**Unit**	**Description**
h	[m]	water depth
Z_s	[m]	free surface elevation
U, V, W	[$\mathrm{m\,s^{-1}}$]	three-dimensional components of velocity
T	[tracer unit]	passive or active tracer
p	[-]	pressure
p_{atm}	[-]	atmospheric pressure
g	[$\mathrm{m\,s^{-2}}$]	acceleration due to gravity
ν	[$\mathrm{m^2\,s^{-1}}$]	velocity and tracer diffusion coefficients
Z_f	[m]	bottom depth
ρ_0	[-]	reference density
$\Delta\rho$	[-]	variation of density around the reference density
t	[s]	time
F_x, F_y	[$\mathrm{m\,s^{-2}}$]	source terms
Q	[tracer unit]	tracer source of sink

Additionally, h, U, V, W and T are the unknown quantities i.e. the computational variables. The source terms F_x and F_y can e.g. denote the Coriolis force, the wind and the bottom friction. The model gives the opportunity to take several tracers into account simultaneously. (TELEMAC, 2017)

To simplify and describe the TELEMAC-3D basic algorithm, equation 12-16, further it can be split up into three computational steps. The first step consists in calculating the advected velocity components by only solving the advection terms in the momentum equations. The second step computes the new velocity components, from the advected velocities, taking into account the source terms and diffusion terms in the momentum equations. Leading to that an intermediate velocity field is obtained. The third step is provided for calculation of the water depth from the vertical integration of the continuity equation and the momentum equations only including the pressure-continuity terms as the other terms have been taken into account in the two earlier steps. (TELEMAC, 2017)

For two-dimensional equations (corresponding to the Saint-Venant equations without source terms, diffusion and advection) is written according to equation 17-19. (TELEMAC, 2017)

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (vh)}{\partial y} = 0 \tag{17}$$

$$\frac{\partial u}{\partial t} = -g \frac{\partial Z_s}{\partial x} \tag{18}$$

$$\frac{\partial v}{\partial t} = -g \frac{\partial Z_s}{\partial y} \tag{19}$$

Where, u and v are the two-dimensional variables of the vertically integrated velocity. Equations 17-19 are solved by TELEMAC-2D and make it possible to get the vertically averaged velocity and water depth. With the water depth, it is possible to recompute the elevations of various mesh points as well as the mesh nodes of the free surface. The computation of U and V can shortly be described by a combination of the equations linking the velocities. With help of the continuity equation, the vertical velocity W is computed. The tracers can as mentioned earlier be either passive or active. Either way, the tracer evolution equation in TELEMAC-3D is formulated according to equation 20. (TELEMAC, 2017)

$$\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial x} + V\frac{\partial T}{\partial y} + W\frac{\partial T}{\partial z} = \frac{\partial}{\partial x}(\nu_T \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(\nu_T \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z}(\nu_T \frac{\partial T}{\partial z}) + Q \tag{20}$$

Where, T [tracer unit] is the tracer either passive or active, ν_T [$\mathrm{m^2\,s^{-1}}$] is the tracer diffusion coefficients, t [s] is the time. Furthermore, x, y, z [m] are the space components and Q [tracer unit] is the tracer source or sink. (TELEMAC, 2017)

The mesh structure in TELEMAC-3D is made out of prisms. First a two-dimensional mesh comprising triangles, which covers the computational domain (the bottom) in a plane is constructed. This in order to prepare the mesh for the 3D flow domain. Secondly, the mesh is duplicated along the vertical direction in a number of curved surfaces so-called planes. The links between the meshed triangles between two planes make up the prisms. At each point, node, of the three-dimensional mesh the computational variables are defined including the bottom and surface. All variables are three-dimensional except the water depth and bottom depth that are only defined along the vertical once and are therefore two-dimensional. In TELEMAC-3D some actions are therefore shared with TELEMAC-2D. An example of how a three-dimensional mesh can look like is seen in figure 3.1. The mesh is prepared by using a mesh generator software adaptable with the TELEMAC system, e.g. BLUE KENUE, that is used in this thesis and described in section 3.1.3 *Blue Kenue™*. (TELEMAC, 2017)

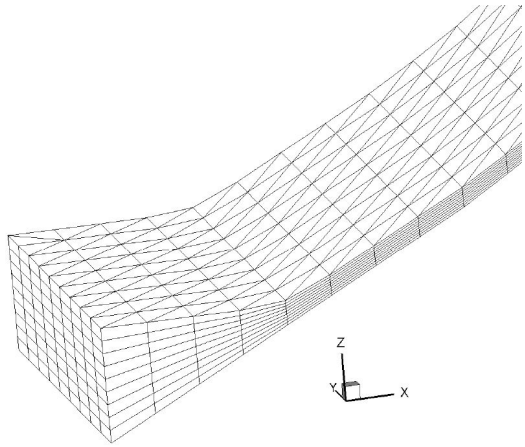

Figure 3.1: An example of a three dimensional mesh (TELEMAC, 2017)

When using a simulation module, the user sometimes needs to programme a specific subroutine, which is not in the code's standard release. This is made creating and changing the Fortran code in the so-called "user" subroutines i.e. subroutines open for users to modify. The subroutine SOURCE_TRAC is the subroutine that the script for this thesis has been developed in. It is further described in section *3.2 Degradation of E. coli coupled to TELEMAC-3D*. (TELEMAC, 2016)

3.1.2 FORTRAN 90

In TELEMAC-3D all the simulation modules are written in the computer language FORTRAN 90 (EDF R&D. 2016). Application areas of FORTRAN are for example numerical weather prediction, computational fluid dynamics and finite element analysis (Bodda S.R., 2009). The name FORTRAN is an abbreviation for *FORmula TRANslator* as it was designed to easily translate mathematical formulas into code. It was first developed in 1954 and commercially released in 1957 by IBM, International Business Machines and by that became the first computer language standard. (IBM, 2017)

FORTRAN has been updated several times since the start to be able to remain competitive with other programming languages. The version FORTRAN 90 was released in 1990 and since then two further updates in 1996 and 2004 has followed. (Encyclopædia Britannica, 2017)

3.1.3 Blue Kenue™

The advanced data preparation, analysis, and visualization tool, Blue Kenue™, for hydraulic modellers is developed by the Canadian Hydraulics Centre of the National Research Council Canada. The programme proposes a state-of-the-art interface, integrating geospatial data with model input and results in data. (National Research Council Canada. 2017) Furthermore, it offers a powerful mesh generation tool and a user-friendly post-processing tool (EDF R&D. 2016). The programme offers direct import of model results from e.g. TELEMAC-3D (National Research Council Canada. 2017). Important to mention is that Blue Kenue™ as well as QGIS are examples of pre- and postprocessing programmes and in this specific case, Blue Kenue™ is used.

3.2 Degradation of E. coli coupled to TELEMAC-3D

The mathematical theory for degradation of E. coli in section *2.3.2 Mathematical model of degradation of E.coli*, equation 11, is added to the existing subroutine SOURCE_TRAC. The subroutine is coupled with already existing hydrodynamic modules, describing the physical transport processes, in TELEMAC-3D described in section *3.1.1.1 TELEMAC-3D*. This to be able to simulate the simultaneous processes of transport, dispersion. Data required for the simulations are concentrations at model boundaries, flow and concentration from pollution sources, water temperature and an influx of light etc. Furthermore, the water temperature or salinity can be results from the hydrodynamic simulations or be specified by a user.

3.2.1 Developed script

In this section information that needs to be highlighted for the developed script is described further to clarify how the script operates. The script was developed with trial and error with no hydrodynamic occurring. It was possible to check if the script was correctly programmed by comparing with analytical calculations due to that no hydrodynamic was included. Additionally, if the script is used with a hydrodynamic model it is important that the model is calibrated in order to assure that the model is accurate. The final script can be seen in Appendix A plus some more specific description of the script can be seen in Appendix B. In the developed script the following assumptions were made to simplify and limit the study. The two first assumptions were made as the mathematical method used did not contain information concerning this, it may however happen in natural environments. The third assumption was made due to the time limit of the project.

- E. coli is only present in the water column and do not re-suspend or accumulate in the sediment.
- Even though the growth of E. coli may occur immediately after discharge it is assumed that no growth occurs.
- The light intensity at the surface is the same throughout the whole day.

In TELEMAC-3D a first-order degradation of tracers can be executed by using either implicit source terms for tracers (S1TA), explicit source terms for tracers (S0TA) or a combination of both. S1TA acts implicitly on the tracer value at the end of the time step of the calculations according to equation 21.

$$TA * (1. - S1TA) = TA + ... + ADVECTION + DIFFUSION. \tag{21}$$

Furthermore, S0TA acts explicitly on the tracer value at the beginning of the time step according to equation 22.

$$TA = TA + S0TA... + ADVECTION + DIFFUSION + ... \tag{22}$$

Where, TA is the concentration at the current time step. The concentration in every time step for every node in all layers are simultaneously calculated with the developed script with help of either S0TA, S1TA or a combination of both. The developed script is introduced in the subroutine SOURCE_TRAC using implicit source terms for tracers. It was with help of trial and error decided to use implicit source terms for tracers, S1TA. S0TA has not been used as it was not understood how to programme the degradation of E. coli with help of SOTA. It is therefore hard to state pro and cons with the usage of SOTA or S1TA. A further investigation concerning how S0TA and S1TA interact within TELEMAC-3D is needed.

The degradation coefficient, k, from equation 11 in section *2.3.2 Mathematical model of degradation of E. coli* can be seen below.

$$C_{E.coli} = C_{E.coli_0} * e^{(-((a_T*T-k_{m0})+(S_m*\frac{(b_T*T+K_{L0})}{(a*S_m-(\frac{1}{a})*S)})*(I_0*e^{-(-ln(\frac{0.15}{SD}))*z}))*t)}$$

The subroutine SOURCE_TRAC has an internal calculation of a first-order degradation model when using S1TA or S0TA. This means that the degradation coefficient is the only part of the equation that needs to be implemented into the subroutine, see below. The minus sign does not need to be implemented as it is already implemented into the subroutine.

$$k = ((a_T * T - k_{m0}) + (S_m * \frac{(b_T * T + K_{L0})}{(a * S_m - (\frac{1}{a}) * S)}) * (I_0 * e^{-(-ln(\frac{0.15}{SD}))*z}))$$

The implementation of the degradation coefficient, k, in the developed script into the subroutine can be seen below. Notice that this is only a part of the developed script and that the whole script can be seen in Appendix A.

```
    ...
    K = ((a1*TA%ADR(1)%P%R(I3D)-KM0)+(SM*(bT*
&       TA%ADR(1)%P%R(I3D)+ KL0)/(a*SM-(1.D0/a)* & TA%ADR(2)%P%R(I3D)))*(I0*
&       DEXP(-(-DLOG(0.15/ZSD))*DEPTH)))
    S1TA%ADR(3)%P%R(I3D) = K/3600.
    ...
```

Comparing, the equation for k with the code for the degradation coefficient, k, it can be observed that `a1` is a_T, Temperature dependency constant for dark reaction, `TA%ADR(1)%P%R(I3D)` is T, water temperature, and `KM0` is k_{M0}, the initial coliform decay rate for dark reaction. Furthermore, `SM` is S_m, Reference salinity, `bT` is b_T, the temperature dependency constant for light reaction, `KL0` is K_{L0}, initial coliform decay rate for light reaction, `a` is a, the correction for salinity, and `TA%ADR(2)%P%R(I3D)` is S, the salinity. Moreover, `I0` is I_0, the light intensity at the surface, `DEXP` is e, `DLOG` is ln, `ZSD` is SD, the secchi depth, and `DEPTH` is z, the water depth. The degradation coefficient k is then added to `S1TA%ADR(3)%P%R(I3D) = K/3600.`. k is divided by 3600 to change the unit from hours to seconds. The reason for dividing with 3600 is that the calculations in TELEMAC-3D have been chosen to execute its calculations in seconds. The variables salinity, water temperature, the initial concentration of E. coli, time step and duration of the simulation are set through a steering file, the "configuration" of the simulation, in TELEMAC-3D. The steering file is the main link between the hydrodynamic calculations and the subroutine SOURCE_TRAC where the code for degradation of E. coli has been added. The concentration in every time step for every node in all layers are then simultaneously calculated with help of `S1TA%ADR(3)%P%R(I3D) = K/3600`. In the developed script with implementation from equation for k, the only variables at the moment that can vary with time are the concentration of E. coli, the water temperature and the salinity.

3.2.2 Limitations in the script

The developed script has some limitations, in addition to the aforementioned simplifications, these are the most important limitations. The first is that the calculations do not take into account the daily variations in solar radiation. It is therefore recommended that a daily variation in solar radiation i.e. that the solar radiation is time-dependent, is added to the developed script. This is a possibility in TELEMAC-3D. Furthermore, in the developed script only the implicit source terms for tracers (S1TA) is used. However, further research on the possibilities to use explicit source terms for tracers (S0TA) and also a combination of the two and how this is programmed in TELEMAC-3D needs further investigation. In this thesis equation 11, has only been implemented with help of the implicit source term (S1TA) and how the explicit source term (S0TA) is implemented has not been understood. Even so, there might be a way of programming S0TA so it also calculates according to equation 11, but little is known about how this is done.

4 Sensitivity analysis

A sensitivity analysis for equation 11 is described in this section. This was done in order to analyse the sensitivity of the used equation in the developed script. First, some background information will be described followed by simulation description and results.

4.1 Background information

A sensitivity analysis was performed by plotting, with help of Python 3.6, equation 11 and changing the different variables and parameters to illustrate the affect a specific variable or parameter has on the degradation of E. coli after five days over a water column. This to study which variable and parameter the degradation of E. coli is more or less sensitive to. Important to notice is that no mixing of water in the water column or hydrodynamic occurs.

For the sensitivity analysis, it was chosen to first focus on the variables: secchi depth, water temperature, salinity, the initial concentration of E. coli and the light intensity at the water surface. Followed by a sensitivity analysis over the six parameters a_T, K_{M0}, SM, a, b_T and K_{L0} described in section *2.3.2 Mathematical model of degradation of E. coli*. This to illustrate how fast the degradation of E. coli has progressed after five days at different depths in a water column depending on the chosen value of a specific variable or parameter for equation 11.

4.2 Simulation

For the sensitivity analysis, each specific parameter and variable had selected values to show the sensitivity of each variable or parameter as well as selected standard values. For each parameter that is varied, the others are kept constant on the selected standard value, these can be seen in table 4.1. Additionally, the total time for calculation of degradation of E. coli was set to 5 days.

Table 4.1: Selected values for the sensitivity analysis for the specific parameters and variables.

Parameter/ Variable	**Description**	**Selected standard values**	**Selected variable values**	**Unit**
C_0	Initial concentration of E. coli	10^7	10^4, 10^5, 10^6, 10^7	$[\mathrm{ml}^{-1}]$
ZSD	Secchi depth	0.9	0.5, 1, 2, 3, 5, 10	[m]
T	The water temperature	20	4, 6, 8, 12, 14, 16, 20, 24, 34	[°C]
S	Salinity	1	0, 1, 10, 20, 30	[psu]
I_0	Light intensity at the surface	200	0, 5, 10, 25, 50, 100, 150, 200, 400, 800	$[\mathrm{W\,m}^{-2}]$
a_T	Temperature dependency constant, dark reaction	0.002425	0.002525, 0.002325, 0.002425, 0.002525, 0.002625	$[(°\mathrm{C} * \mathrm{h})^{-1}]$
K_{m0}	Initial coliform decay rate, dark reaction	0.00826	0.00526, 0.00626, 0.00726, 0.00826, 0.00926, 0.01026	$[\mathrm{h}^{-1}]$
S_m	Reference salinity	34.5	0.5, 1, 2, 3.54, 34.5, 3450	[psu]
a	Correction for salinity	1.54	0.54, 1.54, 2.54, 3.54, 4.54	[-]
b_T	Temperature dependency constant for light reaction	0.000133	0.00000133, 0.0000133, 0.000133, 0.00133, 0.0133, 0.133	$[\mathrm{m}^2\,(\mathrm{W} * \mathrm{h} * °\mathrm{C})^{-1}]$
K_{L0}	Initial coliform decay rate for light reaction	0.002124	0.00002124, 0.0002124, 0.002124, 0.02124, 0.2124, 2.124	$[\mathrm{m}^2\,(\mathrm{W} * \mathrm{h})^{-1}]$

For salinity, the range of values was selected in order to visualize the sensitivity of salinity as clear as possible for Swedish waters. The range of water temperatures was chosen as equation 11 used from section *2.3.2 Mathematical model of degradation of E. coli*, only is valid in the chosen range. The selected secchi depths were chosen to have values including secchi depths used in section *5. Simplified case* and to visualize the affect of secchi depths on light intensity for different depths through Lambert-Beers Law, described in equation 9 and 10.

According to, table 2.7 the estimated standard values for initial concentrations of E. coli are in the range of 10^4 to $10^7\,\mathrm{ml}^{-1}$ and these values were therefore chosen. To visualize the affect of the degradation from the initial concentrations clearer two graphs were plotted for the different concentrations. The selected light intensity at the water surface was chosen to have values including the light intensity at the water surface used in section *5. Simplified case* and to visualize the affect of the selected light intensity at the water surface. For the parameters: a_T, K_{M0}, SM, a, b_T and K_{L0}, the selected values were chosen to illustrate the affect of a changed constant as clear as possible.

4.3 Results

The results from the sensitivity analysis for the variables secchi depth, water temperature, initial solar radiation, salinity and initial concentrations are presented below. Followed by a sensitivity analysis over the six parameters a_T, K_{M0}, SM, a, b_T and K_{L0}. This to illustrate how fast the degradation of E. coli has progressed after five days at different depths in a water column depending on the chosen value of a specific parameter or variable for equation 11. In figure 4.1, the depth is plotted against the concentration of E. coli after five days for salinities [psu] at 0, 1, 10, 20 and 30 psu.

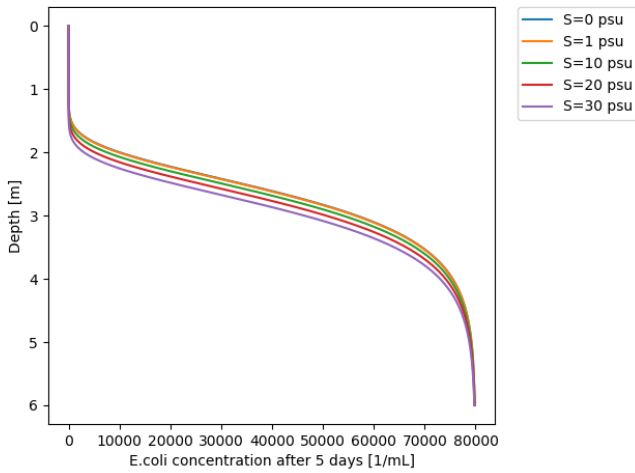

Figure 4.1: Comparison of different values for salinity.

In figure 4.1, it can be seen that the concentration of E. coli after 5 days are lower with higher salinity. However, the degradation of E. coli depending on salinity does not vary considerably between the five different salinities. Additionally, it is observed that the maximum concentration in the graph is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.2 and 4.3, the depth is plotted against the concentration of E. coli after five days for water temperature [°C] at 4, 6, 8, 12, 14, 16, 20, 24 and 34 °C. Two different graphs are shown to clearly see the relation and impact between different water temperatures.

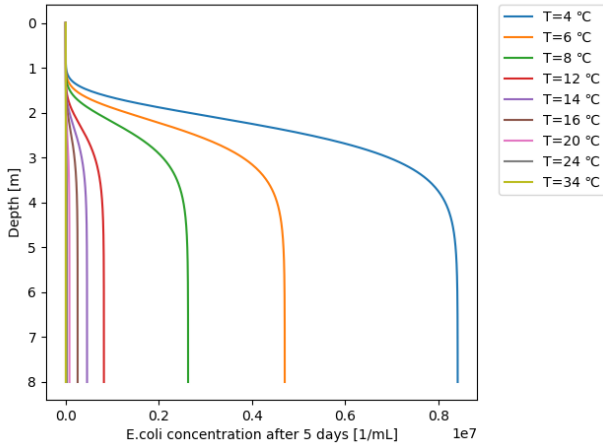

Figure 4.2: Comparison of different values for water temperature.

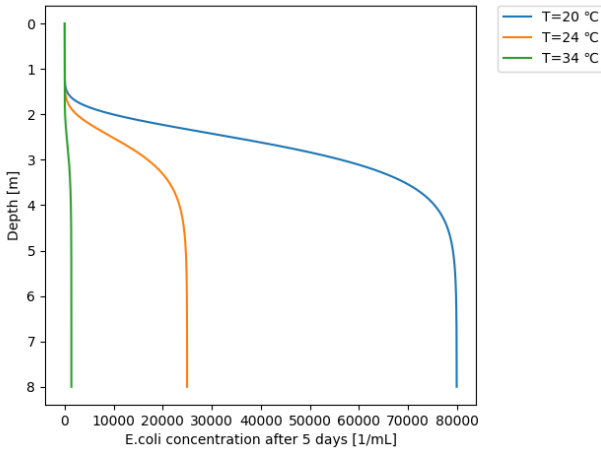

Figure 4.3: Comparison of different values for water temperature.

It can be seen in figure 4.2 and 4.3 that the concentration of E. coli after 5 days are lower with higher water temperature. It is also seen that the water temperature is most important for the degradation of E. coli for a water depth between 1 and 6 m. In figure 4.2 it is seen that the maximum concentration is $0.8 * 10^7$ ml^{-1}, which is 80 % of the initial concentration of E. coli (10^7 ml^{-1}). Additionally, it is observed that the maximum concentration in figure 4.3 is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.4 and 4.5, the depth is plotted against the concentration of E. coli after five days for initial concentrations of E. coli [ml^{-1}] at 10^4, 10^5, 10^6, 10^7 ml^{-1}. It was chosen to do two different graphs to clearly see the relation and impact between different initial concentrations.

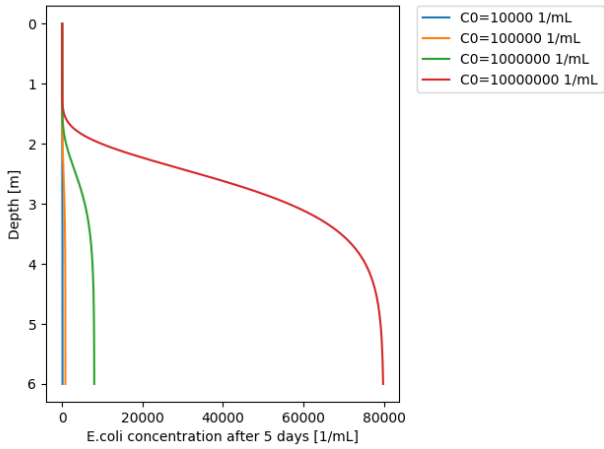

Figure 4.4: Comparison of different values for initial concentration of E. coli.

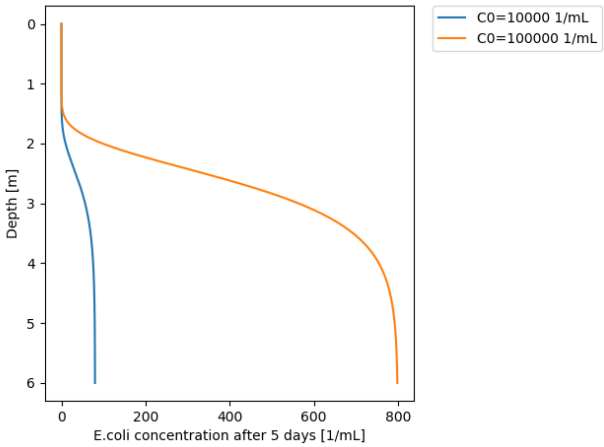

Figure 4.5: Comparison of different values for initial concentration of E. coli.

In the two graphs above, it can be seen that the concentration of E. coli after 5 days are lower with a lower initial concentration of E. coli. The concentration after five days is in relation to the initial concentrations in the same order between each other i.e. all are degraded similarly. To clarify, an initial concentration of 10^4 ml^{-1} gives a concentration at a water depth of 6 ml^{-1} to 80 ml^{-1} and 10^5 ml^{-1} to a concentration of 800 ml^{-1}. Additionally, for a water depth at 0 to 1.5 m, all initial concentrations are around 0 ml^{-1}. It is observed that 0.8 % of each initial concentration of E. coli plotted in the graph is left after 5 days.

In figure 4.6, the depth is plotted against the light intensity over depth (I_z) with Lambert-Beers law in equation 9 and 10 for secchi depths [m] at 0.5, 1, 2, 3, 5 and 10 m.

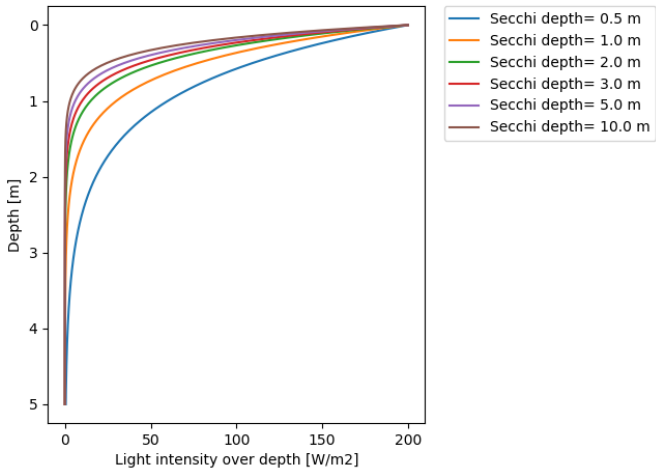

Figure 4.6: Comparison of how the light intensity over depth (I_z) is affected by different secchi depths.

In figure 4.6, it can be seen that with a lower secchi depth the light intensity over depth (I_z) is higher. This trend can be seen up to depths at 4 m were all trials start to behave similarly. Furthermore, the secchi depth has a higher impact on Lambert-Beers law for secchi depths between 0.5 and 3 m than from 3 to 10 m.

In figure 4.7, the depth is plotted against the concentration of E. coli after five days for light intensity at the water surface [$\mathrm{W\,m^{-2}}$] at 0, 5, 10, 25, 50, 100, 150, 200, 400 and 800 $\mathrm{W\,m^{-2}}$.

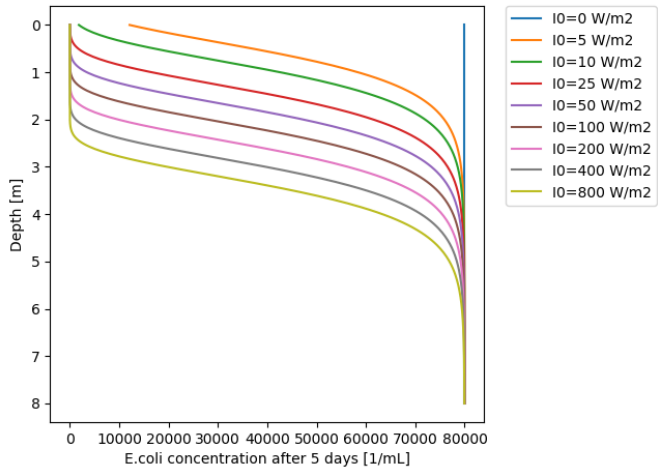

Figure 4.7: Comparison of different values for light intensity at the water surface.

Studying figure 4.7, it is observed that the concentration of E. coli after five days are lower with higher light intensity at the water surface until a water depth between 5-6 m were no difference in degradation can be noticed. If the light intensity at the water surface is chosen to zero no remarkable degradation over the water column can be seen. Additionally, it is observed that the maximum concentration in the graph is 80000 $\mathrm{ml^{-1}}$, which is 0.8 % of the initial concentration of E. coli (10^7 $\mathrm{ml^{-1}}$).

In figure 4.8, the depth is plotted against the concentration of E. coli after five days for the temperature dependency constant for the dark reaction, a_T $[(^{\circ}\mathrm{C} * \mathrm{h})^{-1}]$ at 0.002525, 0.002325, 0.002425, 0.002525 and 0.002625 $(^{\circ}\mathrm{C} * \mathrm{h})^{-1}$, where 0.002425 is the used value in equation 11 for degradation of E. coli.

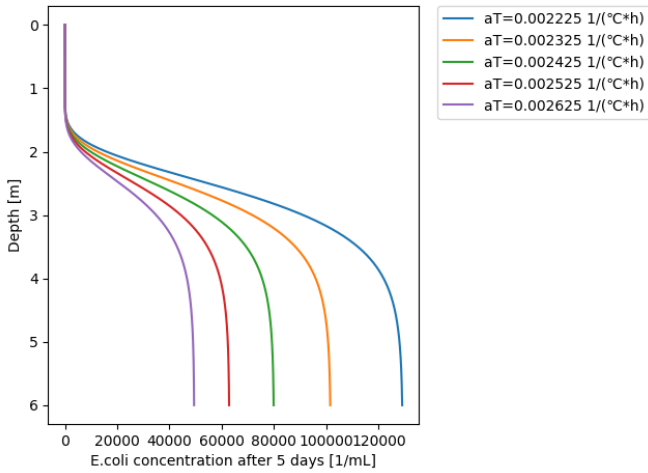

Figure 4.8: Comparison of different values for the temperature dependency constant for dark reaction.

Observing figure 4.8, it is seen that the value of a_T does not have an affect on approximately the first metre in the water column. However, after one metre the degradation of E. coli is higher with higher a_T. It is also observed that the maximum concentration in the graph is approximately 120000 $[\mathrm{ml}^{-1}]$, which is 1.2 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.9, the depth is plotted against the concentration of E. coli after five days for the Initial coliform decay rate, dark reaction, K_{M0} $[\mathrm{h}^{-1}]$ at 0.00526, 0.00626, 0.00726, 0.00826, 0.00926 and 0.01026 h^{-1}, where 0.00826 is the used value in equation 11 for degradation of E. coli.

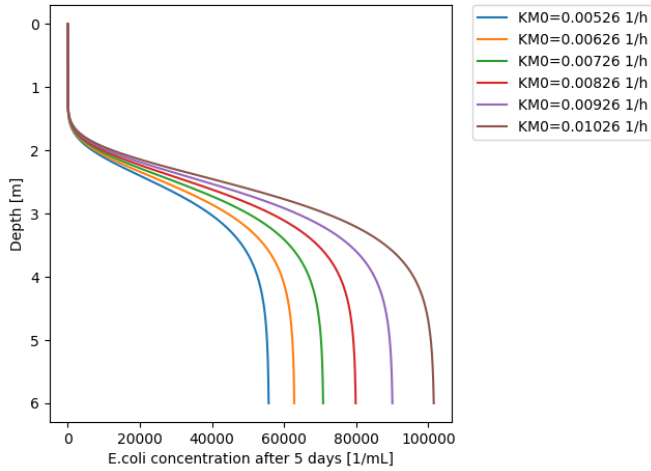

Figure 4.9: Comparison of different values for the Initial coliform decay rate, dark reaction.

It is seen in figure 4.9 that K_{M0} does not have a change in affect depending on the chosen value for K_{M0} for approximately the first metre in the water column. However, after one metre the degradation of E. coli is higher with lower K_{M0}. Additionally, it is observed that the maximum concentration in the graph is 100000 ml^{-1}, which is approximately 1 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.10, the depth is plotted against the concentration of E. coli after five days for the reference salinity, SM [psu] at 0.5, 1, 2, 3.54, 34.5 and 3450 psu, where 34.5 is the used value in equation 11 for degradation of E. coli.

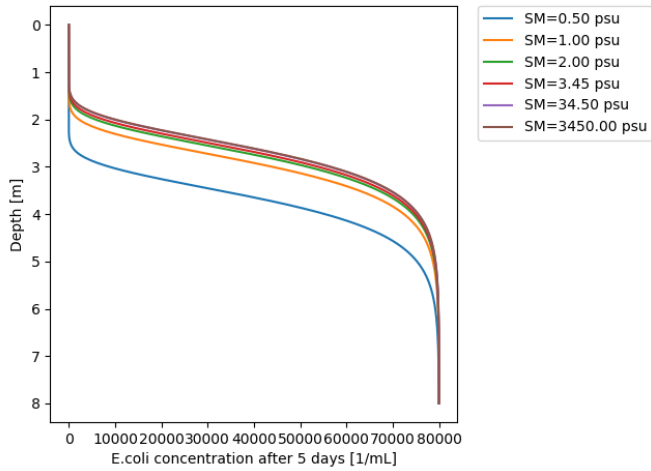

Figure 4.10: Comparison of different values for the reference salinity.

In figure 4.10, SM does not have a change in affect depending on the chosen value for SM for approximately the first metre in the water column. However, between approximately one and six metre, the degradation of E. coli is slightly higher with lower SM. After six meters it can be seen that SM does not have a changed affect between the different values for SM. Additionally, it is observed that the maximum concentration in the graph is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.11, the depth is plotted against the concentration of E. coli after five days for the correction for salinity, a $[-]$ at 0.54, 1.54, 2.54, 3.54 and 4.54, where 1.54 is the used value in equation 11 for degradation of E. coli.

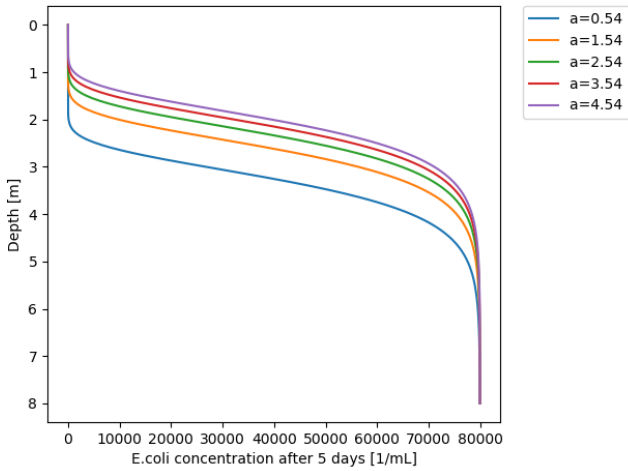

Figure 4.11: Comparison of different values for the correction for salinity.

Studying figure 4.11, a does not have a change in affect depending on the chosen value for approximately the first metre, in the water column. However, between approximately one and six metre the degradation of E. coli is slightly higher with lower a. After six meters it can be seen that a does not have a changed affect between the different values for a. Additionally, it is observed that the maximum concentration in the graph is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.12, the depth is plotted against the concentration of E. coli after five days for the temperature dependency constant for light reaction, b_T, at 0.00000133, 0.0000133, 0.000133, 0.00133, 0.0133 and 0.133 $m^2\ (W * h * °C)^{-1}$, where 0.000133 is the used value in equation 11 for degradation of E. coli.

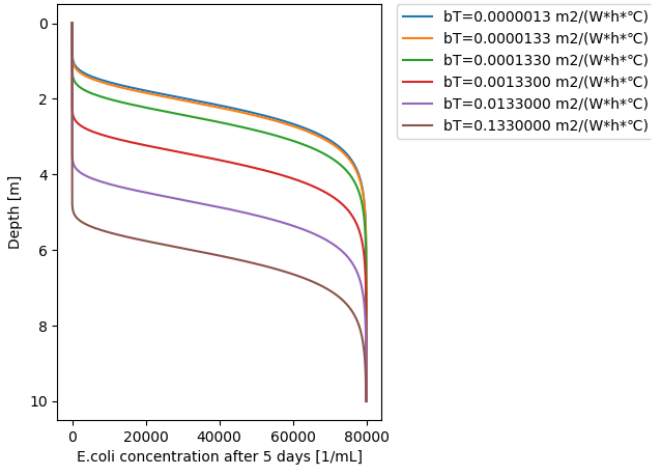

Figure 4.12: Comparison of different values for the temperature dependency constant for light reaction.

Observing b_T in figure 4.12, it is seen that for approximately the first half metre in the water column b_T does not have a change in affect between the different values. However, between approximately the first half metre and seven metre in the water column, the degradation of E. coli is higher with higher b_T. After seven metre it can be seen that b_T does not have a changed affect between the different values. Additionally, it is observed that the maximum concentration in the graph is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

In figure 4.13, the depth is plotted against the concentration of E. coli after five days for the initial coliform decay rate for light reaction, K_{L0}, $[\mathrm{m}^2\,(\mathrm{W} * \mathrm{h})^{-1}]$ at 0.00002124, 0.0002124, 0.002124, 0.02124, 0.2124 and 2.124 $\mathrm{m}^2\,(\mathrm{W} * \mathrm{h})^{-1}$, where 0.002124 is the used value in equation 11 for degradation of E. coli.

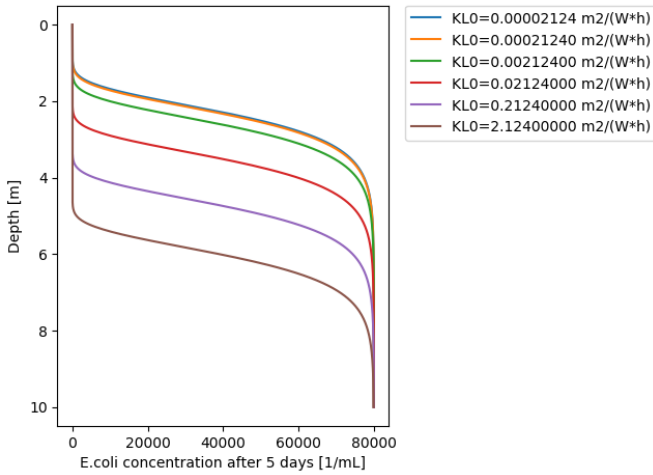

Figure 4.13: Comparison of different values for the initial coliform decay rate for light reaction.

Studying K_{L0} in figure 4.13, it is observed that for approximately the first metre in the water column K_{L0} does not have a change in affect between the different values. However, between approximately the first and seven metre in the water column, the degradation of E. coli is higher with higher K_{L0}. After seven metre it can be seen that K_{L0} does not have a changed affect between the different values. Additionally, it is observed that the maximum concentration in the graph is 80000 ml^{-1}, which is 0.8 % of the initial concentration of E. coli (10^7 ml^{-1}).

5 Simplified case

The developed script was used in a simplified case described in this section. This was done in order to be able to compare the results from the developed script with real data. The experiment and its data will first be shortly described followed by a description of the data used for the simulation and the results.

5.1 Background information

In the report *Decay of Bacteroidales Genetic Markers in Relation to Traditional Fecal Indicators for Water Quality Modeling of Drinking Water Sources* by Sokolova et al. (2011), they studied the decay of total coliforms, E. coli, Intestinal Enterococci, Somatic Coliphages and Bacteroidales so called host-specific genetic markers by performing a microcosm experiment. The experiment was conducted by collecting water samples from the Swedish Lake Rådasjön, untreated wastewater and faecal slurry prepared by mixing 60 g fecal matter and 300 ml of sterile deionized water. The water samples from Lake Rådasjön was collected at a distance of 20 m from the shore and at a depth of 0.5 m. The two experiments were conducted in two aquaria with a total volume of 25 L each. The volume of 25 L consisted of 2.5 L of untreated wastewater and 100 ml of faecal slurry and the rest was water from the Lake Rådasjön. (Sokolova et al., 2011)

The experiment was performed outdoor during a 14-day period in March, August and November in 2012. According to, Sokolova et al.(2011) the time periods were chosen in order to illustrate the varying temperature and light conditions during winter, summer and early spring in Sweden. Furthermore, the experiment was performed outside to optimize the representation of the conditions in Lake Rådasjön e.g. is the light intensity different outdoor and indoors. The experiment consisted of two setups in two aquaria, one protected from light (dark microcosm) and one exposed to natural light (light microcosm). The dark experiment illustrated the bottom and the light the surface of the lake. The dark experiment was covered with aluminium foil and a lid of opaque material to prevent rain and sunlight. Furthermore, the light experiment was covered with a transparent film to prevent from the rain. The experiment were conducted during aerobic conditions, with help of continuous circulation and mixing in the two aquarium. This was done with help of a circulation and air pump in each aquarium. The setup of the experiment can be seen in figure 3.1. To the left in the picture the two aquaria can be seen without lids and to the right the same two aquaria are shown covered with a lid. (Sokolova et al., 2011)

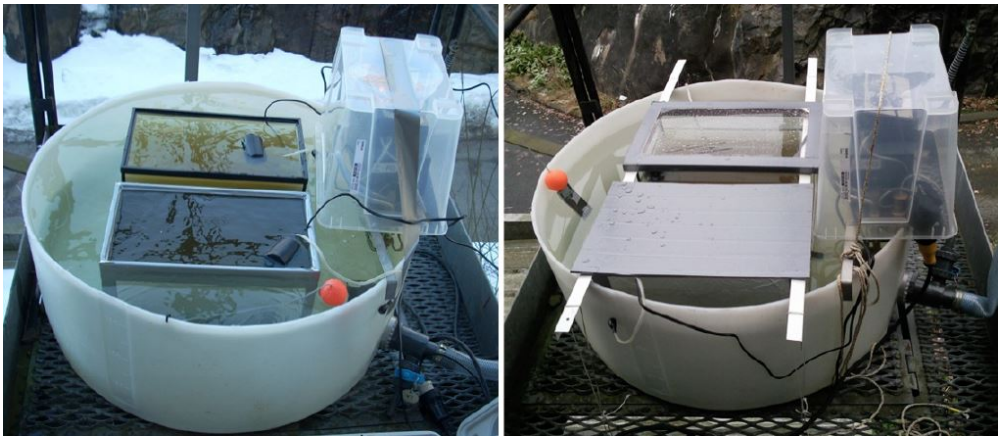

Figure 5.1: The experiment arrangement. At the left side the two aquarium without lids and to the right the same two aquarium covered with lids (Sokolova, 2013a)

During the experiment, the dissolved oxygen concentration exceeded 91 % of the saturated dissolved oxygen concentration in all experiments. The measured data and results from the experiments can be seen in table 5.1. The initial concentrations, $C(0)$, in table 5.1 were detected in the two aquaria on day zero of the performed experiment. In table 5.1, T90-value stands for the persistence of E. coli by the time for a 90 % reduction of the initial concentration of E.coli. (Sokolova et al., 2011)

Table 5.1: Data from the experiment, Light and dark conditions (Sokolova et al., 2011)

Regime	**Season**	**Mean water temperature** [°C]	**Mean solar radiation** [W m^{-2}]	**C(0)** [No $100ml^{-1}$]	**T90-value** [d] (95% Confidence interval)
Light	March	5	74	$3.1 * 10^5$	4.2 (3.3;5.5)
	August	20	127	$1.4 * 10^6$	2.2 (1.8;3.0)
	November	6	22	$6.9 * 10^5$	6.5 (4.3;13.2)
Dark	March	5	74	$2.4 * 10^5$	4.6 (3.2;8.2)
	August	20	127	$1.3 * 10^6$	3.8 (2.7;6.4)
	November	6	22	$1.0 * 10^6$	5.9 (4.1;10.3)

5.2 Simulation

The data from the experiment was used in the developed script to simulate both dark and light conditions for March, August and November. In the simulations, it was assumed that the salinity was 0 psu as the water was taken from a lake and that the dimensions of the aquariums were 0.3 m*0.3 m*0.3 m with a four-layered mesh with depths at 0 m, 0.1 m, 0.2 m, 0.3 m. It was chosen to vary the secchi depths as no information in the experiment concerning the secchi depth was found. According to, VISS (2017) the secchi depths values between 2014 and 2016 ranged from 2.7 to 4.2. Furthermore, in the report, *Vattendragskontroll Mölndalsån* by Göta älvs vattendragsförbund the secchi depths in Lake Rådasjön was 2.3 m on 23 February in 2012 and 3.9 m on 10 August in 2012 (Göta älvs vattendragsförbund, 2013). It was therefore chosen to simulate four different simulation scenarios for both dark and light conditions with secchi depths at 2.5 m, 3.0 m, 3.5 m and 4.0 m.

Additionally, the used equations for degradation of E. coli in section *2.3.2 Mathematical model of degradation of E. coli* were used and calculated directly analytically in Excel i.e. calculated by hand with the same input data as for the simulation. This in order to be able to compare the results from the Experiment, the Simulation in TELEMAC and the theoretical degradation of E. coli calculated by hand in Excel with each other.

According to Sokolova et al.(2011), the persistence of the faecal indicators can be described by the time for a 90 % reduction of faecal indicator concentrations T90-values. To be able to compare the degradation of the Experiment with the Simulated results from TELEMAC-3D and the results calculated by hand in Excel, the time for a 90 % reduction of faecal indicator concentrations T90-values were calculated for the three cases.

From the simulated simplified case, eight T90-values were calculated per each secchi depth, layer in the mesh (0 m, 0.1 m, 0.2 m and 0.3 m) and season (March, August and November). For each secchi depth and season, a mean value was calculated for the T90-value over the whole mesh, i.e. a mean value for all layers in the mesh. Furthermore, the same procedure was done in Excel with calculations by hand based on the same equations for degradation of E. coli. Furthermore, the difference between the T90-values for the three cases was calculated. Three different fractions were also calculated, further described below. All calculations were done for light and dark conditions.

The difference in fraction for the T90-value between the calculated by hand values in Excel and the Simulated results in TELEMAC were calculated according to equation 23.

$$\frac{(T_{90})_{Calculatedbyhand} - (T_{90})_{Simulation}}{(T_{90})_{Calculatedbyhand}} \tag{23}$$

The difference in fraction for the T90-value between the Experiment and the calculated by hand values in Excel were calculated according to equation 24.

$$\frac{(T_{90})_{Experiment} - (T_{90})_{Calculatedbyhand}}{(T_{90})_{Experiment}} \tag{24}$$

The difference in fraction for the T90-value between the Experiment and the Simulated results in TELEMAC were calculated according to equation 25.

$$\frac{(T_{90})_{Experiment} - (T_{90})_{Simulation}}{(T_{90})_{Experiment}} \tag{25}$$

5.3 Results

From the simulated simplified case described in section 5.2, *Simulation* eight T90-values were calculated per each secchi depth, layer in the mesh and season. For each secchi depth and season, a mean value was calculated for the T90-value over the whole mesh. Furthermore, the same procedure was done in Excel by calculating the values by hand based on the same equations for degradation of E. coli. Additionally, the difference between the T90-values for both light and dark conditions were calculated between the three cases: experiment, simulation in TELEMAC and calculations by hand in Excel. The difference in fraction for the T90-values was also calculated for light and dark conditions for the three cases. These results are further described and presented in Appendix C.

Presented in this section are plotted graphs from the calculated results presented in Appendix C. First, a graph over the calculated T90-values for the three scenarios March, August and November are presented in figure 5.2. Where, 1 stands for March, 2 for August and 3 for November. In figure 5.2 all calculated T90-values are presented for the calculated by hand values in Excel, simulated values and the values from the experiment for both light and dark conditions. The specific simulated values and the calculated by hand values can be seen in Appendix C, table 1 and 2. The T90-values from the experiment can be seen in section *5.1 Background information*, table 5.1. In the graph light stands for light conditions and dark for dark conditions i.e. *Simulated values, light* stands for calculated T90-values from the simulations in TELEMAC with light conditions.

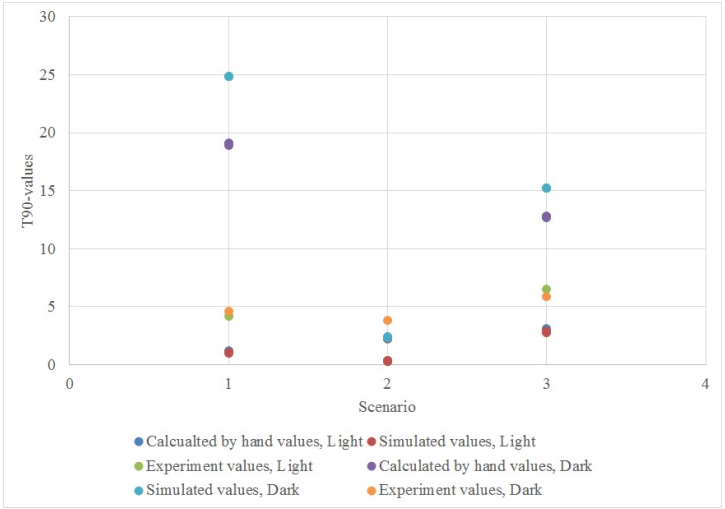

Figure 5.2: Comparison of T90-values for March (1), August (2) and November (3) for light and dark conditions.

In figure 5.2, it is seen that the T90-values for scenario 1, March, has the highest variation followed by scenario 3, November, and that number 2, August, has the smallest variation between its T90-values.

5.3.1 Difference in T90-values

The results from the difference between the T90-values from the calculations by hand, the simulation in TELEMAC and the experiment for light and dark conditions are presented in figure 5.3-5.6.

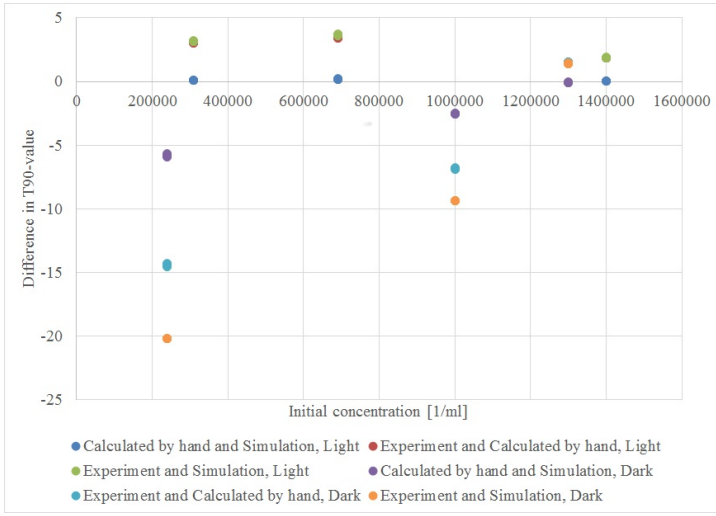

Figure 5.3: Comparison of difference in T90-values and initial concentrations.

Studying the difference in T90-values against initial concentrations it is seen that for dark conditions the difference in T90-values increases with lower initial concentrations. Nonetheless, for light conditions, the difference is quite similar even though the initial concentrations vary. The initial concentration, therefore, seems to have a higher impact on the degradation of dark conditions.

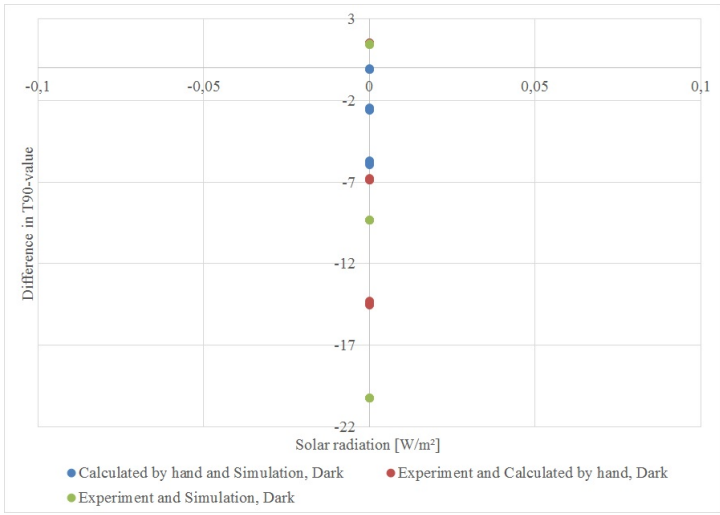

Figure 5.4: Comparison of difference in T90-values and solar radiation for dark conditions.

In figure 5.4 the difference in T90-values has the highest difference and variation for *Experiment and Simulation, Dark* followed by *Experiment and Calculated by hand, Dark* and the lowest variation can be seen for *Calculated by hand and Simulation, Dark*.

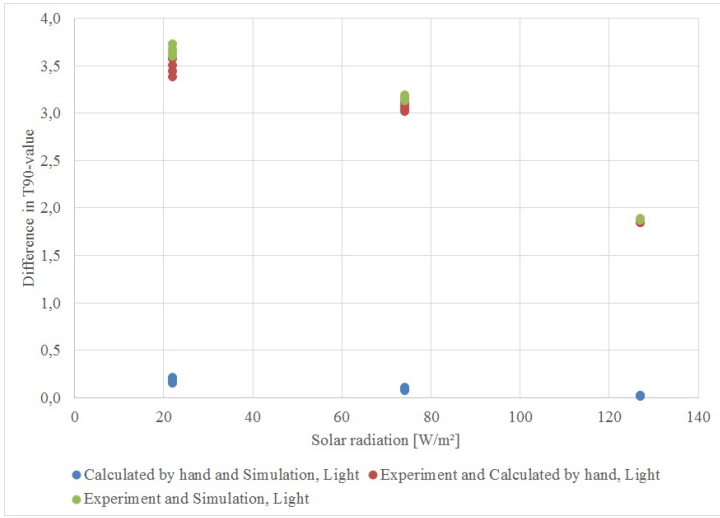

Figure 5.5: Comparison of difference in T90-values and solar radiation for light conditions.

For light conditions, the difference in T90-values for *Experiment and Calculated by hand, Light* and *Experiment and Simulation, Light* follows the same trend with higher difference than *Calculated by hand and Simulation, Light*. Furthermore, the difference for *Calculated by hand and Simulation, Light* are relatively constant with only a slight decrease even though the solar radiation changes. However, for *Experiment and Calculated by hand, Light* and *Experiment and Simulation, Light* the difference in T90-values decreases with higher solar radiation.

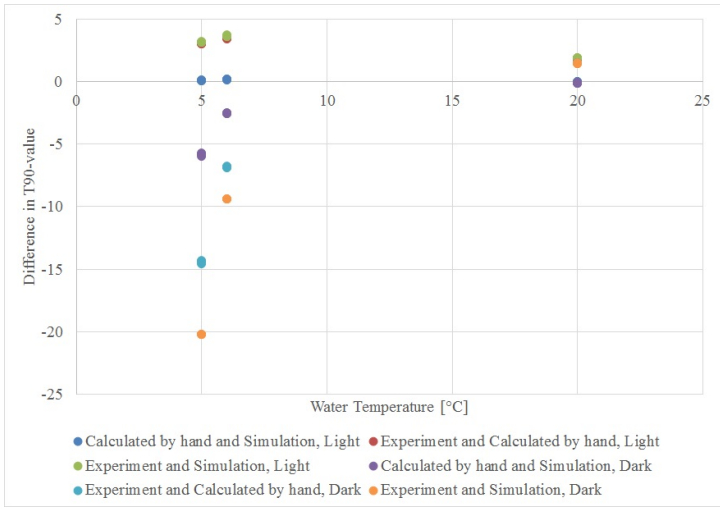

Figure 5.6: Comparison of difference in T90-values and water temperature.

Studying the difference in T90-values for both light and dark conditions for the three water temperatures 5, 6 and 20 °C it can be seen that the highest variation is for 5 °C followed by 6 °C and the lowest variation is for 20 °C. In other words, according to figure 5.6 the higher the water temperature is the lower is the difference in T90-values for both light and dark conditions.

5.3.2 Calculated difference in fraction for T90-values

The results from the difference in fraction for T90-values from the calculations by hand, the simulation in TELEMAC and the experiment for light and dark conditions are presented in figure 5.7-5.10.

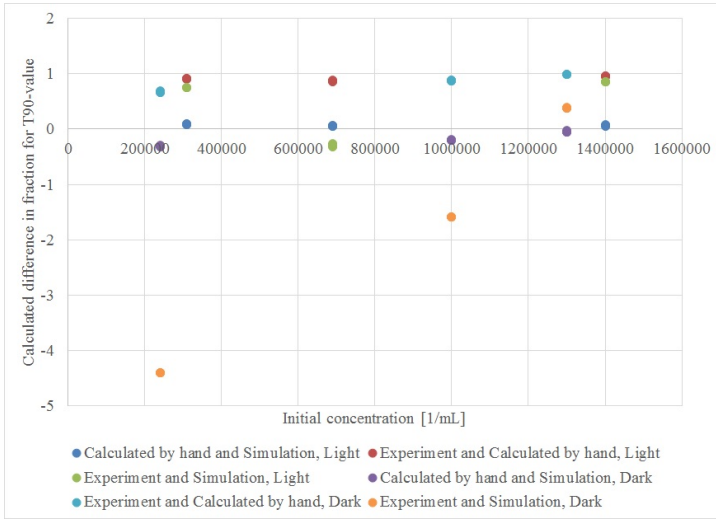

Figure 5.7: Comparison of difference in fraction for T90-values and initial concentrations.

For the calculated difference in fraction for T90-values in comparison with initial concentrations, all scenarios are between minus one and one except for *Experiment and Simulation, Dark*. For lower initial concentrations *Experiment and Simulation, Dark* are between minus 5 and minus 4, with a decreasing difference in fraction for T90-values with increasing initial concentration.

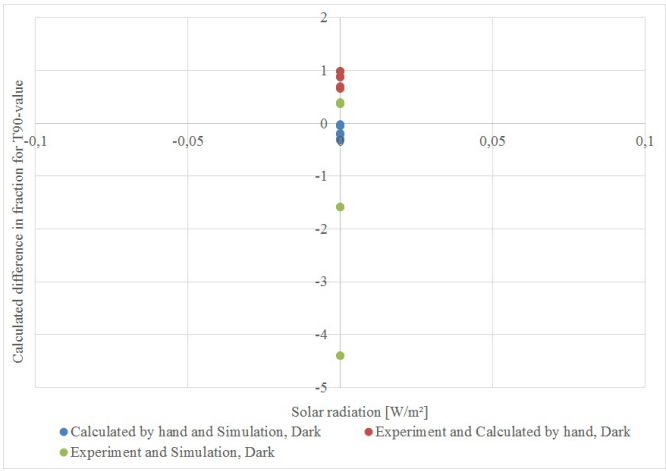

Figure 5.8: Comparison of difference in fraction for T90-values and solar radiation, dark conditions.

For figure 5.8 the highest variation for the calculated difference in fraction for T90-values is *Experiment and Simulation, Dark*. *Calculated by hand and Simulation, Dark* has the lowest calculated difference in fraction for T90-values followed by *Experiment and Calculated by hand, Dark*.

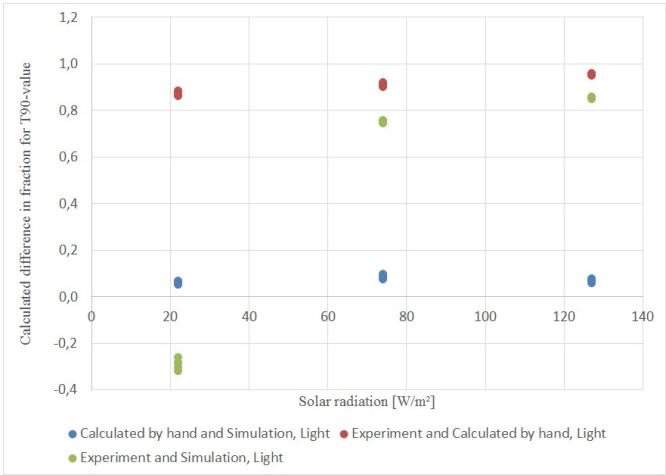

Figure 5.9: Comparison of difference in fraction for T90-values and solar radiation for light conditions.

The variation of calculated difference in fraction for T90-values in figure 5.9 is highest for *Experiment and Simulation, Light*. The calculated difference in fraction for T90-values are lowest for *Calculated by hand and Simulation, Light*. *Experiment and Calculated by hand, Light* and *Experiment and Simulation, Light* have quite the same calculated difference in fraction for T90-values. However, the variation of calculated difference in fraction for *Experiment and Calculated by hand, Light* are much smaller compared with *Experiment and Simulation, Light*.

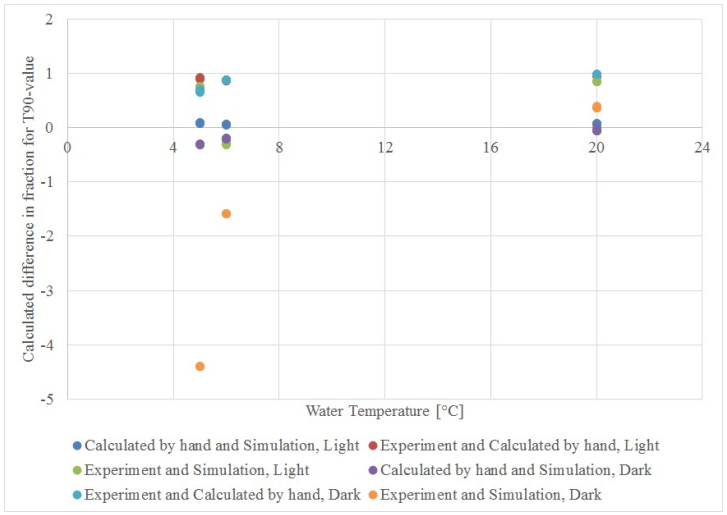

Figure 5.10: Comparison of difference in fraction for T90-values and water temperature.

In figure 5.10, the calculated difference in fraction for T90-values are altogether around zero to one except for *Experiment and Simulation, Dark* that has a decreasing difference in fraction for T90-values with higher water temperature, where the difference is highest for 5 °C and lowest for 20 °C.

6 Discussion

The discussion is structured in four parts, *Developed script*, *Sensitivity analysis*, *Simplified case* and *Future studies*.

6.1 Developed script

For the developed script some uncertainties of the used equation 11 are apparent. Firstly, no clear information of which approximations that the equation is based on has been found. Secondly, in the report by Erichsen et al. (2006), no clear information of how the parameters have been developed has been found. At last, the equation only includes information of salinity, water temperature, light intensity and depth. Comparing the used exponential first-order degradation model for E. coli (equation 11) with the literature study, the major factors controlling the degradation of E. coli is included in the used method such as the light intensity and the water temperature. However, some variables that according to the literature study that has been found important has been neglected in equation 11, such as SPM. A reason for this might be that it is hard to have reliable data for such a variable.

Some limitations in the developed script can be highlighted in relation to concentration levels of E. coli. For example, has the affects of tide and SPM concentrations not been taken into account in the used exponential first-order degradation model for E. coli and therefore also not in the developed script. First, according to a study by Chan et al. (2013) tidal levels were found to be the second most important factor for the abundance of E. coli after solar radiation. However, the tidal affects may not be important in Sweden as the tidal differences are low but in e.g. the UK or the Netherlands it might be of higher importance as the tidal affects in these regions are more distinct. Secondly, according to the article by Perkins et al. (2016), it was found that SPM concentrations had none or a minimal influence on the decay rates of E. coli in freshwater. However, it was observed that the decay rates increased with an increased SPM concentration in brackish waters. This indicates that salinity may not have a direct influence on the degradation but indirectly as it affects the SPM in the water, which then affects the concentrations of E. coli. At last, according to the study by Schernewski et al. (2012), the abundance of E. coli was found to be positively correlated with turbidity. The authors also found that high organic carbon content and small particle size in coastal sediments improved the survival of E. coli. Comparing, the used equation 11 that only takes four variables into consideration with the literature study it can be said that the degradation of E. coli is more complex. It is depending on the location, SPM, tidal levels or organic matter. However, the used equation for the implementation of the developed script includes the two major factors light intensity and water temperature for the degradation of E. coli. Even so, it can be concluded that the degradation of E.coli is very complex and that further investigation of the factors that affect E. coli needs to be done.

Looking, more specifically at the developed script, it is recommended that the daily variation of solar radiation is implemented. Information of how S0TA and S1TA are integrated and coupled to TELEMAC-3D has been limited. It is, therefore, hard to know if the script could be more optimized or not by adding S0TA to the script.

To sum up, it is believed that there is insufficient information or that the information is hard to find on how E. coli is affected in aquatic environment and why it degrades or grow outside a host. In addition, there is very little information about the few equations found and how they were developed. Information concerning how the parameters in the used method were developed was not found. The questions that then arise are if the information about the equations is inadequate. Furthermore, if the information concerning the equations are inadequate how can the model then be reliable? It may, therefore, be more reliable to simulate a simple dilution and dispersion model. It may be important to consider if the studied body of water is a small lake, bay with low residence time or the ocean. In smaller lakes, the rate of degradation is probably important. However, in the ocean where currents are stronger and the volume of dilution is high, the rate of degradation may not be so important and the usage of the degradation model might give overestimated values of the degradation of E.coli. If forecasts are made where the rate of degradation is overestimated, there is a risk that non-healthy baths will not be detected and warned. Despite the uncertainty of the model, it is still good to develop such tools to complement water sampling as it is costly and rarely taken plus that short-term contamination may be missed without the usage of models.

6.2 Sensitivity analysis

For the affect of salinity on the degradation of E. coli after five days figure 4.1 indicate that the different values of salinity do not have a major impact for water depth between zero to one and a half metre in the water column. Furthermore, the same trend seems to occur over the whole water column. Even though, a slight difference in the values of salinity can be seen for water depths from one and a half to five metres in the water column. Additionally, according to Schernewski et al. (2012), the abundance of E. coli is inversely correlated with salinity. This correlation can slightly be seen in figure 4.1 even if the difference in degradation between the different salinities is very low. It may, therefore, be said that salinity is not one of the variables that mostly affects the degradation of E. coli.

Moreover, if looking at how the water temperature affects the degradation in figure 4.2 and 4.3 it is first important to state that equation 11 only is valid between 12 and 24 °C. However, Erichsen et al. (2006) propose that equation 11 can be used for temperatures down to 4 °C as the light contribution to the water also is lower and that it will therefore not give rise to major problems. Even so, this is a weakness of the used equation, which may cause errors and misleading results for simulations under 12 °C. This indicates that both equation 11 and the developed script is most suitable for modelling of bathing water quality during the summer. Continuing to analyse figure 4.2 and 4.3, it is seen that the higher the water temperature is the higher is the degradation of E. coli.

It also seems like the water temperature has a major impact on the degradation as the percentage of the concentrations after 5 days varies between 0.8 % and 80 % depending on which water temperature that is selected. This is in correlation with the literature study where both Krstulovic'et al. (2007) and Sokolova (2013) found that the water temperature was one of the major factors controlling the degradation of E. coli. Additionally, concerning the water temperature in the developed model no temperature stratification has been taken into account. According to, Sokolova (2013a) a vertical temperature stratification highly effects the degradation. As the stratification is most present during the summer and the bathing water quality mostly is of interest during the summer season it may be an important factor to take into consideration when analysing the bathing water quality. This is also a variable that I did not study for my developed script. However, it is recommended to implement as the developed script is coupled to a hydrodynamic model in TELEMAC-3D.

Studying the two figures 4.4 and 4.5 it may be concluded that the relation between the different initial concentrations and concentration of E. coli after 5 days at a water depth at six meters is of the same magnitude, with a difference in 10^1. The initial concentrations seems to affect the concentrations mostly for water depths at 1.5 to 4 metres in the water column. However, the change in concentration from initial to after five days is directly depending on the decay factor in equation 11, which also indicates that the concentrations should be of the same magnitude.

Observing, the change in light intensity over depth (I_z) with different secchi depths in figure 4.6, it is seen that the light intensity is lower with higher secchi depth. This is in correlation with the used equations 9 and 10 for calculations of (I_z) through Lambert-Beers law. Additionally, Lambert-Beers law seems to be most affected by secchi depth between approximately the surface and a water depth at four meters.

For the light intensity at the surface in figure 4.7 it is clearly seen that the degradation of E. coli is highly dependent on light intensity. It can be observed that with no light intensity substantially less of the E. coli is degraded. It is also seen that the degree of degradation after five days increases with increased light intensity at the surface. Comparing figure 4.6 with 4.7, the light intensity at the water surface (I_0) is a more important variable for the degradation of E.coli than secchi depth. This can be concluded even though, an increased secchi depth leads to a decreased light intensity over depth (I_z) as the degradation of E. coli decreases with increased light intensity at the surface. Furthermore, if comparing figure 4.7 with figure 4.1 to 4.6 it can be observed that the light intensity affects the degradation to a deeper water depth in the water column compared with the five other figures. This may be an indication that the light intensity at the surface is one of the most important variable among the six variables in the figures 4.1 to 4.7.

In the literature study the article *Some environmental factors affecting survival of fecal pathogens and indicator organisms in seawater* by El-Sharkawi et al. (1989) it was concluded that the exposure to sunlight was the most important factor for self-purification of water polluted with sewage outfalls. Furthermore, Evison (1988) also found that the affect of light was important along with Krstulovic' et al. (2007) that found that the major factor controlling the survival of faecal coliforms in seawater was the presence of sunlight. At last, Sokolova et al. (2013a) also came to the conclusion that the main factors affecting degradation are exposure to sunlight and the water temperature. From this, it can, therefore, be concluded that the major factor controlling degradation of the six variables studied in figure 4.1 to 4.7 are the light intensity at the surface and the water temperature.

For the two parameters temperature dependency constant for dark reaction, a_T, and initial coliform decay rate, dark reaction, K_{M0} in figure 4.8 and 4.9. It is seen that the parameters in the surface, approximately first metre in the water column, are not very sensitive for a change of value. However, the deeper the water depth is in the water column the more difference in concentration of E. coli after five days is seen even though the difference in values for a_T and K_{M0} are quite low. This indicates that the parameters a_T and K_{M0} are sensitive for change.

Analysing, the parameter reference salinity, SM, in figure 4.10, it may be seen that the parameter is not sensitive at the surface (0-1.5 m) or after 6 m in the water column. For water depths between 1.5 and 6 m, the degradation tends to be more sensitive to low values for SM in the range (0.5 to 1 psu) than for higher values. In figure 4.11 the correction for salinity, a, follows the same pattern as SM but seems to be more sensitive then SM as the difference between the values of a are lower than those of SM. Comparing, SM and a with a_T and K_{M0} it may be concluded that the degradation of E. coli is less sensitive to changes in the parameters SM and a then a_T and K_{M0}. However, the degradation of E. coli is more sensitive to changes in a compared with SM.

The temperature dependency constant for light reaction, bT, in figure 4.12 and the initial coliform decay rate for light reaction, K_{L0}, in figure 4.13 has similar patterns with increasing degradation in the water column with increased b_T and K_{L0}. For both figures, it may be observed that the two parameters affect the degradation mostly from one and a half metre to eight and a half metre. The parameters, therefore, do not have a large impact on the surface of the water column. On the overall, it may be said that all parameters are sensitive to change. Furthermore, as limited information concerning how the parameters are developed were found it is hard to say if equation 11 really is reliable.

Comparing, the sensitivity analysis with the literature study it can be said that the light intensity at the surface and the water temperature are important factors for degradation of E. coli. Furthermore, comparing the percentage of the remaining concentration of E. coli from the initial concentration of E. coli for the different graphs in the results it can be concluded that the degradation is most sensitive for changes in water temperature. This indicates that the variables that is most important for the degradation of E. coli is the water temperature. While the percentage of the remaining concentration of E. coli from the initial concentration of E. coli for the other graphs are quite similar. Leading to that the rest of the variables has quite the same impact of sensitivity on the degradation of E. coli. However, in the literature study variables affecting the degradation of E. coli, which was not included in equation 11 also exists. Examples of this were turbidity and SPM-concentrations. This may be a weakness in the equation as the natural environments are more complex and that many factors may affect the degradation rate of E. coli. However, these factors may be difficult to measure and therefore it might not be that it is more reliable to take these factors into consideration. Another vagueness for equation 11 is that information concerning how the parameters specifically were developed were not found. If this information existed then an indication of how ambiguous the results from the developed script are would be better understood.

To sum up, degradation rate is very sensitive to variations in the parameters and variables involved. It seems that the equation is most sensitive to changes in the water column for depths between one and eight metres. The reason for this might be that the degradation of E. coli is high on the surface even if the parameters or variables are changed. This might be explained by that the water depth and the light intensity at the surface are important factors for degradation. If the water depth is low then the degradation becomes higher and if the light intensity at the surface is separate from zero then the degradation is not highly affected by a change in the variables for the first metre in the water column. However, in natural waters there will be a mix between the different depths so there will not be as much difference between different depths. Further, it can be noticed that bathers usually only bath a few metres deep in a water column and that the degradation of E. coli, therefore, is of most interest for the lower depths. Additionally, for the sensitivity analysis, the water temperature seems to be the most sensitive variable but the other variables and parameters are also sensitive. This may be an indication that equation 11 might be unreliable and when using it or the developed script this is important to take into consideration. Further on, it may be important to notice that sometimes measurements are not always found for variables such as secchi depth, solar radiation and water temperature for specific locations. This is also an uncertainty when using models as the accuracy of results for a model is directly depending on input data.

6.3 Simplified case

For the simplified case it may overall be said that the experiment, the simulation in TELEMAC-3D and the analytical calculations quite well agrees with each other for high water temperatures and high values for light intensity at the surface. For all the other cases the simulation in TELEMAC-3D and the analytical calculations correlates much better compared to the experiment.

Looking more specific at figure 5.2, the lowest variation is for August either if it is the analytical calculation by hand in Excel, simulated values from TELEMAC or values from the Experiment. The highest variation for all three methods is seen for March. Figure 5.2 indicates that the higher the water temperature and light intensity is the lower variation occurs. However, for March the light intensity is higher than in November, which also indicates that the water temperature is the main factor controlling the variations.

Furthermore, for figure 5.3 it is observed that the model is more sensitive to dark conditions than light. This is the case as the lower initial concentrations gives the higher difference in T90-value for dark conditions, a trend that cannot be seen for light conditions. In figure 5.4 an indication that the analytical calculations by hand and the simulation in TELEMAC-3D are more accurate for dark conditions is observed as the variation in T90-value is lowest. The same indication that the analytical calculations by hand and the simulation in TELEMAC-3D are most accurate also for light conditions can be observed in figure 5.5. It can also be noticed that the variation is reduced with higher light intensity at the surface, which implies that the light intensity at the surface is an important factor for degradation of E. coli.

Continuing to, figure 5.6 it is seen that the higher the water temperature is the lower is the variation in T90-values for both light and dark conditions. This indicates that the temperature is an important variables when using equation 11. For figure 5.7 it is hard to see a clear trend, however, it seems that the initial concentration may have a small influence with lower variation as the initial concentration increases especially for dark conditions. In figure 5.8 and 5.9, it is clearly seen that the difference is lowest for the analytical calculations made by hand in Excel and for the simulation made in TELEMAC-3D for both dark and light conditions. For the difference in fraction for T90-values compared with the water temperatures a slight or none change with increased water temperature can be seen. This is not in correlation with the earlier discussion that the water temperature is an important factor for the degradation of E. coli.

Overall, it can be said that the analytical calculations and the simulations in TELEMAC-3D have a higher correlation when compared to each other. However, why the simulation in TELEMAC-3D and the analytical calculations have a slight difference is difficult to say but it shows that the implementation of the used method may not have been entirely correct performed. The correlation is lower when the experiment is compared to both the analytical calculations and the simulation. A reason for this may be that information concerning the experiment were limited. Furthermore, for dark conditions, the results tend to differ more and the reason for this may be that the experiment does not really have a dark conditions. In figure 5.1 it can be seen that the dark condition not really is dark condition as the aquarium is not entirely covered from light intensity. This may have affected the results of the experiment and be a reason for the difference. Furthermore, the experiment was conducted with continuous circulation and mixing which the performed simulation in TELEMAC-3D and the calculations by hand in Excel did not take into consideration. Additionally, the experiment was conducted in aquarium of a volume of 25 L but the simulation in TELEMAC-3D was performed for a mesh which consisted of 27 L of water with the dimensions 0.3*0.3*0.3 m^3. These factors may have given rise to different results as for example the water depth is not known. However, as little is know about both the experiment and the equations used for implementation of the developed script and the analytical equations calculated by hand in Excel it is difficult to know the reason for the large differences.

Even so, it may be concluded that empirical evidence is missing and that further research both in field and how to mathematically describe the degradation of E. coli is needed. Additionally, the results from the simplified case show how difficult it is to perform experiments that resemble the reality as well as to resemble the reality in models. The simplified case shows that a model is highly dependent on the input and that the results do not have a higher accuracy than the model.

6.4 Future studies

In this section, a couple of suggestions for future studies are recommended. At first to add a variation of solar radiation to the script. Further on, an investigation concerning if the script can be optimized by implementing S0TA or a combination of S0TA and S1TA would be recommended. It should also be considered if using this script would give uncertain results due to that so little is known about the degradation of E. coli and the implemented exponential first-order degradation model for E. coli. Therefore, more field studies are needed to ensure that the model shows what is aimed. Further research is also needed to deepen the knowledge of the used exponential first-order degradation model for E. coli that the script in TELEMAC-3D is based on. Solar radiation and water temperature were found to be the most important physical variables. However, some aspects are important to take into account, for both of them it is difficult to find good measurements plus that they vary over time and between different locations. It might, therefore, be interesting for the future to develop a general exponential first order degradation model for E. coli that is only time-dependent, but has factors that describe temperature and solar radiation representative of the summer for different locations in Sweden. However, in order to produce such a model a lot of measurements are needed to verify its reliability.

7 Conclusions

The main objective of this thesis was to develop and evaluate a script for biodegradation of the faecal indicator bacteria E. coli in a marine environment. It can be concluded that a script for degradation of E. coli has been developed and is operating in accordance with the used exponential first-order degradation model for E. coli. However, little empirical evidence was found of how E.coli is degraded and it may be because there is limited information for how E. coli is affected in natural environments and how to describe the degradation of E. coli mathematically. Further research of how E. coli is degraded and factors affecting E. coli is needed both in field and how to describe it mathematically. An uncertainty of the developed script is if it is adequate to use as information concerning the implemented exponential first-order degradation model of E. coli is limited.

From the performed sensitivity analysis it can be concluded that the degradation rate is sensitive to variations in both parameters and variables. The major factors controlling the degradation of E. coli are light intensity at the surface and water temperature. It seems that the used exponential first-order degradation model of E. coli is most sensitive to changes in the water column for depths between one and eight metres. Additionally, only limited information were found of how the implemented degradation model of E. coli was developed, which indicates that it may not be entirely reliable to use the implemented degradation model of E.coli. Before further development and verification are possible, it may be more reliable to model dilution and dispersion instead of using the developed script. Depending on the body of the water the usage of a degradation model may be more or less important. For example in the case of the ocean, it may give overestimated values for degradation of E.coli. If forecasts are made where the rate of degradation is overestimated, there is a risk that non-healthy baths will not be detected and warned.

For the simplified case it can be concluded that the calculations by hand and the simulations in TELEMAC-3D correlate better with each other, while the experiment differs more compared to the other two. A reason for this may be that information concerning the experiment was limited and that the dark conditions during the experiment did not fully occur. On the other hand, that the calculations by hand in Excel and the simulation in TELEMAC-3D are correlating shows that the developed script is working in accordance with the implemented exponential first-order degradation model of E. coli.

On the whole, it can be said that empirics and research of degradation of E.coli are restricted and further research is needed to gain a deeper knowledge of bathing water quality.

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Appendix

Appendix A

Developed script

```
                              SUBROUTINE SOURCE_TRAC
!-----------------------------------------------------------------------------
USE BIEF
USE DECLARATIONS_TELEMAC3D
USE DECLARATIONS_WAQTEL, ONLY ZSD
IMPLICIT NONE
!-----------------------------------------------------------------------------
INTEGER ITRAC
INTEGER I2D, I3D, IPLAN
DOUBLE PRECISION, PARAMETER ::  a1 = 0.002425D0
DOUBLE PRECISION, PARAMETER ::  KM0 = 0.00826D0
DOUBLE PRECISION, PARAMETER ::  a = 1.54D0
DOUBLE PRECISION, PARAMETER ::  SM = 34.5DO
DOUBLE PRECISION, PARAMETER ::  bT = 0.000133D0
DOUBLE PRECISION, PARAMETER ::  KL0 = 0.002124D0
!-----------------------------------------------------------------------------
!  UNIFORM DECAY RATE FOR TRACER NUMBER 3 (%ADR(3))
 ZSD = 0.9D0    !SETS SECCHI DEPTH TO 0.9
 I0 = 200.D0    !SETS THE LIGHT INTENSITY AT THE SURFACE TO 200
 IF(NTRAC.GE.3) THEN
   S1TA%ADR(3)%P%TYPR='Q'
   !SETS SOURCE TERMS TO Q INSTEAD OF 0 IN TYPR IF NOT NIL
   DO I2D=1, NPOIN2
   DO IPLAN=1, NPLAN
   I3D= I2D + NPOIN2*(IPLAN-1)
   DEPTH = DMAX1(1.D-12,Z(I2D+NPOIN2*(NPLAN-1))-Z(I3D))
   PRIVE%ADR(1)%p%R(I3D) = DEPTH
   K = ((a1*TA%ADR(1)%P%R(I3D)-KM0)+(SM*(bT*
&      TA%ADR(1)%P%R(I3D)+ KL0)/(a*SM-(1.D0/a)* & TA%ADR(2)%P%R(I3D)))*(I0*
&      DEXP(-(-DLOG(0.15/ZSD))*DEPTH)))
   S1TA%ADR(3)%P%R(I3D) = K/3600.
   ENDDO
   ENDDO
   ENDIF
```

Appendix B

Some parts of the script will be further described below to clarify parts of the code in the developed script in Appendix A. In the following part of the script S1TA is implemented into the script.

```
IF(NTRAC.GE.3) THEN
  S1TA%ADR(3)%P%TYPR='Q'
  !SETS SOURCE TERMS TO Q INSTEAD OF 0 IN TYPR IF NOT NIL
  ...
 ENDIF
```

In the code above `IF(NTRAC.GE.3)THEN` starts the computation of the developed script. Where, `NTRAC` are the number of tracers and `NTRAC.GE.3` stands for that the number of tracers are equal to three or higher. So if the number of tracers are equal to three, the computation starts. In TELEMAC-3D, the water temperature is the first tracer and salinity the second making, in this case, E. coli the third tracer. In `S1TA%ADR(3)%P%TYPR='Q'` S1TA for the third tracer is set to Q in order for the user to select the source term for E. coli in TELEMAC-3D.

The depth of any 3D node is calculated with the following section of code. The basis is to loop all 2D nodes first (bottom plane only, NPOIN2) and then on the vertical planes (PLAN).

```
...
DO I2D=1, NPOIN2
DO IPLAN=1, NPLAN
I3D= I2D + NPOIN2*(IPLAN-1)
DEPTH = DMAX1(1.D-12,Z(I2D+NPOIN2*(NPLAN-1))-Z(I3D))
...
ENDDO
ENDDO
...
```

In the script the value for `I2D+NPOIN2*(NPLAN-1)` is the surface node corresponding to the initial 2D node (bottom plane).`Z(I2D+NPOIN2*(NPLAN-1)) - Z(I3D)` gives the distance between the surface and the nodes located on the planes below along the same vertical, Z stands for the elevation in the specific node. In other words, the depth is calculated from the elevations in every layer of the mesh for each node. The max of the `DEPTH` and a very small value `1.D-12`, meaning 10^{-12}, is taken in order to avoid nil or any negative depth values that might trigger some mistakes in the code as LOG laws are used.

In the following part of the script the degradation of E. coli is implemented.

```
    ...
    PRIVE%ADR(1)%P%R(I3D) = DEPTH
    K = ((a1*TA%ADR(1)%P%R(I3D)-KM0)+(SM*(bT*
&       TA%ADR(1)%P%R(I3D)+ KL0)/(a*SM-(1.D0/a)* & TA%ADR(2)%P%R(I3D)))*(I0*
&       DEXP(-(-DLOG(0.15/ZSD))*DEPTH)))
    S1TA%ADR(3)%P%R(I3D) = K/3600.
    ...
```

In the script the depth is created to a user variable in form of a vector that contains the depth value at every 3D node, this is made by using private variables, `PRIVE%ADR(1)%P%R(I3D) = DEPTH`. The aim for this is to see in the mesh that the calculations for the depth is correct. Furthermore, the k from equation 11 (or 23) is added in the script by `K = ((a1*TA%ADR(1)%P%R(I3D)-KM0)+(SM*(bT*TA%ADR(1)%P%R(I3D)+KL0)/(a*SM-(1.D0/a)*TA%ADR(2)%P%R(I3D)))*(I0*DEXP(-(- DLOG(0.15/ZSD))*DEPTH)))`, which is written at different lines in the code as the k is to long for one line in TELEMAC-3D. In the code for k, `TA%ADR(1)%P%R(I3D)` stands for the water temperature and `TA%ADR(2)%P%R(I3D)` for the salinity in each I3D node in the whole mesh. At last k is added to `S1TA%ADR(3)%P%R(I3D) = K/3600.`. k is divided by 3600 to change the unit from hours to seconds. The reason for dividing with 3600 is that TELEMAC-3D execute its calculation i seconds. `S1TA%ADR(3)%P%R(I3D) = K/3600.` then calculates internally in TELEMAC-3D the degradation of E.coli in the form of a first-order degradation for all 3D-nodes in the mesh.

Appendix C

From the simulated simplified case described in section 5 eight T90-values were calculated per each secchi depth, layer in the mesh (0 m, 0.1 m, 0.2 m and 0.3 m) and season (March, August and November). For each secchi depth and season, a mean value was calculated for the T90-value over the whole mesh, i.e. a mean value for all layers in the mesh. Furthermore, the same procedure was done with calculations by hand in Excel based on the same equations for degradation of E. coli. Additionally, the difference between the T90-values for both light and dark conditions were calculated between the three cases: Experiment, Simulation in TELEMAC-3D and calculations by hand in Excel. The difference in fraction for the T90-values were also calculated for light and dark conditions for the three cases. The results are here presented in tables. In table 1 and 2 the maximum and minimum values for the T90-values are also added to illustrate the variation of T90-values.

Table .1: Results from the Simulation in TELEMAC-3D for the light and dark conditions

Season	**Secchi depth**	**Mean T90-value [days], Light**	**Min and Max value of T90, Light**	**Mean T90-value [days], Dark**	**Min and Max value of T90, Dark**
March	2.5	1.01	(1.01; 1.01)	24.8	(24.8; 24.8)
	3.0	1.03	(1.03; 1.04)	24.8	(24.8; 24.8)
	3.5	1.05	(1.05; 1.06)	24.8	(24.8; 24.8)
	4.0	1.07	(1.07; 1.07)	24.8	(24.8; 24.8)
August	2.5	0.31	(0.31; 0.32)	2.31	(2.31; 2.31)
	3.0	0.32	(0.32; 0.32)	2.38	(2.38; 2.39)
	3.5	0.32	(0.32; 0.33)	2.38	(2.38; 2.39)
	4.0	0.33	(0.32; 0.33)	2.38	(2.38; 2.39)
November	2.5	2.77	(2.77; 2.78)	15.3	(15.3; 15.3)
	3.0	2.82	(2.82; 2.82)	15.3	(15.3; 15.3)
	3.5	2.86	(2.86; 2.86)	15.3	(15.3; 15.3)
	4.0	2.90	(2.90; 2.90)	15.3	(15.3; 15.3)

Table .2: Results from calculations by hand made in Excel for the light and dark conditions

Season	**Secchi depth**	**Mean T90-value [days], Light**	**Min and Max value of T90, Light**	**Mean T90-value [days], Dark**	**Min and Max value of T90, Dark**
March	2.5	1.09	(0.7; 1.56)	18.9	(16.9; 20.7)
	3.0	1.13	(0.7; 1.64)	18.9	(16.9; 20.9)
	3.5	1.16	(0.7; 1.71)	19.1	(16.9; 21.0)
	4.0	1.18	(0.7; 1.78)	19.1	(16.9; 21.1)
August	2.5	0.33	(0.22; 0.46)	2.26	(2.21; 2.31)
	3.0	0.34	(0.22; 0.48)	2.27	(2.21; 2.31)
	3.5	0.35	(0.22; 0.50)	2.27	(2.21; 2.31)
	4.0	0.35	(0.22; 0.51)	2.27	(2.21; 2.32)
November	2.5	2.92	(2.00; 3.96)	12.7	(11.7; 13.5)
	3.0	2.99	(2.00; 4.12)	12.7	(11.7; 13.6)
	3.5	3.06	(2.00; 4.26)	12.8	(11.7; 13.7)
	4.0	3.11	(2.00; 4.39)	12.8	(11.7; 13.7)

In table 3 and 4, the difference between the T90-values for the Experiment, Simulations in TELEMAC-3D and Calculations bu hand in Excel are presented. In the two tables, the difference between i.e. the T90-values from the Experiment and Simulated results has been calculated. The same method has been used for *Calculated by hand and Simulated results* and *Experiment and Calculated by hand results*.

Table .3: Calculated difference for T90-values for light conditions

Season	**Secchi depth**	**Experiment and Simulated results**	**Calculated by hand and Simulated results**	**Experiment and Calculated by hand results**
March	2.5	3.19	0.08	3.11
	3.0	3.17	0.09	3.07
	3.5	3.15	0.11	3.04
	4.0	3.13	0.12	3.02
August	2.5	1.89	0.02	1.87
	3.0	1.88	0.02	1.86
	3.5	1.88	0.03	1.85
	4.0	1.87	0.03	1.85
November	2.5	3.73	0.15	3.58
	3.0	3.68	0.18	3.51
	3.5	3.64	0.21	3.44
	4.0	3.60	0.21	3.39

Table .4: Calculated difference in T90-values for dark conditions

Season	**Secchi depth**	**Experiment and simulated results**	**Calculated by hand and simulated results**	**Experiment and Calculated by hand results**
March	2.5	-20.22	-5.95	-14.3
	3.0	-20.22	-5.85	-14.4
	3.5	-20.22	-5.76	-14.5
	4.0	-20.22	-5.68	-14.5
August	2.5	1.49	-0.04	1.54
	3.0	1.42	-0.12	1.53
	3.5	1.42	-0.11	1.53
	4.0	1.42	-0.11	1.53
November	2.5	-9.35	-2.59	-6.77
	3.0	-9.35	-2.54	-6.81
	3.5	-9.35	-2.50	-6.85
	4.0	-9.35	-2.46	-6.89

In table 5 and 6, the difference in fraction for the T90-values for the Experiment, Simulations in TELEMAC-3D and Calculations by hand in Excel are presented. The calculations were performed with the method described in section *5. Simplified case*, equation 23-25.

Table .5: Calculated difference in fraction for T90-values, light conditions

Season	**Secchi depth**	**Experiment and simulated results**	**Calculated by hand and simulated results**	**Experiment and Calculated by hand results**
March	2.5	0.76	0.07	0.92
	3.0	0.75	0.08	0.92
	3.5	0.75	0.09	0.91
	4.0	0.75	0.10	0.90
August	2.5	0,86	0.06	0.96
	3.0	0,86	0.07	0.96
	3.5	0,85	0.07	0.95
	4.0	0,85	0.08	0.95
November	2.5	-0,26	0.05	0.89
	3.0	-0,28	0.06	0.88
	3.5	-0,30	0.06	0.87
	4.0	-0,32	0.07	0.86

Table .6: Calculated difference in fraction for T90-values, dark conditions

Season	**Secchi depth**	**Experiment and simulated results**	**Calculated by hand and simulated results**	**Experiment and Calculated by hand results**
March	2.5	-4.40	-0.32	0.69
	3.0	-4.40	-0.31	0.68
	3.5	-4.40	-0.30	0.67
	4.0	-4.40	-0.30	0.66
August	2.5	0.39	-0.02	0.99
	3.0	0.37	-0.05	0.99
	3.5	0.37	-0.05	0.99
	4.0	0.37	-0.05	0.99
November	2.5	-1.59	-0.20	0.89
	3.0	-1.59	-0.20	0.88
	3.5	-1.59	-0.20	0.88
	4.0	-1.59	-0.19	0.87