Development of a Hydroinformatics Software Tool

Enteric Bacteria Transport Modelling Associated with Sediment Transport

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DECLARATION

This work has not previously been accepted in substance for any degree and is not concurrently being submitted in candidature for any degree.

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Date   14th Nov. 2005

STATEMENT 1

This thesis is the result of my own investigations, except where otherwise stated. Other sources are acknowledged by footnotes giving explicit references. A bibliography is appended.

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Abstract

This study presents investigations on microbiological water quality numerical modelling. Emphases have been laid on the model development by implementing state-of-the-art technologies in terms of the new research branch in water science, established in 1980s – hydroinformatics.

In the study, new mathematical equations for modelling bacterial re-suspension from bottom sediments and disappearance due to sediment deposition are established. Therefore, the bacterial re-suspension from bottom sediments is firstly modelled. The bacterial sedimentation equations presenting bacterial disappearance due to sediments settling process in natural waters is also introduced, which is independent from the well-known first order decay model.

Based on the new equations, an integrated 1-D and 2-D hydroinformatics water quality simulation model has been developed, carrying out sediment transport associated bacteriological water quality modelling. The model therefore performs modelling work including hydrodynamic modelling, sediment transport modelling and bacterial decay modelling which is associated with the sediment transport processes. The new bacterial decay model encompasses the terms of bacterial first order decay, bacterial resuspension and the bacterial deposition.

Object-oriented methodologies are employed in the integration of the sediment-associated multi-dimensional water quality model to encompass well-tested existing modules, by implementing Fortran 90 and Visual Basic 6.0 programming languages to deploy the advanced numerical schemes and provide a state-of-the-art GUI system.

Validation and calibration of the integrated sediment-linked water quality model has been carried out in its application to the Bristol Channel and Severn Estuary by using vast volumes of data from in-situ field measurements including: diffuse faecal indicator sources of 29 riverine inputs; point faecal indicators sources of 34 WwTW outfalls; daily-recording hourly observed sunlight radiation data; downstream real-time tidal water elevation boundary data; upstream Severn River flowrate variations; and the bathymetry data across the 1-D and 2-D domain. Satisfied calibration results were obtained and the model was successfully validated to estimate the enterococci concentration levels at beach bathing water compliance locations, thereby could now be applied to other estuarine environments.

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Chapter 1

GENERAL INTRODUCTION

This study addresses the new and developing field of hydroinformatics. At the beginning when the study started, the objective of the research project was to develop a software tool for water quality modelling. The questions confronted by this objective were: What kind of software was going to be? Which kind of water quality problem would be solved?

The answer to the first question was a 'hydroinformatics software tool' integrating existing and newly developed sub-models via object-oriented technologies to construct numerical modelling tools for integrated catchment areas. The answer to the second question was to model the 'enteric bacteria transport processes' in natural waters. These questions were followed by what kind of problems could be solved whilst a lot of these modelling tools had already been established and what were the new investigations in enteric bacteria processes modelling?

With these questions in mind, the research study outlined herein can be described from four main areas. Expressed in keywords these four areas are given as: hydroinformatics, object-oriented methods, graphical user-friendly interfaces and the investigation of enteric bacteria transport processes. Firstly, hydroinformatics is a new research branch and a post-modern technology. Any new field undoubtedly needs researchers making an effort to explore, improve and to implement the techniques. So this study could be firstly placed in the field of hydroinformatics.

In recent years more emphasis has been focused on the demand for upgrading existing numerical models by making them more user-friendly, with easy to use graphical user interfaces (GUI). This is because water environmental assessment projects have been developed not just among professionals, but also amongst a wide rang of professions for societal needs. The joint efforts from non-experts are increasingly challenging modellers to have more user-friendly visualization capabilities and thus the implementation of the GUI facilities forms a key aspect of this study.

The main part of the study focuses on the modelling of enteric bacteria transport processes. It is known that, in general, microbiological numerical modelling predictions comprise three parts: 1) hydrodynamic modelling, i.e. studying the current patterns, to give a description of the water movements and provides templates for runs on bacteriological modelling; 2) transport modelling, studying the bacteria advective /dispersion transport processes resulting from the flow fields, i.e. computes the bacterial levels from pure dilution effects by transport of the flow flux; 3) bacteriological decay modelling, i.e. studying the kinetic principles of bacteria transformation in the natural water environment, including any source entries and disappearance, including both die-off and physical losses.

To-date there have been well documented details of a wide range of hydrodynamic and transport models of coastal and estuarine waters, with water quality modelling started in the 1960s and 70s (Heaps, 1969; Thomann, 1972, 1987; Abbott, 1979; Fischer et al., 1979; Orlob, 1982; McCutcheon, 1989; Falconer and Cahyono,1994; etc). However, there is still a major lack of knowledge in the third aspect, i.e. bacteriological decay modelling. In recent years, more emphasis has been focused on studies examining the relationship between sediments and the bacterial population and higher heterotrophic activity. Although the abundance of microbial populations and their heterotrophic activity in the water column and in the bed sediments have been studied simultaneously in both field and laboratory experiments in the past, numerical modelling studies on these aspects have been rarely reported. The author has noted that the relationship between bacteria transferring from the sediments to the overlying water has not carefully investigated to-date, in particular, no quantitative relationships have been established. These key references will be described in detail in Chapter 2 – Literature Review.

The main focus of this research study has therefore been to reveal the mechanisms of the enteric bacteria transport processes in coastal waters in the natural environment, via computer numerical modelling studies. The numerical model developed not only applies the well-known first order decay model, but also with additional bacterial deposition fluxes due to sediments settling out and additional bacterial re-entraining due to bottom being re-suspension into the water column. These new investigations are outlined in Chapter 4 of the study.

1.1   Hydroinformatics

Hydroinformatics is a rapidly growing research field, since its introduction in the late 1980s (Abbott 1999). This relatively new discipline is a branch of science concerned with the applications of information technology (IT) in the engineering and research field of water science and technology. There are two main aspects within hydroinformatics. On the one hand, hydroinformatics is a new technology related to the study of water, with this technology raising a new concept of multi-technology systems. It is the integration and linking of various domains in water science, including hydraulics, hydrology, water chemistry, physics and biology, with all of these embedded in water resources and the water cycle.

On the other hand, hydroinformatics is a software system. The application of the state-of-the-art information technology and modelling capabilities lies at the heart of the hydroinformatics. Hydroinformatics depends upon computers and is developing along with the continuing improvements in computing. As this was born out of the computer skills, hydroinformatics presents all of the advantages from computer science at its start. The use of the computer provides more accurate, simpler and quicker processes predictions in comparison with traditional calculation, design and management processes for the water industry and resource management. Firstly, by undertaking the calculations on a computer to get automatic calculations makes the process quickly and also automation gives the possibility to water engineers and scientists to explore many different designs to determine which is optimal. This automation changed the traditional design procedures into simply clicks of a button. Secondly, after debugging and model

validation, the automatic calculation program created above can be re-used in any future calculations without errors.

Although the advantages taken from modern day computers are the key feature of hydroinformatics, the emphasis of this discipline is placed on solving water problems for the water industry and water resources. The study is based on developing and improving engineering technologies and scientific research for water by using modern information technology. Therefore, hydroinformatics also can be said to be an applied water science based on the assistance of computers.

Over the past 20 years the key developments in hydroinformatics have been: data mining; modelling; integration technology; process control; design and management, with each of reviewed briefly below.

◆ Data mining

Environmental water engineers and scientists often work with large amounts of data. The exploration of data or data analysis is often very difficult due to the form of the recovery of knowledge from classical statistical and physical models, due to the complexities in the large amount of data sets and the limits in the analysis methods. This leads to the new technique of data mining methods being involved in the field of hydroinformatics.

The technique of data mining in hydroinformatics has its potential uses in two contexts. Firstly, it has considerable benefits in terms of searching data, collecting data, data acquisition and visualization. These data management facilities are important parts of hydroinformatics software tools, as data are the information resource for most practical environments. Secondly, data mining is useful in terms of the transformation of data to knowledge. This is also called data mining for knowledge discovery.

The data used today are generally raw and abundant and not exploited because of a lack of tools, a lack of the means to transform them into information and a lack of the developed market (Cunge 1999). Hydroinformatics is the technology growing in this area and aimed at overcoming these difficulties. An example is the D2K project (http://projects.dhi.dk/dzk) which used large-scale data mining in hydroinformatics. Some scientific numerical methods have been integrated within the hydroinformatics

discipline to solve this problem. Artificial neural network (ANN) tools and evolutionary algorithms (EA) are methods that allow the establishment of physical laws from the raw data.

One function of data mining for knowledge discovery in hydroinformatics is presented as data assimilation, which is a method that combines a model of a system with measurements in order to obtain a better knowledge about the state of the system (Babovic and Fuhrman 2002). Applications of data assimilation have been increasingly developed in the field of hydroinformatics (e.g. Savic et al 1999, Babovic and Fahrman 2002, Hugen and Parrish 2002). Data mining methods have been adapted from IT and have a wide use in hydroinformatics, those methods include: 1.data selection, 2.pre-processing, 3.data mining, 4.post-processing, 5.interpretation and evaluation, 6.knowledge discovery (Fayadd et.al. 1996).

◆ Modelling

Computer modelling is a methodology by which a mathematical formulation is used to describe a physical process. The appearance of hydroinformatics arose from the development of the fourth generation of modelling tools in the mid-1980s (Abbott 1999) whereas numerical modelling has been frequently used in water engineering applications since the 1960s. Hence the development of hydroinformatics has started from the application of computer numerical modelling tools. Computer modelling provides powerful tools that offer the possibility of testing numerically scenarios that could never be tested physically, even if it could be performed at any spatial and temporal scales.

◆ Integration technology

In the case of hydroinformatics, more concerns arise in solving problems as a result of increasing complexity and social aspects of the problems. Whereas a single modelling tool maybe used to solve specific process, integration technology allows a modelling system to combine or co-ordinate different modelling compartments to solve large systems problems. In real-time studies large system problems occur most commonly in the water environment. Nevertheless this integration technology employs object oriented methods with implementing geographical information systems (GIS) and provides user-friendly graphical interfaces to allow the numerical techniques be easily set-up and

operated and then used in various forms to provide invaluable information to public society.

◆ Design and Process control

Hydroinformatics was first developed from numerical modelling techniques associated with computational hydraulics. It is well-known that computational hydraulics was the mainly component used to design water supply systems or wastewater networks, and sewerage networks etc. Design work in hydroinformatics has many advantages as the water-related industries needed to recognise any environmental impacts for social aspects. By providing the less trained technologists with user-friendly tools, then the results and design processes in hydroinformatics were more readily understood and easily interpreted by the public.

Computer-aided process control has been widely used in the industrial world but has not been so widely used in the water industry. The other advance within hydroinformatics have been the development of process control as applied in the water industry, such as the on-line control of operations in water and wastewater treatment works. This is not the main focus of the thesis, but is worthy of note at this stage.

◆ Management

Management is the domain containing all analysis of the above mentioned techniques and involves comprehensive multi-function, multi-purpose processes. The objective is to maintain the water resources in an environmentally-friendly and sustainable manner. Water resource management therefore refers to two individual aspects. One is the scientific and technical issues and the other is the social and economic aspects. Therefore the decision-making process in water resource management not only includes the engineers, the managers, the police-makers, but also a whole ranges of stake holders and their associative and political representatives as well as the information carriers such as the media.

The shortage of water is a world-wide problem existing in many countries. This water shortage problem is partly due to more water pollution from modernization and waste disposal thereby reducing the usability of limited water resources; and also from the

uneven distribution of rainfall events across the seasons causing serious water quantity shortages in dry weather and high flood-risk during wet seasons.

The need to solve these water shortage problems and manage the world's limited water resource becomes more and more urgent with time. Hydroinformatics software tool have great potential for improving the planning and management of water resources. Flood management from flooding forecasts, to the impact of flooding and then flood protection, is one of the main subjects for decision-making. Hydroinformatics tools can meet the target to compare alternative decisions taking into account scientific, social and economical parameters. Furthermore, hydroinformatics tools can potentially benefit the modelling tasks by interconnecting between ground water and surface water systems in water resources management. Another task is the water quality management of water resources, to reduce the water pollution as much as possible. The importance of this task is dramatically increases rapidly with growth of the economy and population. This study will focus on this topic – that is water quality assessment in coastal waters.

The discussion has so far been limited only to the contents of the field of hydroinformatics. This field has such a wide range of scope that it is possible to be defined as a new platform, and any development or application to water science and technology placed on this platform will provide benefits for the future.

1.2   Water Quality Indicators – Enteric Bacteria

The measurement of the abundance of enteric bacteria (i.e. total coliform, faecal coliform and faecal streptococci or enterococci) is one of the most commonly used methods to establish the quality of natural waters. These measurement data are very much a part of coastal management, as monitoring the enteric bacteria counts in the water environment is one of the main tasks in water quality control, and is especially important as a standard parameter for the usage of water against human pathogens in bathing beaches, high-use recreational areas and water for food productions.

Research on the survival of enteric bacteria in the water environment has received considerable attention in recent years because of their usage as the indices of water

quality for the use of bathing, water recreations and shellfishing. Furthermore, discovering relationships within these measurement data and building up a mathematical modelling tool for further predictions, even for the predictions at some specific sites that were impossible for physical measurement either temporally or spatially, will lead to a more efficient control on water quality in coastal zones.

Therefore, in order to protect natural waters from enteric bacteria pollution, coastal management practices must involve both monitoring and modelling of enteric bacteria and finally to have decision-making according to the monitoring data and the modelling assessments.

In past studies, most effort has concentrated on field investigations and laboratory studies but only limited studies have been focused on modelling. Hence this study will lay the emphasis on modelling enteric bacteria transport processes, which is entirely new established and associated with sediment transport in coastal waters.

1.3   Research Aims and Objectives

The main aims of the current research study reported herein can be summarised as follows:

1. Develop a hydroinformatics software tool.

2. Solve a practical problem by applying the hydroinformatics software tool for a real-time water quality modelling study of Bristol Channel and Severn Estuary.

3. Implement object orientated (OO) technology to combine existing and well-tested models into the software tool to most efficiently and quickly improve the power of the software tool.

4. Apply GUIs in the software tool to present user-friendly capabilities and include data mining techniques.

5. Build up the new investigations on enteric bacteria in transport modelling. This is a key issue in the research and firstly the topic will be reviewed in Chapter 2 – Literature Review. There are many researches historically focused on the enteric bacteria contamination as this topic is so close linked to daily public health. However, there is a research dearth needs to be fitted, that is to reveal the paradigm of bacteria contamination coming from bed sediments as well as settling down to the bed in a quantitative way. This research project goes on to build up these mathematical equations and solve the equations numerically; hence a model which performs the most comprehensive bacteria transport modelling process in natural waters is investigated (see Chapter 4).

1.4   Overview of the Thesis

Chapter 1 provides a brief introduction to introduce the concept of hydroinformatics and lead to the basis of this research.

Chapter 2 provides an overview of the historical research undertaken in the area of survival and contamination of enteric bacteria in natural waters. In this chapter the confronted problem from the review of historical research on bacteria modelling is found to be the greet needs in developing the new models for enteric bacteria transport modelling to include the bacterial entrainment from the bed sediments and the bacterial sedimentation due to the SS depositions.

Chapter 3 presents the theoretical background describing the foundation of numerical modelling for bacterial water quality assessment. This chapter introduces the basic theoretical background of bacterial water quality numerical modelling, including the standard governing equations and the algorithms of the numerical solution.

Chapter 4, the most important issue in the thesis demonstrates a new investigation for bacteria transport modelling associated with sediment transport in natural waters. It describes the basic concept model, mathematical model, numerical model, and finally illustrates the whole process of the new modelling approach of bacteria transport

processes, which are associated with the sediment transportation. Also the mechanics of sediment transport modelling processes which are linked to the bacteria transport modelling are discussed in this chapter.

Chapter 5 describes the implementation of object orientated (OO) technology in the hydroinformatics software system. It is an attempt to explain the OO technology in a core position in this research, which integrates existing and well-tested models into the simulation model. This chapter details the development of the integrated simulation model system, which is capable of predicting water elevations, velocities, cohesive and non-cohesive sediment concentration distributions, and the bacteria contaminations associated with or without the suspended sediments. Chapter 5 also details the development of GUIs provided to the hydroinformatics software tool. Emphasis is placed on the construction of the interface for existing model. The facilities within the interface not only have the easy-access "windows", but also include data management and storage tools, as well as the graphic and tabular visualization functions.

Chapter 6 presents the application of the model to the Bristol Channel and Severn Estuary. The application is carried out to illustrate the model's various capabilities on modelling each related process. In this application, excellent hydrodynamic calibration and satisfactory enterococci calibration were achieved.

Chapter 7 analyses the different uncertainty levels of the model results by taking into account the selection of model parameters with the selection of different model assumptions. The sensitivity of bacteria decay rate, bacteria bed concentration and the flux of sediment loads and flow effects etc. have been studied under a series of model tests.

Chapter 8 draws the conclusions from the research project and discusses the scope for future development.

Chapter 2

LITERATURE REVIEW

In water quality management, the use of enteric bacteria i.e. total coliform (TC), faecal coliform (FC) and faecal streptococci or enterococci as public health parameter for indicating pollution of natural waters (such as lake, river, coastal and estuarine water) is widespread. It is therefore of critical concern to predict the fate of enteric bacteria in natural waters. There have been many studies reported in the literature and focusing on this subject. This chapter focuses on gaining an insight into these historical research details not only for the physical experimental survival studies, but also for studies of mathematical or computer modelling of bacteria die-off. This review progresses through survival studies, both in water column and the bottom sediments. The review reveals that further research efforts need to be focused on investigations of developing modelling tool for enteric bacteria die-off (or survival). In particular, investigations on modelling of the die-off or survival associated with bottom sediments are of the greatest concern for research focus.

2.1   Enteric Bacteria in Natural Water Environment

Natural water basins often receive large amounts of waste and wastewaters, arising from rapid modernisation and economical development in surrounding towns and cities, and this amount of waste and wastewaters are always increasing. This leads to a worldwide-spread of water pollution problems, including enteric bacteria contamination.

2.1.1   Sources of enteric bacteria to natural waters

In order to control water pollution, an investigation first needs to be undertaken of the pollutant sources. Although wastewater outfalls are generally the main source of enteric bacteria, many other sources are also frequent. There are often multiple sources of enteric bacteria to natural water systems.

♦ WwTW outfalls

There are always one or more wastewater treatment works (WwTW) in each city. The WwTW outfalls generally release either into the sea or to rivers and are the most significant sources of enteric bacteria in the natural environment. For example, in this study the data provided by the Environmental Agency indicated there were 34 WwTW outfalls located in the Bristol Channel and Severn Estuary, with the faecal indicator bacteria concentrations being up to millions of counts. Usually WwTW outfalls are the major sources of faecal organisms to natural waters; however, levels of bacterial indicators in effluents from a properly functioning sewage treatment plant using disinfection will be considerably reduced (Miescier and Cabelli, 1982). In some environments, for example, Fujioka et al. (1995) found that the ocean sewage outfall was not the major source of elevated concentrations of faecal bacteria recovered from shoreline beach sites near and around Kailua Beach.

♦ Storm sewer outfalls and Sewage overflows

During storm events, storm sewers contribute water to the natural water resources (lake, river, estuary or sea) and this added flow can possibly contain elevated faecal bacteria concentrations, which come from field and street surfaces (Hunter, et al. 1992; Coyne, et al. 1995 and Roll and Fujioka, 1997). A sanitary sewer source is also a possibility, since storms can aggravate infiltration and inflows, thereby causing an indirect connection to the waters through sewage overflows, especially when a combined sewer system is used (Richman, 1996 and Solo-Gabriele, et al. 2000).

♦ Rainfall and surface runoff

It is very usual for faecal bacteria concentrations to be elevated during or after rainfall events. Solo-Gabriela et al.(2000) reported their 7-day autosample experiments in a coastal waterway, where the first and most obvious relationship was the extremely high E. coli concentrations observed during periods of rainfall. The experimental results are

plotted in Figure 2.1, where E. coli concentration was counted in a most probable number (MPN) per 100ml of water by using a defined substrate technology known as Colilert-18.
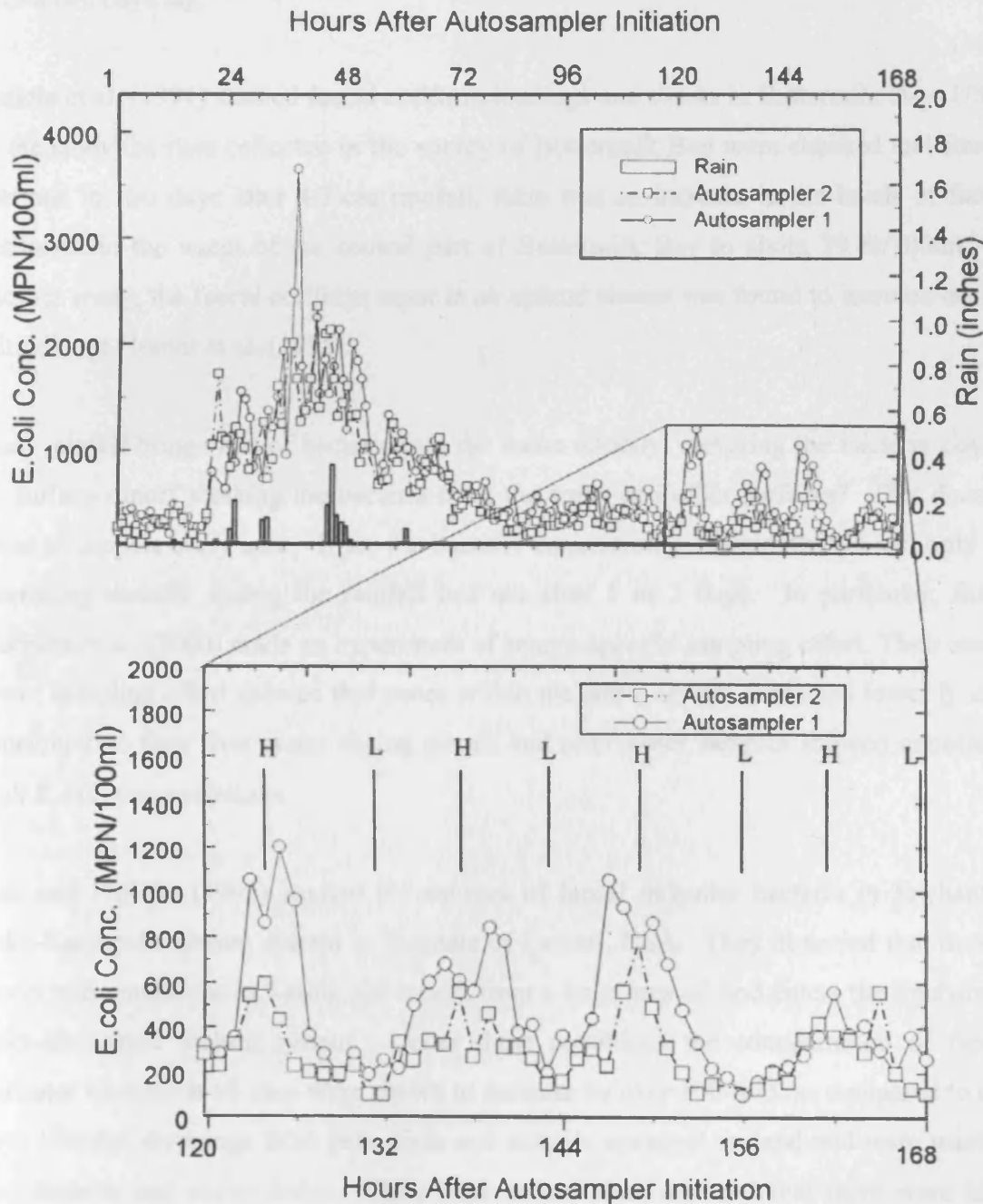
Figure 2.1   Results of 1-week auto-sampler experiment. H, high tide; L, low tide.
(after Solo-Gabriela et al., 2000)

Figure 2.1 shows two distinct relationships between E. coli levels and hydrologic conditions. The first obvious relationship was the extremely high E. coli levels observed during rainfall (as shown in the figure in day 2 and day 3). The second peak occurred from day 6 to day 7, so it shows that after the rainfall there was a second peak occurring with a two days lag.

Valiela et al. (1991) studied faecal coliform loadings and stocks in Buttermilk Bay, USA. In the study the data collected in the survey of Buttermilk Bay were checked and shown that one to two days after 4.7 cm rainfall, there was an increase in the levels of faecal coliforms in the water of the central part of Buttermilk Bay to about 79 fc/100ml. In another study, the faecal coliform input to an upland stream was found to increase during rainfall, see Hunter et al. (1992).

Does rainfall brings lots of bacteria into the water directly, elevating the bacteria counts by surface runoff washing the bacteria from the street and other surfaces? This doesn't seem to support every case. If so, the bacteria concentration should always and only go increasing directly during the rainfall but not after 1 or 2 days. In particular, Solo-Gabriela et al. (2000) made an experiment of source-specific sampling effort. Their storm sewer sampling effort showed that water within the storm sewers contained lower E. coli concentration than river water during storms and river water samples showed extremely high E. coli concentrations.

Roll and Fujioka (1997) studied the sources of faecal indicator bacteria in Enchanted Lake-Kaelepulu Stream system in the state of Hawaii, USA. They observed that during heavy rain conditions in Kailua, the runoff from a large area of land enters the Enchanted Lake-Kaelepulu Stream system. Under these conditions the concentration of faecal indicator bacteria at all sites were shown to increase by over 100-fold, as compared to dry days. Faecal droppings from pets, birds and animals occurred on land and were washed into streams and storm drains. Their experiments also indicated that there were high concentrations of nutrients being washed from the catchments into the lake stream system. The results of the nutrients experiment provided a good resource to conclude that the added nutrients from land surface runoff could support bacterial rapid-growth after rainfall in a one- or two-day later. Therefore rainfall can either wash faecal bacteria or

nutrients which support the bacteria growth from farm land surface runoff to enter the catchment stream or drainage system.

Crowther et al.(2001) studied the relationship between FC, TC and FS concentrations and environmental conditions in coastal recreational waters by in-situ monitoring of 8 bathing water sites during the bathing season (May to September) with two experimental series undertoken in two periods of pre-schemes and post-schemes (i.e. before and after a new WwTW had been completed). The study found that concentration of FC, TC and FS were all significantly increased following rainfall for the pre-schemes period, even with minor rainfall events. For the post-schemes period rainfall was still a significant factor but only the effect of higher magnitude rainfall events was of importance.

◆ **Upstream river inflows**

Streams usually contain high concentrations of faecal bacteria as reported in many publications. A study by Roll and Fujioka (1997) revealed that streams (in uplands) are major external sources of faecal bacteria and nutrients entering Enchanted Lake and Kaelepulu Stream. The source of stream water was usually rainfall in the mountains. As cited above, the surface runoff brings loads of bacteria from the land surface into the stream water system. There is little doubt that the upstream stream/river inflows are one of the major sources of faecal indicator bacteria in lakes, rivers, estuaries and coastal waters.

◆ **Groundwater discharge**

In the study of Solo-Gabriele et al. (2000), stage measurements of the canal and groundwater during tidal conditions indicated that groundwater contributions are strongest during low tide, including contamination of groundwater from septic tanks and sanitary sewers, as a source of E. coli contamination.

◆ **Water creatures**

The study of Roll and Fujioka (1997) reported that animal faeces on land were a source of faecal bacteria which were washed into streams and storm drains by rain. Some animals such as ducks discharge faeces directly to streams on a daily basis. In the study, four samples of duck faeces obtained from the banks of Kaelepulu Stream were determined to contain average concentrations (CFU/gram of faeces) of $1.6*10^6$ E. coli, $7.6*10^5$ faecal coli, $1.4*10^6$ enterococci and $2.9*10^5$ C. perfringens.

♦ River bank (soil)

Solo-Gabriele et al. (2000) reported that river bank soils were found to be a significant source between storms, with the largest E. coli concentrations observed during high tide. The study indicated that both storm surface runoff and incoming tidal flow could flush the E. coli from the bank soils into the river water column. Another mechanism by which direct runoff or up-going tidal flow acts as a source is by washing in faecal matter deposited by animals who foraged along the river bank. Hardina and Fujioka (1991) reported high concentrations of faecal indicators in soils of Hawaii. Their further study (Roll and Fujioka, 1997) indicated that soil, rather than sewage or animal faeces, was the major environmental source of faecal indicator bacteria recovered from streams as they found the presence of high concentrations of faecal coliform, E. coli and enterococci in soil but low concentrations of C. perfringens in the soil, corresponding to the same relative concentrations of these bacteria in streams.

♦ Intertidal beaches

Obiri-Danso and Jones (2000) studied intertidal sediments as reservoirs for faecal indicators in bathing waters by analysing intertidal sediment samples taken in Morecambe, a seaside resort in Morecambe Bay in the north west of England, which has a high tidal range, from 7.5 to 10.2 m. At low tide there is a vast area of exposed intertidal sediments (31086 ha of sand and mudflats) which are foraged by large numbers of waterfowl leaving their faeces. They reported that sediments at the northern part of Morecambe contained on average 1000-6500 faecal coliforms cm^{-3}, 200-700 faecal streptococci cm^{-3} and 3-13 Campylobacter cm^{-3} (assuming 1g dry weight cm^{-3}). The measurements showed that the faecal indicators were not found in subsurface sediments and mainly stayed within the first 1 cm layer. Therefore these bacteria are readily entrained into the water column by tidal action.

♦ Bottom sediment re-suspension

The microbiological quality of sediments at the sediment-water interface in bathing waters is receiving increased attention. The re-suspension of sediment-bound indicator bacteria, which raised significant public health hazards for the overlying water column has been documented by many studies (Grimes, 1975, 1980; Gerba and McLeod, 1976; Laliberte and Grimes, 1982). The study of faecal coliform loadings and stocks in Buttermilk Bay in USA by Valiela et al. (1991) deduced one conclusion as below:

"The amounts of faecal coliforms brought into the bay by waterfowl, surface runoff, groundwater and streams are an order of magnitude smaller than the losses by mortality and tidal removal. This implies that there is an additional source of faecal coliforms within the bay. We suggest that resuspension of the upper layers of sediments can easily account for the faecal coliform present in the water."

There is an evidence that faecal indicator and pathogenic bacteria survive in sediments for longer than in overlying water and it has been proposed that sediments serve as reservoirs for faecal bacteria with the potential to pollute the overlying bathing waters (Valiela et al., 1991; Ashbolt et al., 1993; Nix et al., 1993; Ghinsberg et al., 1994; Howell et al., 1996).

Grimes (1975) reported a study which examined membrane filter faecal coliform (FC) densities in a relatively nonpolluted reach of the Mississippi River prior to, during and after a large dredging operation. It was found that FC concentrations in water samples collected downstream (0 to 1 km) from the dredging were significantly greater than in upstream samples and the water samples collected during dredging had significantly higher FC densities than before or after. These increased counts were obviously attributed to the disturbance and relocation of bottom sediments by dredging with concomitant release of sediment-bounded FC to the overlying water column. In another study, Grimes (1980) further reporting the bacteriological water quality effects from bed sediments by hydraulically dredging, found that TC and FC densities in water samples taken below the dredging discharge pipe were approx. 4 times the corresponding upstream values; and FS densities were approx. 50 times the corresponding upstream values. His correlation analysis indicated that mean turbidity values downstream of the dredging operation were directly and significantly (the correlation coefficient, r>0.94) related to the corresponding TC, FC and FS densities, revealing that the increased bacteria counts from the re-suspension of bed sediments were significantly high.

Crabill et al. (1999) studied the impact of sediment faecal coliform reservoirs on seasonal water quality in Oak Creek, Arizona, and their results showed that sediment agitation by recreational activity and storm events associated with the summer storm season were responsible for the impact to water quality.

♦Growth in water

There has been an increasing body of evidence indicating that faecal indicator bacteria are capable of limited growth both in polluted fresh water and sea water. After a series of studies on growth of enteric bacteria in river water (Hendricks and Morrison, 1967, and Hendricks, 1970, 1971, 1972), Hendricks et al. indicated growth of faecal coliforms in autoclaved polluted stream water, but not in unpolluted water. Shuval et al. (1973) found re-growth of these organisms in chlorinated sewage effluents. Gerba and McLeod (1976) observed growth of E. coli in sea water. They used autoclaved natural seawater taken from both domestic wastes polluted and unpolluted sites. The experimental results showed E. coli rapidly died away in water from the unpolluted sites, but after a lag period of 5 to 6 days an increase in the number by 2 logs (i.e. from 10^3 E. coli/ml to 10^5 E. coli/ml) was usually observed in water taken from polluted areas (shown in Figure 2.2). It was also concluded that the growth was always more gradual in seawater alone and never reached numbers as high as those observed when sediment was present. The observation that E. coli always persisted much longer when sediment was presented was very significant.

Symbols:

o - seawater from site7 (an area receiving no domestic wastes);

▲ - seawater from site1;

● - sediment from site7;

■ - sediment from site1.
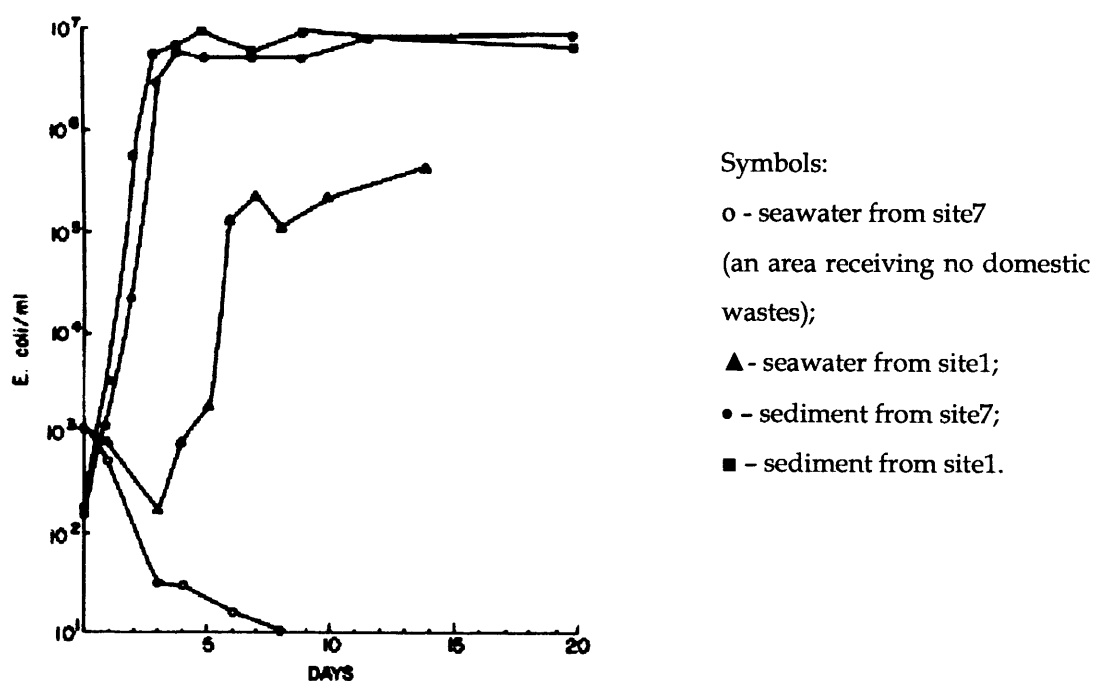
Figure 2.2   Growth of E. coli in nutrients eluted from autoclaved sediment.

(after Gerba and McLeod, 1976)

Tassoula (1997) studied the growth possibilities of *E. coli* in natural waters. His experiments have provided a significant result for sewage disposal in natural waters. It was found that, for 0 up to 35‰ salinities, covering the salinity range of natural waters, the E. coli number increased, as long as there was present an organic load. Hence in raw sewage disposal areas around the diffusers, especially on and near the bottom where deposition of sediment loads takes place, as well as in sludge disposal areas of sewage treatment plants, one would not expect decay of E. coli, but to the contrary growing E. coli growth at high rates. For example, the experiment of artificial sewage with 9‰ salinity showed an increase in the E. coli concentration from 10^3 up to 10^7 counts/ml for the first 2 days of experiments, and subsequently the E. coli concentrations remained nearly at the same level for the remaining 28 days of the experiment. Growth was also observed in the sewages with 0‰ and 35‰ salinities, although these were for slightly lower growth rates, of from 10^3 up to 10^6 and 10^5 E.coli/ml after the first two days respectively. Therefore, the area around the sewage disposal diffusers should be considered suspect for E. coli growth whether the water is saline or not.

2.1.2   Survival of enteric bacteria in natural waters

2.1.2.1   T90

The survival of enteric bacteria in natural waters, which are from the discharge of sewage as well as other sources, as discussed in the above sections, has been the subject of substantial research over the past decades. Many environmental individual factors affecting the coliform survival have been studied, including: solar radiation; turbidity; sedimentation; nutrients and other physico-chemical factors; biological factors etc.

Most of the survival studies observed that the enteric bacteria decay in natural waters follows a first order decay model, known as Chick's Law (1908). As a tool for engineers, the decay rate is usually expressed in the form of T90, which is the time for 90% bacteria to die (or become inactivate). So T90 values frequently appeared in documented survival studies, showing a wide range of variations from 0.5 hour to several days (or even weeks) according to the environmental conditions (Chamberlin and Mitchell, 1978; Solic and Krstulovic, 1992; Pommepuy et al. 1992; Guillaud et al. 1997 and Wait and Sobsey, 2001).

For example, Pommepuy et al. (1992) studying the survival of enteric bacteria experimentally in two coastal regions, observed that on Mediterranean coasts, oligotrophic water and high solar radiation due to the climate greatly diminish the survival time of faecal bacteria in surface waters: T90 values were very short (< 2 hours) at the surface. However in deep water in the same region, where the wastewater plume was trapped under the thermocline, the T90 values were much longer (several tens of hours). In the English Channel, waters and sediments were rich in organic matter, with high turbidity significantly increasing faecal bacterial survival: T90 were very long, from several tens to hundreds of hours. A diurnal T90 variation of less than 1 hour at noon to 40 hours at night time was found in an experimental study by Bellair et al. (1977). Dupray et al. (1995) reported that in estuarine water, where shellfish are farmed, T90 was observed to be several days; the presence of organic matter and osmoprotective compounds were used to increase the faecal coliforms survival.

2.1.2.2 Factors affecting bacteria die-off

Several factors have been proposed which considerably affect the survival rates of faecal bacteria in natural water environments, including sunlight, temperature, turbidity (or SS concentration), nutrients concentration, salinity, predation, and sunlight-related water depth, etc. Among these factors sunlight was thought as being the most important factor (Chamberlin and Mitchell, 1978).

2.1.2.2.1 Sunlight

Gameson and Saxon (1967) indicated that the sunlight significantly affected the mortality of coliform bacteria. Bellair et al. (1977) studied the rate of die-off of faecal coliform in-situ experimentally and found a significance of diurnal variations in faecal coliform die-off rates, mainly related to the variation of solar radiation (see in Figure 2.3). The T90 values observed in the experiments can be related to the sunlight intensity as follows:

$$T90 = 3.4 \, I^{-0.42} \hspace{4cm} 2.1$$

where: T90 is in hours,

I is hourly solar radiation, in $MJ \, m^{-2} h^{-1}$.

Pommepuy et al. (1992) studied the survival of enteric bacteria in different environments depending on turbidity, nutrient and sunlight penetration. A close relationship was found

between the light intensity received by bacteria and the T90 value, which was similar to the findings reported by Bellair et al. (1977). This relationship was given as:

$$T90 = 1.2 \times 10^4 \, I_n^{-0.56} \qquad\qquad 2.2$$

where: T90 is in hours,

I_n is the light energy received by bacteria, $\mu E \, m^{-2} \, h^{-1}$, which is the function of turbidity and water depth.
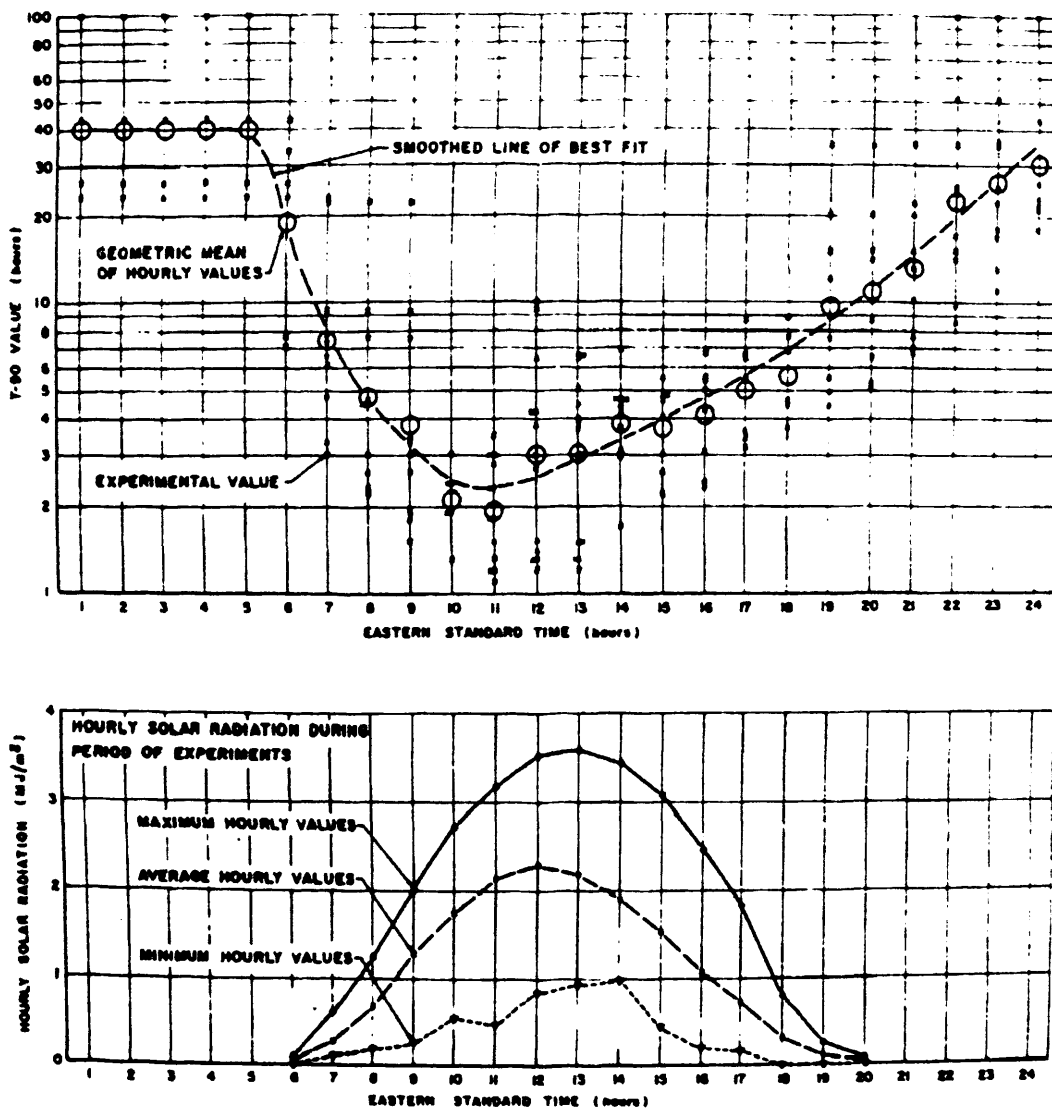
Figure 2.3   Summary of hourly values of T90 and solar radiation.

(after Bellair et al., 1977)

Alkan et al. (1995) studied the survival of enteric bacteria exposed to a sunlight simulator in varying conditions of light intensity, turbidity, sewage content, degree of mixing and temperature under controlled laboratory conditions. The variability of bacteria die-off due to the effect of light was linearly increased with the light intensity, except when a high sewage content of 3.0 % occurred where there was no die-off observed in E. coli population for the light intensity levels of up to 500 W/m^2. Above that value, the linear relationship between the die-off and the light intensity rose again for the high sewage content. Taking into account a combined coefficient, the relationship discovered can be presented as:

$$K_{EC} = A_{EC} + 1.3 \times 10^{-5} I_L \qquad\qquad 2.3$$

$$K_E = A_E + 1.1 \times 10^{-5} I_L \qquad\qquad 2.4$$

where: K_{EC}, K_E is the die-off rates for E. coli and Enterococci respectively, min^{-1};

A_{EC}, A_E is the combined coefficients for E. coli and enterococci, which are related to three other factors, namely: turbidity, sewage content and mixing effects;

I_L is the surface light intensity, $W\ m^{-2}$ (or $J\ m^{-2}\ s^{-1}$).

Guilland et al. (1997) studied the survival of E. coli in laboratories and in-situ under sunlight illuminations with the impacts of sewage and SS concentrations. The relationship between light intensity and T90 was found as below:

$$T90 = 53683\ I_m^{-0.666} \quad (n = 56;\ r^2 = 0.73) \qquad\qquad 2.5$$

Where: T90 is in hours;

I_m is the mean light intensity in the vertical water section, $\mu E\ m^{-2}\ h^{-1}$, which is a function related to surface light intensity, water depth and SS concentration.

2.1.2.2.2 Temperature

Wait and Sobsey (2001) reported that water temperature influenced the survival of test bacteria and viruses in the laboratory experiments, with 2-11 fold lower times for T90 values at 28°C than at 6°C. However, this relationship was not consistently observed in the in-situ field experiments, perhaps because of some other factors influencing the microbial survival. Hence for in-situ conditions there was no clear association between microbial survival and water temperature. Similarly, in the study of Alkan et al. (1995), temperature was proved not to exert any significant effect on bacteria survival in sea

water in the presence of light. The die-off rates were found not to be altered significantly by the variation in temperatures from 10°C to 30°C. This finding was attributed to the fact that the effect of light on the die-off rate overrides the effect of temperature.

Howell et al. (1996) reported that temperature significantly affected both FC and FS mortality (p=0.001). The experiments showed as temperature increased from 4°C to 25°C, mortality rates increased from 0.047 d^{-1} to 0.097 d^{-1} for faecal coliform and from 0.018 d^{-1} to 0.079 d^{-1} for faecal streptococci.

Korhonen and Martikainen (1991) made two sets of experiments using bottles incubated at 25°C and 4°C. The results showed that temperature hardly affected the survival of E. coli., but Campylobacter jejuni survived better at 4°C than at 25°C, and this was also observed by Blaser et al. (1980).

According to Flint (1987), he concluded that E. coli survive better at 4°C than at 25°C. Davenport et al. (1976) reported coliform bacteria to survive lengthy periods in water at 0°C. In earlier years, reports usually said that higher temperature increased bacterial mortality but it could also promote FC regrowth in aquatic environments (Stephenson and Street, 1978; Doran and Linn, 1979). Rhodes and Kator (1988) observed that E. coli cells initially exhibited multiplication (large negative values of the mortality rate coefficient, k) in membrane-filtered water (0.2um) at elevated temperatures in Chesapeake Bay.

The literature dealing with the role of temperature on the in-situ survival of E. coli in saline waters appears equivocal; the findings are confused concerning correlations of temperature and survival. It could be understood as the net effect either significant or not will depends on local environmental conditions.

2.1.2.2.3 Turbidity (or SS concentration)

It has been of increasing concern that high levels of turbidity (or suspended matters) are responsibly for the survival of enteric bacteria in water. Serrano et al. (1998) studied the influence of environmental factors on microbiological indicators of coastal water pollution. Their on-site sampling analysis showed the bacteria indicators in bathing water presented high counts associated with high turbidity.

Although the behaviour of faecal coliforms in natural waters is mainly light-dependent (Gourmelon et al., 1994), the turbidity of water plays an important role on bacteria survival, as the light intensity received by the bacteria in the field is a function of the turbidity and the depth of water (Pommepuy et al. 1992; Guillaud et al. 1997).

Pommepuy et al. (1992) found that according to Lambert's law, the light attenuation coefficient was related to the SS concentration accordingly:

$$k = 0.22 \times SS^{0.78} \qquad\qquad 2.6$$

Where: k is extinction coefficient in m^{-1}; SS is suspended solids concentration in $mg\ l^{-1}$. They also indicated that the direct effects of sunlight on the survival of enteric bacteria were limited in highly turbid waters.

Guillaud et al. (1997) found in their experiments that the extinction coefficient, which is associated with SS concentration for light intensity received by bacteria, was:

$$k = 0.189 \times SS^{0.799} \qquad\qquad 2.7$$

Where: k is in m^{-1}; SS is suspended solids concentration in $mg\ l^{-1}$.

Lambert's law can be written as (Guillaud et al., 1997):

$$I_m = I_o\,[(1-e^{-kh})/kh] \qquad\qquad 2.8$$

Where: I_m is mean light intensity received by bacteria, $\mu E\ m^{-2}\ h^{-1}$;

I_o is light intensity at the surface of seawater, $\mu E\ m^{-2}\ h^{-1}$;

h is water depth, m;

k is the extinction coefficient in m^{-1}.

Tunnicliff and Brickler (1984) suggested that turbidity might be a useful tool to quantitatively model FC loadings because a positive correlation between turbidity and FC densities was observed in the study (see Figure 2.4).

Alkan et al. (1995) also studied the turbidity effect on survival of enteric bacteria in marine waters and found a non-linear relationship between the die-off rates and the turbidity, as below:

$$K_{EC} \propto -3.77 \times 10^{-2}\,U + 2.52 \times 10^{-2}\,U^2 \qquad\qquad 2.9$$

$$K_E \propto -3.45 \times 10^{-2}\,U + 2.13 \times 10^{-2}\,U^2 \qquad\qquad 2.10$$

where: K_{EC}, K_E is the die-off rates for E. coli and enterococci respectively, min^{-1}; U is the turbidity (absorbance, 0-1; λ=288 nm). In this study, it was clearly shown that the die-off rate increased as a function of light intensity for turbidity levels between approx. 0.6 and 0.86 (at a very slow rate), whereas the effect of turbidity was much more pronounced when it was below 0.6 and the increase in die-off rate was considerably higher.
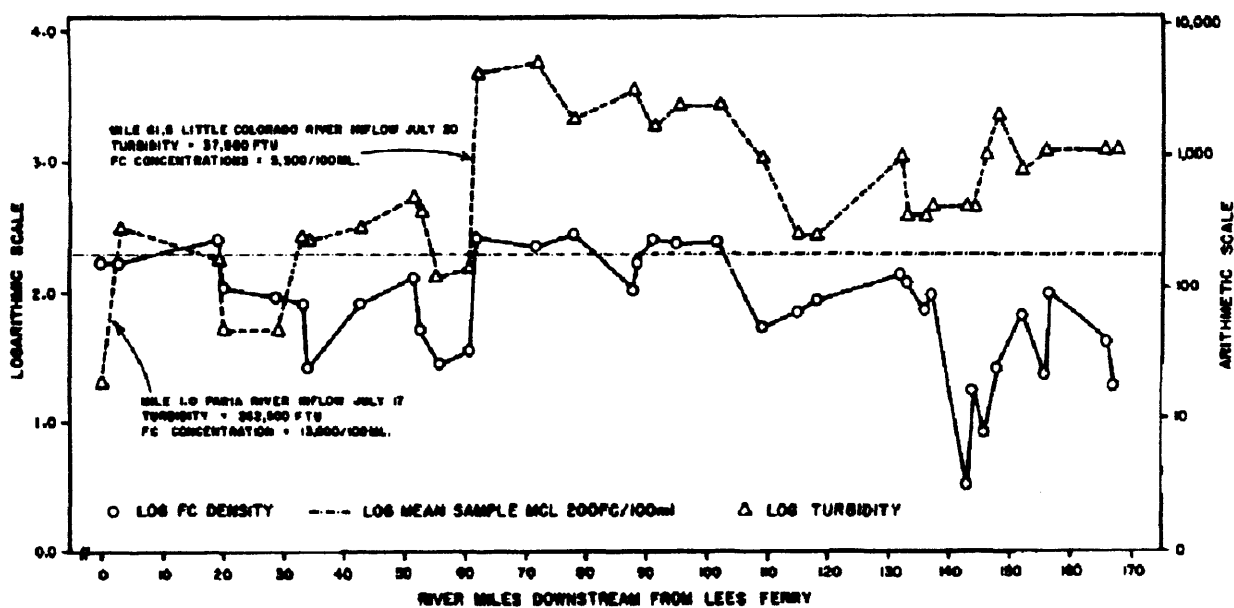
Figure 2.4   FC densities and turbidity in the Colorado River, 1981.

(after Tunnicliff and Brickler, 1984)

2.1.2.2.4 Water depth

Light intensity decreased with depth below the ocean surface and thus, by carrying out simultaneous die-off experiments at different depths, the influence of light intensity for different depths can be observed, such as: reported by Gameson and Saxon (1967); Bellair et al. (1977) and Pommepuy et al. (1992).

In the study by Bellair et al. (1977), a number of die-off experiments were carried out using bottles suspended at depths varying from 0.5 m to 5 m (in Gameson and Saxon's study (1967), depths were designed to vary from 0.5 to 4 m) and it was found that the instantaneous light intensity at 0.5, 2 and 5 m depth was approximately 80, 40 and 10 percent, respectively, of that at the surface. This experiment revealed that the hourly solar radiation at each depth was varying significantly.

2.1.2.2.5 Sewage contents (or nutrients)

Alkan et al. (1995) found that the effect of sewage content on the E. coli die-off rate was significant with inverse linear relationship, the die-off rate reduced dramatically when the sewage content was increased. This was explained as the sewage provided more nutrients to support bacterial life and also led to higher turbidity to protect the bacteria from light radiation.

Tassoula (1997) studying the growth possibilities of E. coli in natural waters, designed his experiments for two cases: the first case was exceptionally polluted with sewage (COD = 100-200 mg/l) and second case was nearly clean water (COD < 3 mg/l). The experimental results proved that in natural waters (0-35‰ salinity) growth of E. coli could be observed as long as there was a significant organic load or decay of E. coli when the organic load was low (COD < 3mg/l). Conclusively, the E. coli survival in natural waters was influenced essentially by the sewage contents and this determined whether growth or decay of E. coli occurred.

As mentioned in the previous section, an increased concentration level of faecal indicators in natural waters was frequently observed after rainfall events for a lag period of 1-2 days, such as in Buttermilk Bay reported by Valiela et al. (1991) and in a coastal waterway located in Ft. Lauderdale, Fla. by Solo-Gabriela et al. (2000). In these studies the data collected in the survey were checked and showed the 1 to 2 days time gap for the appearance of the peak bacteria indicator concentration. Does rainfall brings lots of bacteria into the water directly, elevating the bacteria counts by surface runoff washing the bacteria from streets and other surfaces? This doesn't seem to be supported for every case. If so, the bacteria concentration should always go on increasing directly during the rainfall but not after about 1 or 2 days. In particular, Solo-Gabriela et al. (2000) made an experiment of source-specific sampling effort. Their storm sewer sampling effort showed

that water within the storm sewers contained lower E. coli concentrations than river water during storm conditions and the river water sample showed extremely high E. coli concentrations. The most reasonable explanation is the rainfall washing up large amounts of organic matter from the upstream catchments and sometimes also bringing more sewage content from combined sewer overflows into the water system, which provides rich nutrients for the bacteria in waters to grow rapidly within the following 1 to 2 days. Hence balancing the normal die-off rate to make extended survival or in many cases to have net growth. Actually in natural environments, with large amount of organic matter, bacteria could find both nutrients and osmoprotectors.

2.1.2.2.6 Salinity

High salinity was found to be a significant factor contributing to the death of faecal bacteria in seawater by Pike et al. (1970).

Tassoula (1997) studied the influence of salinity on the growth limitation of E. coli in natural waters. The observation showed that salt concentrations (weight fraction) greater than 9‰ had a negative effect, which was clearly more intense under starvation conditions (clean natural water with a COD level lower than 3mg/l).

The negative effects of salinity could be overridden when bacteria indicators were in the waters with rich sewage contents and this was found in the studies of Gerba and McLeod, 1976; Alkan et al., 1995; and Mezrioui et al., 1995. Not only rich nutrient foods in the sewage content enabled the bacteria to grow, but also the presence of osmoprotectors (glycine-betaine, trehalose, amino acids) could help to increase survival rates of faecal bacteria in salt environments (Pommepuy et al., 1992). Pommepuy et al. (1992) quoted several studies about the role of organic matter on the salt-tolerance and observed an increase in the salt-tolerance induced by organic matter in their experiments.

2.1.2.3 Rates of die off between different species

The comparison between survivals of different bacterial species and viruses under different conditions is noteworthy of properly choosing the microbial indicator for faecal contamination. Fujioka et al. (1981) investigating the effect of sunlight on sewage-borne faecal coliform and faecal streptococci under field conditions (15°C -25°C), found that the

T90 was 0.5 hour and 1 hour respectively, in exposure to sunlight. Some other researches also found the longer survival times for enterococci in comparison with faecal coli (Gameson, 1984).

Korhonen and Martikainen (1991) studied the survival of C. jejuni and E. coli in lake water using viable counts and found that E. coli survived for all of the test conditions better than C. jejuni. E. coli could be the valued indicator of the potential presence of C. jejuni.

Alkan et al. (1995) in comparing the survival of E. coli and enterococci, in relation to solar radiation and other environmental factors, in marine waters concluded that the two indicator species might survive equally in sunlight conditions, although one of the experimental results obtained from the bottom of the water column indicated that the survival of enterococci was better than that of E. coli (the ratio of T90 was Enterococci/E.coli = 98.8/91.6 = 1.08:1).

Wait and Sobsey (2001) studied the comparative survival of E. coli, Salmonella typhi, Shigella sonnei and enteric viruses in Atlantic Ocean seawater, where it was found that E. coli was inactivated more rapidly than any other test microbe under laboratory conditions. But during in-situ field studies, the inactivation of E. coli was not significantly different from the inactivation of the other bacteria and viruses. By using of resuscitation and repair plating procedures for the enumeration of bacteria, it was found that the enteric viruses did not survive appreciably longer than enteric bacteria under field condition.

2.2   Enteric Bacteria in Bottom Sediments

Ritterberg et al. (1958) found extensive fields of coliform bacteria in sediments covering several square miles and extending right up to the water line at nearby bathing beaches that were close to marine sewage outfalls. In addition, Weiss (1951) showed that E. coli readily adsorbs to silt found in estuaries, and it would seem logical to conclude that many of the coliforms that reach marine waters find their way into sediments. Originally the enteric bacteria in sediments are deposited from the overlying water column and then have some ability to multiply their populations.

2.2.1 Survival time

Many authors have studied survival times of enteric microorganisms in sediment. Sediments protect bacteria from sunlight radiation, in addition to procuring osmoprotectors and providing nutrient elements which are more easily utilized types for the coliforms. Survival times are very long for faecal bacteria in sediments. They can vary from several days to several weeks, and even months (Marino and Gannon, 1991; Pommepuy et al., 1992; Burton et al., 1987).

Gerba and McLoed (1976) observed that E. coli survival increased rapidly when either autoclaved or fresh estuarine sediments were added to estuarine water. Hood and Ness (1982) found that E.coli could survive better in non-sterile (fresh) estuarine sediments than in estuarine waters (whether sterile or non-sterile). Burton et al. (1987), using continues-flow chambers containing lake or river sediments, artificially constituted water, and streptomycin-resistant bacteria, found extended bacterial survival in sediments compared to survival in water. The extended survival results in sediments were being found while water populations were reduced to acceptable levels, which were the observations concluded by Davies et al. (1995) who commenced a study to monitor faecal microorganisms in marine water and inshore sediments.

The survival of high concentrations of bacteria indicators in sediments has been recognised as a possible health hazard. One is the risks for people who contact directly with the sediments, such as, children playing on the beach. Another is the water recreational activities would resuspend sediments and their bacterial loads, thus increasing the health risks in such waters.

Van Donsel and Geldreich (1971) firstly reported a T90 value of both FC and Salmonella spp. for 7 days in various sediments. Marino and Gannon (1991) found that FC and FS in the sediments remained stable for up to 6 days at 10^4-10^5 counts/100ml in their Creek field studies, whereas the FC and FS water column counts for this period were <400 and <700 per 100ml, respectively. In another study, Burton et al. (1987) observed that the sediment reservoir allowed enteric and pathogenic bacteria to survive, possibly for several months; thus they suggested that the resuspension and human ingestion in primary-contact waters created a real possibility of raising potential health hazard.

2.2.2   Population in bottom sediment

Buckley et al. (1998) found that total coliform concentration in streambed sediments were on average about 1000 times greater than in the overlying water column, (95% c.i. 760-1560). In the study a total of 240 samples were analysed for total coliform. The mean TC concentration in streambed sediments was 0.5×10^6 cfu/100ml during the dry season and 1.2×10^6 cfu/100ml during the wet season.

The ratio between the coliform concentration in the sediments and waters was within the range of 760-1000, with this beling found by van Dansel and Geldreich (1971), and Stepheson and Rychert (1982). In addition, Ashbolt et al. (1993) found that sediments containing 100-1000 times as many faecal indicator bacteria as the overlying water. Tunnicliff and Brickler (1984) examined the Colorrado River and tributaries were found to harbour sediments with FC in densities averaging 10 to 100 times those in the overlying waters, with the water counts of ≤ 20 FC/100ml.

Doyle et al. (1992) studied FC concentration distributions in water and related beach sediments with sampling over 50 days. Results showed that both water and sediment FC populations were highly variable over time and the ratio of sediment FC to water FC was found to be 10-100:1. The mean sediment FC density was about 10^3 MPN/100ml.

Obiri-Danso and Jones (2000) conducted sampling experiments for intertidal sediments in Morecambe Bay in the UK for a period over 12 months to measure the faecal bacteria contamination of the bed sediments underlying the bathing waters. The results are presented in Table 2.1. The results show that the numbers of faecal indicators in sediments are at least an order of magnitude higher than in overlying water column (Obiri-Danso and Jones, 1999).

In another study, conduced by Crabill et al. (1999), sediment sampling sites were identified with very high FC counts in Oak Creek, averaging 2200 times larger than the FC counts of the water column. The measured mean sediment FC population (cfu/100ml) was 1.5×10^5, 7.8×10^3 and 1.0×10^5 for Summer, Winter and Year mean respectively.

Table 2.1   A comparison between the numbers (MPN) of faecal indicators and Campylobacters in the surface sediments and the overlying seawater in Morecambe bay in 1996. (after Obiri-Danso and Jones, 2000)

Indicator	Bathing water site	Geometric mean (g dry weight cm^{-3}) sediment	Geometric mean (100ml^{-1}) water	Geometric mean (100g dry w. cm^{-3}) sediment
Faecal coliform	Site 1	1096	2951	75624
	Site 2	724	3981	57196
	Site 3	107	758	8132
Faecal streptococci	Site 1	204	281	14076
	Site 2	229	398	18091
	Site 3	13	120	988
Campylobacter	Site 1	3	22	207
	Site 2	2	13	158
	Site 3	3	26	228

2.2.3   Growth in bottom sediment

In contrast to die-off in water columns, most studies found growth for faecal indicators in bottom sediments. This could be one of the reasons why the bacteria counts in bottom sediment are generally 2-3 logs higher than water counts. Davies et al. (1995) reporting their monitoring study on survival of faecal indicators in marine and freshwater sediments, indicated that the usual exponential decay model could not be applied to the sediment survival data but were confounded by a complex relationship between growth and predation. Throughout the duration of the experiments (68 days), the same proportion of E. coli organisms remained culturable, suggesting that sediment provides a favourable non-starvation environment for the bacteria.

Laliberte and Grimes (1982) studied the survival of E. coli in lake bottom sediments using in-situ experiments with unsterile sand and mud sediment samples analyzed for a 5-day period, for each sediment type. Daily most-probable-number determinations indicated that there was a rapid growth in the autoclaved sand and mud samples during the first 24 h, followed by a stationary period of 2 to 3 days and then by a decline of 1 log in day 5. The mud sediment inoculated with 1.0×10^6 bacteria per g increased to 2.2×10^8 bacteria per g in 3 days, while the sand sediment inoculated with 1.2×10^5 cells per g,

increased to 5.4×10^7 bacteria per g. This study indicated that E. coli has the ability of rapidly growing in lake bottom sediments in the first three days.

Marino and Gannon (1991) attempted to find if the indicator bacteria were capable of multiplying in the aquatic sediments in designed laboratory and field experiment studies. The field study ensured that the same FC and FS populations were monitored throughout a given inter-storm period with no additional bacterial supplementation. The laboratory studies determined the effect of biotic and abiotic factors, and demonstrated reproductive capability in low nutrient, sterile sediments. These results indicated that faecal bacteria (particularly FC) may indeed multiply in aquatic sediments, since the populations maintained themselves at high densities in the presence of constant predation and competition/antagonism effects and without significant external supplementation.

2.2.4 Factors affecting growth in sediments

The growth of enteric bacteria in sediments can be attributed to several factors although this hasn't been fully investigated.

♦ Nutrients

Chan et al. (1979) found extended Enterobacter aerogenes survival in nutrient-rich, fine-grained sediments. Burton et al.(1987) studied the survival of pathogenic bacteria in various freshwater sediments and found that E. coli and S. newport survived longer in lake sediments containing at least 25% clay, which was attributed to higher organic matter and nutrient contents held by the clay. The fastest die-off for E. coli, S. newport and K. pneumoniae was observed in sandy river bed sediments, which contained 98% sand and 2% clay, with the lowest organic matter contents of 0.7%.

Gerba and McLeod (1976) studied nutrients' effects to the survival of E. coli in marine waters and indicated that there were sufficient nutrients present in estuarine sediments from both polluted and unpolluted sites, and in water from polluted sites, to support the growth of E. coli. Results of the study revealed that E. coli was capable of utilizing nutrients absorbed to estuarine sediments from areas where sewage effluents were being discharged as well as from areas free of such pollution. In general, sediments either at polluted sites or at unpolluted sites contain more nutrients (or organic matter) than the overlaying water. They further indicated that the types of nutrients present in the

sediments were different from those present in the water and were more easily utilized by faecal coliforms.

Hendricks (1970) was unable to obtain significant quantities of nutrients from the fresh water sediments within a river to those values already found in the water. Gerba and McLeod (1976) also found that nutrients bound up in the sediment material were not easily released into the natural seawater unless the sediments had been autoclaved or were added to artificial seawater. So the most possible means by which faecal bacteria can grow is in the bottom sediments, but much less chance in the water column.

◆ **Sediment type (or size)**

Tate (1978) suggested that E. coli could catabolize organic soil constituents, and he found that such substrates maintained populations three times greater than sand, so concluded that small sediment particle sizes increased E. coli survival rates. However, the study by Lalilerte and Grimes (1982) revealed that this was not the case for unsterile sediment samples, which had a mean FC per gram in sand of 5.6 times higher than in mud. The results of the sediment analyses demonstrated distinct physical differences between sand and mud: sand sediments with 71.1% sand, 28.8% clay and silt, and had 0.6% organic material; mud sediment with 22.7% sand, 75.4% clay and silt, and had 5.8% organic material. However the effect of sediment type on E. coli survival had no clearly results. Once autoclaved, the two inoculated sediment types maintained comparable FC numbers.

Sherer et al. (1992) observed that FC survived longer in fine sediments than in coarse sediments and found no differences in the FS survival rates between fine and coarse sediments.

Three sediment types were designed in a study to consider the effect of sediment particle size by Howell et al.(1996), these were 1) sand with 100% sand; 2) loam with 41% sand, 49% silt and 10% clay; 3) clay with 100% clay. The results revealed that: faecal coliform mortality rates were significantly less in clay-sized sediments than in coarse sediments, whereas faecal streptococci mortality rates were not significantly less.

Albrechtsen (1994) studied the distributions of bacteria in different size fractions of aquifer sediment. Sediment samples were fractionated into 500, 100, 55, 20, 1.2 and 0.2

µm sizes by filtering a sediment suspension successively through progressively smaller mesh-sizes filters. In all sediment samples, even where abundance of coarse particles was high, 91.9-100% of the viable number of bacteria in the fractionated sediments were found in the 1.2-100 µm fraction; 40-96% in the 1.2-55 µm fraction, and only 0.01-0.04% in the 0.2-1.2 µm fraction.

◆ **Soil moisture**

Solo-Gariele et al. (2000) reported that laboratory analysis of soil collected from riverbanks showed an increase of several orders of magnitude in soil E. coli concentrations and determined the growth of the E. coli within riverbank soils. The ability of E. coli to multiply in the soil was found to be a function of soil moisture content, presumably due to the ability of E. coli to outcompete predators in relatively dry soil. The importance of soil moisture in regulating the multiplication of E. coli was found to be critical in tidally influenced areas due to periodic wetting and drying of soils.

2.3   Modelling Enteric Bacteria Die-Off

There are frequently a range of urban structures near any coastline. It has been a critical concern for coastal waters continuously to receive sewage disposals and hence to be harmfully polluted. In many water basins, one of the main water management tasks is the monitoring of the bacterial indicator levels by field sampling measurements. Perhaps justifiably, there are enormous amounts of time, money and effort that need to be spent on these kinds of water quality sampling tasks. However, years of water quality sampling have not generated adequate information from which to establish environmental standards or management tools. Comprehensive developments in computer modelling have increased the need to gathering more water quality data to verify modelling tools; this is necessary before using them either to review the past or predict the future in terms of water pollution.

The use of computer models requires large quantities of data from diverse sources to predict enteric bacteria populations in natural water environments and numerical modelling has been successfully applied in this field, particularly in two contexts – hydrodynamic modelling and advective/dispersion modelling.

Microbiological numerical modelling processes comprise three parts: 1) hydrodynamic modelling, i.e. predicting the currents, and giving a description of the water movements, which provides the template for simulations of bacteriological modelling; 2) advective /dispersion modelling, where the bacteria transport processes are predicted from the water movements, giving bacterial levels from pure dilution effects; 3) bacteriological decay modelling studying the kinetic principles of bacteria survival in natural water environment, which takes into account any source entries and total disappearance (i.e. both die-off and physical disappearance). In the following sections, the third phase of bacteriological decay modelling is reviewed in more details.

2.3.1   Modelling based on first order decay model

Many bacterial survival studies (Kittrell and Furfari, 1963; Hanes and Fragala, 1967; Klock, 1971; Canale et al., 1973; Thomann and Mueller, 1987; Salomon and Pommepuy, 1990; Bell et al., 1992; Canale et al., 1993; Alkan et al., 1995; Guillaud et al., 1997; etc) found that the first order decay model, known as the Chick's Law(1908), could be sufficiently accurate to describe the measured bacteriological data, and obtain a reasonable level of accuracy. The typical form of the first order decay model can be written in equation 2.11. However, most of these studies were experimental in nature, whilst a few of the studies (such as Canale et al., 1973; Salomon and Pommepuy, 1990; etc) included computer numerical modelling for comparisons with the experimental measurements.

The bacterial first order decay model is given by Chick's Law (1908):

$$dC/dt = -KC \qquad\qquad 2.11$$

where: K is the decay coefficient, h^{-1}.

In engineering studies, another parameter for representing the decay rate is used, namely T90, which is the time needed for 90% of the bacteria to die off. It has the relationship with decay rate K, as:

$$T90 = \ln 10/K. \qquad\qquad 2.12$$

where: T90 is in hours; K is in h^{-1}.

Salomon and Pommepuy (1990) reported their numerical modelling on bacterial contamination in the Morlaix Estuary (France). They used the first order decay model for decay modelling. Two different T90 values under Summer conditions (with low river flows) and Winter situation (with high river flows) were chosen to present the highly varied values, yet constant decay rates were used in each case. Survival trials were carried out in-situ to determine the decay rates, which ranged from 2h to 1 week. For the summer situation, the simulation results including bacterial dispersion and decay were observed for a T90 value ranging between 2 and 8 hours did not induce great differences. Physical factors (such as dilution) were thus the dominant mechanisms, which confirmed their experimental data obtained when considering transit times. However, they found that T90 at 2 h led to concentrations which were much too low and did not appear to be realistic values. The best agreement was obtained for T90 at about 24 hours. In the case of winter condition, best results were obtained for distinct T90 values throughout the estuary: 8 days upstream and 2 days downstream. Comparing the summer situation, physical dilution appeared to be even more efficient than mortality in the estuary.

Due to the complexities of the living mechanism of bacteria in natural environments, in practical modelling researchers prefer varying decay rates, which depend on available local varying environmental factors to make predictions more accurate. Canale et al. (1973) studied the coliform modelling and found that bacterial die-off in the Great Lakes was a function of water temperature and the state of local waters which included (a) algal toxins, (b) bacteriophage, (c) predators, (d) sedimentation and adsorption, (e) bacteria nutrients and (f) sunlight. This research suggested that the first order die-off rate coefficient, K, could be modified as:

$$K = 0.2 + 0.0223 \times T \qquad\qquad 2.13$$

where: T is the temperature in °C.

This relation indicated that summer die-off rates were approximately 3 times greater than those for the winter season.

Mancini (1978) integrated the data found from other studies into a model for coliform mortality in river and estuary waters considering the parameters of temperature, solar radiation and salt content of the water. He presented a model based on first order die-off

with the death rate coefficient, k, modified by terms of some considered factors. The modified die-off rate k_t was:

$$\frac{k}{k_t} = 0.8 + 0.006(\%seawater) \times 1.07^{(T-20)} + \frac{I_A}{k_e H}[1 - \exp(-k_e H)] \qquad 2.14$$

where: k, k_t is the constant and modified first order die-off rate respectively.

T is the temperature in °C;

I_A is the average daily surface solar radiation, Langley $ha^{-1} d^{-1}$;

k_e is the light extinction coefficient in water, m^{-1};

H is the completely mixed depth of water, m.

Bell et al. (1992) undertook numerical modelling studies to predict microbial concentration levels from multiple outfalls using time-varying inputs and decay rates (T90). The study laid the emphasis in their advective/dispersion and decay modelling on the using of realistic bacteria decay rates, which would apply: 1) varying decay rates during each half hour of a diurnal cycle; 2) reduced decay rates at depth below the surface. The variability of these decay rates was due to the change of the first important killing bacteria factor, namely solar radiation. The disadvantage was that they used two patterns – summer and winter for the diurnal decay rates, hence not including the distinct daily changes in solar radiation.

Occasionally, the first order decay model has been utilised by modifying a specific decay rate (either k or T90) to suit different local environmental conditions. From the literature it can be seen that the special modified first order decay rate is integrated for all of the environmental factors which affect the survival of the modelled bacteria indicators (e.g. Canale et al., 1973; Mancini 1978; Salomon and Pommepuy , 1990; Bell et al., 1992).

2.3.2 Modelling of decay with separated deposition

Adsorption of bacteria onto marine and estuarine sediments has been shown to play an important role in the disappearance of bacteria. Waksmann and Vartiovaara (1938) demonstrated that marine organisms might be strongly adsorbed by marine mud. In another study, Weiss (1951) carried out extensive investigations on bacterial adsorption by river and estuarine silts. They both reported that E. coli removals of > 50% were dependent on turbidity and the characteristics of the particular sediment.

Milne et al. (1986) experimentally studied the effects of sedimentation on the removal of faecal bacteria in estuarine waters, aiming to establish the principles of deposition to substantiate the theory of the finding reported by the above two studies, which was the hypothesis that the bacteria disappeared due to deposition. The work showed that the deposition of SS in estuarine waters was a function of time, and that most deposition took place in a 3 hours period. The deposition of FC in estuarine waters was also a function of time and the FC deposition rate was directly proportional to the SS concentrations (25-100 mg/l range). The series of adsorption efficiency experiments implied immediate adsorption of about 20% of FC onto estuary water particles. They concluded that the results certainly indicated that FC were adsorbed onto estuarine particles in the water column, and might be deposited onto the estuary bed.

Rarely have researchers modelled bacterial decay by including deposition theory. Canale et al. (1993) modelled faecal coliform bacteria contamination in a polluted urban lake, by separating the bacterial sedimentation losses from the decay term. In the study the losses due to sedimentation and death were performed in separate sub-models. They documented the modelling work as presented below:

"Kinetic mechanisms were represented in the bacteriological decay modelling by the overall loss coefficient, K:

$$K = k_d + k_i + k_s \qquad 2.15$$

where: k_d is dark death rate coefficient, d^{-1};

k_i is the irradiance-mediated death rate coefficient, d^{-1};

k_s is the sedimentation loss coefficient, d^{-1}.

The irradiance-mediated death rate coefficient was given by:

$$k_i = aI \qquad 2.16$$

Where: a is the irradiance proportionality constant, $cm^2\ cal^{-1}$;

I is the irradiance intensity, $cal\ cm^{-2}\ d^{-1}$.

Light was averaged over the layer depth:

$$I_{avg} = \frac{I_{o,avg}}{\eta z}[1 - e^{(-\eta z)}] \qquad 2.17$$

where: I_{avg} is average irradiance in the layer, $cal\ cm^{-2}\ d^{-1}$;

$I_{o,avg}$ is average incident irradiance, $cal\ cm^{-2}\ d^{-1}$;

η is vertical irradiance attenuation coefficient, m^{-1};

z is the layer depth, m.

The sedimentation loss coefficient was calculated from:

$$k_s = v/z \qquad\qquad 2.18$$

where: v is the sedimentation velocity, $m\ d^{-1}$.

Substituting equations (2.15), (2.16), and (2.17) to (2.18) yields the kinetics sub-model:

$$K = k_d + a\frac{I_{o,avg}}{\eta z}[1 - e^{(-\eta z)}] + \frac{v}{z} \qquad\qquad 2.19$$

Note that since $I_{o,avg}$ is 0 in the bottom layer of most lakes, the k_i term drops out of equation (2.19) when modelling bottom cells."

Although the study of Canale et al. (1993) reported that different submodels were used to predict separately the bacterial losses due to sedimentation and die-off, the mathematical model (i.e. Equation 2.19) actually used the simplest sedimentation process (i.e. $k_s = v/z$) in the modelling, and finally the deposition process was still being combined into the overall first-order decay rate K (see Equation 2.19). This work is thought to be the only published attempt to include deposition in the bacterial kinetics.

2.4   The Lack of the Historical Research in Bacterial Modelling

2.4.1   Entrainment from bed sediment

As cited in section 2.1.1 bottom sediment re-suspension is known to be reasonably responsible for the overlying bathing water pollution. Many studies have revealed that the bottom sediments serve as reservoirs for faecal bacteria, with the potential to pollute the overlying bathing waters. However, no modelling work involving this kind of re-suspension has been reported in the literature.

In a study of a modelling procedure reported by Salomon and Pommepuy (1990), a detailed examination showed that, very near the upstream extremity, low tide measurements of E. coli were about three times higher than their model results. They explained that this could be attributed either to an incomplete lateral mixing of the effluent in the estuarine waters, or to the high turbidity existing at that time when previously released bacteria were put in re-suspension, this re-suspension could not be

confirmed because no suspension modelling procedure was included in their model. Hence there is a dearth of research in the modelling of bacterial entrainment from bottom sediments.

2.4.2   Deposition term

Although a few studies have considered the bacteriological decay modelling with a separate deposition term, the deposition theory raised in the studies (Waksmann and Vartiovaara, 1938; Weiss, 1951; Curran and Wilson, 1986; Milne et al., 1986) was presented in such a simple way that the process representation could not fully represent the in-situ sediment deposition processes. As mentioned previously Canale et al (1993) used separated sub-models for the different losses due to die-off and sedimentation. However, the principles of sedimentation adopted in their modelling was to consider the sedimentation loss coefficient k_s as a part of the overall loss coefficient (k), which is included in the first order decay model. Therefore, this kind of separated deposition modelling work belongs to the work of modifying a specific decay rate and integrating all the local environmental effects together.

A modelling study concerned with deposition processes to reflect the in-situ complicated suspended sediment deposition processes, which are based on the deposition principles describing the bacterial deposition loss as a function of time and SS concentrations etc, is the second dearth of research from the literature.

Chapter 3

THEORETICAL BACKGROUND OF SURFACE WATER QUALITY NUMERICAL MODELLING

3.1   Water Quality Numerical Modelling Process

Coastal water pollution has been an increased concern worldwide due to rapid economic development and urbanization along the coastal lines. Water quality numerical modelling software as an essential management tool is in great need in the field of coastal water management including water pollution control.

In recent years, water quality numerical models have been successfully applied to predict water pollution in natural waters. The modelling results can provide useful information to help protect the water environment adequately and economically. The process of the water quality numerical modelling can be described in six steps, which is illustrated in a simplified diagram drawn in Figure 3.1.

In a practical project, once a problem has been identified existing models should first be checked and any suitable ones should be chosen as this will not only save the running costs and time, but also the project will benefit from knowledge and experience obtained from the previous studies. However, for some water quality modelling problems an existing modelling tool is unavailable or, some concerns are just raised recently, the

problems even are never modelled before. In such cases a new model needs to be developed (Chapra, S.C. 1997).

The process of developing a new model is the process diagrammed in the schematic form of Figure 3.1. It outlines six steps for the water quality modelling process as: 1) analyse the physical phenomenon; 2) build up the mathematical equation; 3) solve the equation using numerical solution; 4) develop the model using programming language; 5) calibrate and validate the model by field or experimental data; 6) use the calibrated model for
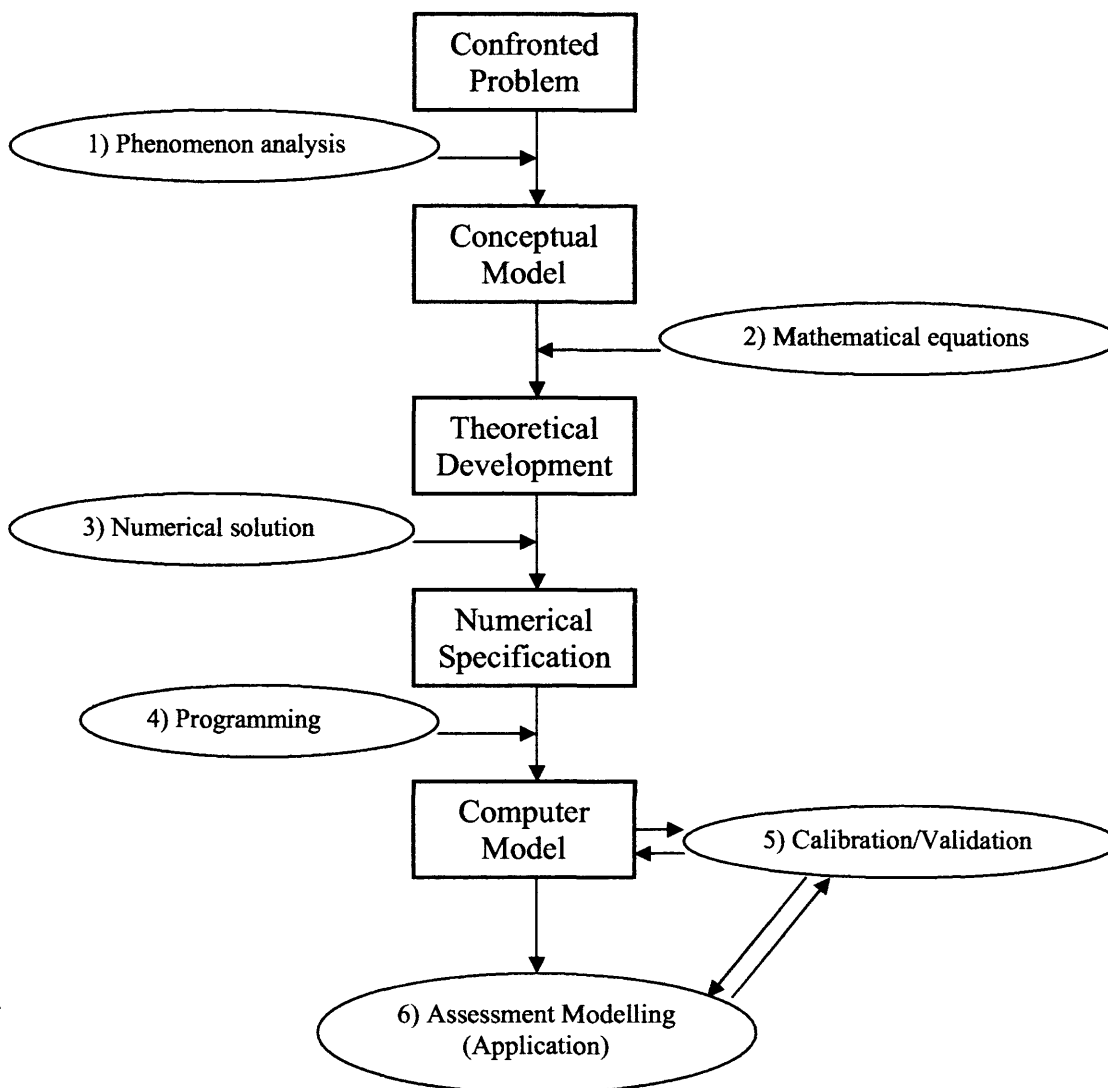
Figure 3.1   The Process of water quality numerical modelling

assessment in application of real case study. In this thesis, the steps 1, 2 and 3 are dealt with in Chapter 3 and 4; step 4 is addressed in Chapter 5; last two steps 5 and 6 are demonstrated in both Chapter 6 and Chapter 7.

As described in chapter 2, in this study enteric bacteria are selected as the water quality indicators. In general, microbiological numerical modelling process comprises three parts: 1) hydrodynamic modelling, i.e. studying the flow current patterns, which aims to give the description of the water movements and which provides the template for runs on bacteriological modelling; 2) transport modelling, studying the bacteria advective/dispersion transport processes caused by the water movements, which computes the bacterial results from pure dilution effects by the flow flux; 3) bacteriological transformation modelling, studying the kinetic principles of bacterial transformations in natural water environment, taking into account any source entries and sinks including bacterial decay and physical disappearance.

To-date there have been well implemented models for the hydrodynamic modelling and transport modelling. However, there is still a major lack of knowledge in the third aspect – the bacteriological transformation modelling (Rauch et al., 1998; Shanahan et al., 1998; Somlyody et al, 1998). As reported in the literature, the survival of enteric bacteria in the coastal environment is controlled by many physical, chemical and biological factors, including the sediments contained in water and the bed. Sometimes the sediment factor even becomes the predominant variable responsible for the bacterial contamination. However, the mechanisms of how sediments impacting on the bacterial population are still not fully understood. Based on this concept, Chapter 3 and 4 are drawn to introduce the mathematical models needed for representing the theoretical background of the sediment-associated bacterial water quality numerical modelling. The knowledge about the bacteriological transformation modelling will be introduced in Chapter 4. This chapter deals only with the fundamental principles of water quality modelling, i.e. the basic theories in hydrodynamic modelling and solute/sediment transport modelling with the advective/dispersion processes.

3.2   Basic Concept of Numerical Method

Numerical methods became widely used after the invention of computers. Today they are used in such a wide field that they almost get into all the disciplines in engineering. As we know analytical solutions are often very difficult to obtain, especially for practical engineering problems. In contrast, numerical approximations can always be found resulting in problem solving. So, the numerical methods are used to "get answers" when the analytical solution is not available.

Table 3.1   Finite difference formulae for higher-order derivatives

Forward difference approximations:

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x}$$

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{\Delta x^2}$$

$$f_i''' = \frac{f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i}{\Delta x^3}$$

Backward difference approximations:

$$f_i' = \frac{f_i - f_{i-1}}{\Delta x}$$

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{\Delta x^2}$$

$$f_i''' = \frac{f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}}{\Delta x^3}$$

Central difference approximations:

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

$$f_i''' = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2\Delta x^3}$$

There are many methods for obtaining a numerical approximation for problem solving. The finite difference methods play a major role in fluid-flow computations. The fundamentals of the finite difference methods are illustrated in the formulas listed in

Table 3.1 (Mayo and Cwiakala 1991), which are derived from the definition of the derivative equations as:

$$f'(x) = \lim_{\Delta x \to 0}\left(\frac{\Delta f(x)}{\Delta x}\right) = \lim_{\Delta x \to 0}\frac{f(x + \Delta x) - f(x)}{\Delta x}$$

In the process of developing a numerical model for problems solving, two important issues are the accuracy and stability. Accuracy deals with how closely the numerical results match the true solutions. Different methods may have different degrees of accuracy because of the number of calculations and the method of solving the problem. Accuracy states errors containing 1) calculation errors associated with the way that computers store numbers and 2) calculation errors that is built into the methods of which the function is solved. Stability is the issue in numerical methods which tells us whether there is a possibility that the method may not return the answer at all. This is especially a concern with techniques that use successive approximations based on previously calculated results. In this study a higher accurate numerical scheme namely Ultimate Quickest (Lin and Falconer, 1997) scheme is deployed in the modelling tool for solving the transport governing equations.

3.3 Governing Equations for Hydrodynamic Process

3-D, 2-D and 1-D standard governing equations describing the hydrodynamic process of fluid flow are the basis of hydrodynamic numerical modelling, which predict the water elevation and velocity field distributions in coastal, estuarine and riverine waters.

3.3.1 2-D governing equations

The 2-D hydrodynamic equations are generally based on the depth-integrated 3-D Reynolds equations (for details, see Falconer et al, 1991) for incompressible and unsteady turbulent flows, with the effects of the earth's rotation, bottom friction and wind shear being included (Falconer, 1993):

$$\frac{\partial \zeta}{\partial t} + \frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} = 0 \qquad\qquad 3.1$$

$$\frac{\partial Q_x}{\partial t} + \beta\frac{\partial U Q_x}{\partial x} + \beta\frac{\partial V Q_x}{\partial y} = f Q_y - gH\frac{\partial \zeta}{\partial x} + \frac{\tau_{xw}}{\rho} - \frac{\tau_{xb}}{\rho} + \overline{\varepsilon}H\left[\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right] \qquad 3.2$$

$$\frac{\partial Q_y}{\partial t} + \beta\frac{\partial U Q_y}{\partial x} + \beta\frac{\partial V Q_y}{\partial y} = f Q_x - gH\frac{\partial \zeta}{\partial y} + \frac{\tau_{yw}}{\rho} - \frac{\tau_{yb}}{\rho} + \overline{\varepsilon}H\left[\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}\right] \qquad 3.3$$

where: ζ = water elevation above (or below) datum;

U, V = the depth averaged velocity components in x, y directions;

h = bed level below datum;

H = ζ+h, is total water depth;

Q_x=UH, Q_y=VH, is unit width discharge components in x, y directions;

β = momentum correction factor;

f = Coriolis parameter due to the Earth's rotation;

τ_{xw}, τ_{yw} = surface wind shear stress components in x, y directions;

τ_{xb}, τ_{yb} = bed shear stress components in x, y directions;

$\overline{\varepsilon}$ = depth averaged eddy viscosity coefficient.

3.3.1.1   *The momentum correction factor*

In 2-D flow, the total momentum flux through a cross-section is estimated from the average flow velocity times the total cross-sectional area, assuming that the velocity does not vary with the depth. If the velocity distribution does vary with the depth, the correct total flow flux is obtained by summing the flux through each element. The momentum correction factor is the ratio of the true total momentum flux to the flux estimated from the average flow velocity. Its value increases as the velocity distribution becomes more non-uniform.

For an assumed logarithmic vertical velocity profile, the momentum correction factor may be calculated from:

$$\beta = 1 + \frac{g}{C^2 \kappa^2} \qquad 3.4$$

where: κ=0.4 is von Kaman's constant.

For an assumed seventh power law velocity profile the value of β is 1.016 and 1.20 for an assumed quadratic velocity profile (Falconer & Chen, 1991).

3.3.1.2 Coriolis parameter

The Coriolis term describes the effect of earth rotation on the flow. It is a function of the latitude and the force acts at right angle to the flow. On the coast it affects the magnitude of tidal currents, causing the flow to rotate around points of zero amplitude. In estuaries, the Coriolis effect is usually small compared with other effects, unless the modelling domain is very large.

$$f = 2\omega \cdot Sin\phi \qquad\qquad 3.5$$

where: ϕ = geographical angle of latitude;

$\omega = 2\pi/(24\times3600)$ is angular rotation speed of the Earth.

3.3.1.3 The effect of wind

Wind exerts a drag force as it blows over the water surface. The wind stress plays a critical role in the open sea and in lakes, but for water bodies with strong currents such as those in estuaries and rivers, the wind stress is often small compared to the bottom shear stress. The wind shear stress at the air-water interface is calculated by assuming that it is proportional to the square of the wind speed at a particular height above the water surface. Various empirical formulae have been proposed to calculate an air-water resistance coefficient similar to the drag coefficient in turbulent flow field. In this study, Wilson's value (Weiyan, 1992) is used, which refers to the resistance height z =10m above the water surface.

3.3.1.4 Bottom friction

Bottom friction has a non-linear, retarding effect on the flow. The Chezy coefficient is a semi-empirical bottom friction coefficient, which was originally developed to describe uniform flow in open channels. Under rough turbulent flow, i.e. for Reynolds number Re>>1000 and an assumed logarithmic velocity-depth profile, the Chezy bottom friction coefficient is assumed to be independent of the flow and varies only with the relative roughness height of the bed:

$$C = -18.0 \times Log_{10}\left[\frac{k}{H \times 12.0}\right] \qquad\qquad 3.6$$

Under transitional flow conditions, i.e. if Re= 2000-4000, the Chezy coefficient varies with the flow conditions. It is calculated by iteration using:

$$C = -18.0 \times Log_{10}\left[\frac{k}{H} + \frac{5}{Re \times 18.0}C\right] \qquad\qquad 3.7$$

where: k = roughness length;

> Re_{min} = minimum Reynolds number for calculation of Chezy coefficient under transitional conditions, 1000 is used in the current study.

3.3.1.5 Turbulence

Turbulent shear stress refers to the flow resistance associated with the random fluctuation of water in space and time. The momentum exchange brought about by turbulence causes the velocity-depth distribution to be more uniform than under laminar conditions. For shear stress between the fluid layers, the Boussinesq's representation for the mean shear stress is used:

$$\tau_e = \varepsilon\frac{dV}{dy} \qquad\qquad 3.8$$

where ε is the eddy viscosity, which is a function of the turbulence characteristics of the flow and maybe thousands of times larger than molecular viscosity. If turbulent shear stress is dominated by bottom friction, a relationship between the Chezy coefficient and the eddy viscosity exists. The depth-integrated eddy viscosity is calculated from:

$$\overline{\varepsilon} = C_e\frac{H}{C}\sqrt{g\left(U^2 + V^2\right)} \qquad\qquad 3.9$$

where Ce = eddy viscosity coefficient. Fischer's (1979) suggestion of Ce =0.15 is used.

3.3.2   1-D governing equations

The 1-D hydrodynamic governing equations for describing flows in rivers and narrow estuaries are based on the St Venant equations for 1-D unsteady open channel flow. Various forms of the St Venant equations were introduced in the field of unsteady open channel flow since 1950's when the electronic computer was developed. The most often used form in practice can be written as (Cunge et al, 1980):

$$T\frac{\partial \varsigma}{\partial t} + \frac{\partial Q}{\partial x} = 0 \qquad\qquad 3.10$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\beta\frac{Q^2}{A}\right) + gA\frac{\partial \varsigma}{\partial x} + g\frac{Q|Q|}{C^2 AR} = 0 \qquad\qquad 3.11$$

where: T = top width of the channel;

> x = flow direction or streamwise coordinate;

ζ = water elevation above (or below) datum;

Q = discharge;

β = momentum correction factor due to the non-uniform vertical velocity profile;

g = gravity acceleration;

C = Chezy coefficient;

A = wetted cross-sectional area;

R = hydraulic radius.

Comparing with 2-D hydrodynamic governing equations, the basic assumptions for 1-D flow are that hydrostatic pressure distribution is true in the vertical direction and Coriolis accelerations may be neglected.

3.4   Advective Diffusion Equation

The basic governing equation describing the transport processes of water quality indicators in fluid flow is the well-known advective diffusion equation (ADE), written (Rauch,W. et al, 1998) as:

$$\frac{\partial S}{\partial t} = \underbrace{-U\frac{\partial S}{\partial x} - V\frac{\partial S}{\partial y} - W\frac{\partial S}{\partial z}}_{(1)} + \underbrace{\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial S}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial S}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial S}{\partial z}\right)}_{(2)} + \underbrace{r(s,p)}_{(3)} \qquad 3.12$$

where: S = water quality indicator's concentration;

U, V and W = velocity components in x, y and z directions;

ε_x, ε_y and ε_z = turbulent diffusion coefficients for x, y and z directions;

r = 3-D vector of rates of change of the indicator due to chemical, biological and other conversion processes as a function of concentration (S) and model parameter (P, subject to calibration).

Equation 3.12 specifies that the local concentration change is composed of three terms, which are: term (1) - advective effects; term (2) - diffusion/dispersion transport; and term (3) - sources or sink terms, which refers to those changes caused by either physical (e.g. outfall discharge and settling loss), chemical or biological transformations.

It is recognised that in water quality modelling accurate numerical models have been developed for representing term (1) and term (2) very successfully ever since water quality modelling first started in the 1960s and 70s. The emphasis that further research should be placed on is the investigation of the complexity in the sources and sink terms (Somlyody, L. et al, 1998). As physical, chemical and biological reactions in natural waters for water quality indicators are very complicated and all different from each other, many of the reactions have not yet been fully understood, new development in future for water quality modelling will be mostly focused on the investigation of the refinement of the sources and sink terms.

Equation 3.12 is used for 3-D flows, from which 2-D and 1-D advective diffusion equations can be derived by integrating over the depth or cross-sectional area to get depth-integrated 2-D ADE or cross-section integrated 1-D ADE.

For a shallow water nearly horizontal flow, the 2-D advective diffusion equation is given as:

$$\underbrace{\frac{\partial SH}{\partial t}}_{(1)} = \underbrace{-\frac{\partial SUH}{\partial x} - \frac{\partial SVH}{\partial y}}_{} + \underbrace{\frac{\partial}{\partial x}\left(HD_x \frac{\partial S}{\partial x}\right) + \frac{\partial}{\partial y}\left(HD_y \frac{\partial S}{\partial y}\right)}_{(2)} + \underbrace{\sum \Phi_s}_{(3)} \qquad 3.13$$

where: S = depth-averaged water quality indicator's concentration;

   D_x, D_y = depth-averaged dispersion coefficients in x, y directions;

   $\sum \Phi_s$ = sources and sink terms, which may include one or several sources or sinks subject to the case conditions.

For a one-dimensional unsteady non-uniform flow, the advective diffusion equation can be written as:

$$\underbrace{\frac{\partial SA}{\partial t}}_{(1)} = \underbrace{-\frac{\partial SUA}{\partial x}}_{} + \underbrace{\frac{\partial}{\partial x}\left(AD_x \frac{\partial S}{\partial x}\right)}_{(2)} + \underbrace{\sum \Phi_s}_{(3)} \qquad 3.14$$

where: S = cross-section averaged water quality indicator's concentration;

   U = cross-section averaged velocity in streamflow direction;

   x = streamflow direction or streamwise coordinate;

   D_x = longitudinal dispersion coefficient.

3.4.1   Advection and diffusion/dispersion terms

The ADEs describe how water quality indicators (or pollutants) behave in natural waters, which can be divided into two general categories: the physical transport, including term (1) Advection and term (2) Diffusion/Dispersion; the other kinetics, which is term (3) Sources and Sinks.

The advection refers to the transport of the pollutants by an imposed current system, such as that due to a tide in estuarine and coastal waters. So term (1) of ADEs refers to the pollutants transport along the advective flux.

Diffusion refers to the movement of pollutants' mass due to random water motion or mixing. In which, molecular diffusion results from the random Brownian motion of water molecules and this is usually negligible in turbulent flow. Turbulent diffusion results from a random motion that occurs on a large scale due to eddy. Diffusive transport has a tendency to reduce concentration gradients by moving mass from regions of high to low concentration. Generally speaking, diffusion makes the pollutants to spread out.

In ADEs' term (2) the coefficient D is a lumped coefficient that incorporates the effects of both turbulent diffusion and dispersion. Dispersion is a related process that also causes pollutants to spread. However, the diffusion is caused by the random water motion in time; in contrast, dispersion is due to the velocity gradients in space.

In numerical modelling, both diffusion and dispersion can cause mixing of the pollutants and to enhance the stability of numerical solution although the effect varies in different flow patterns. It is important to note that the value of D displays great variation in different flow conditions. For example in rivers and estuaries, dispersion usually predominates because of the strong shears developed by the large flow fluxes (river flow or tides). For lakes and other wide bodies of water, diffusion tends to predominate.

3.4.2   Sources and sink terms - $\Sigma\Phi_s$

$\Sigma\Phi_s$ summarises all other sources and sinks of the modelled pollutant apart from advective effects and diffusion/dispersion transport. The sources and sinks may be a physical exchange caused by such actions as outfall discharge, river lateral inflow or settling loss, may also be chemical reactions such as BOD de-oxygenation or a chemical biological process such as the decay of bacteria. In addition it may be composed of two or several different exchange processes and this even is the usual case in real environment, so that in ADEs the $\Sigma\Phi_s$ is used to express the sources and sink terms.

3.4.2.1   Outfalls in 2-D model

For a 2-D model either a wastewater treatment work (WwTW) discharge or a river inflow bringing sewage into 2-D domain can be treated as an outfall discharge during modelling process. The source term for outfalls is:

$$\Phi_s\big|^{outfall} = \frac{Q_o}{A_o}S_o \qquad\qquad 3.15$$

where: Q_o = outfall discharge rate;

A_o = horizontal outfall discharge area (the area of a grid cell);

S_o = outfall discharge concentration.

3.4.2.2   Lateral inflows in 1-D model

For a 1-D model the WwTW outfall discharge and river inflow enter the model segment as lateral inflows, which have the source term as:

$$\Phi_s\big|^{lateral} = \frac{Q_l}{\delta x}S_l \qquad\qquad 3.16$$

where: Q_l = flow rate of lateral inflow, negative value for outflow;

δx = mean segment length in streamwise direction;

S_l = lateral inflow (or outflow) concentration.

3.4.2.3 Conservative tracer

Salinity can be regarded as a conservative tracer having no kinetic exchanges in the transportation. The source term of a conservative tracer is termed as:

$\Phi_s|^{tracer} = 0.$

3.4.2.4 Bacteria decay

The bacteria's decay model, which is widely used in bacterial water quality modelling, is the first order decay equation, known as the Chick's law. The decay source term has slightly different forms for 1-D and 2-D applications.

For a 2-D problem:

$$\Phi_s|^{decay} = -KHS \qquad\qquad 3.17$$

where: K = decay rate;

H = total water depth;

S = depth-averaged concentration.

For a 1-D problem:

$$\Phi_s|^{decay} = -KAS \qquad\qquad 3.18$$

where: K = decay rate;

A = cross-section of the streamflow;

S = cross-section averaged concentration.

3.4.2.5 Other sources

Further analysis on other sources and sink terms is to be carried out in chapter 4.

3.5 Numerical Solution in Water Quality Modelling

The numerical techniques applied in solving the governing equations for water quality modelling have been well developed and widely used since 1970s. Taking advantage of these techniques, the technique of numerical solution adopted in this study is the ULTIMATE QUIKEST (Lin and Falconer, 1997; Lin et al., 2001) scheme for solving the

water quality indicator's transport equation based on finite difference and finite volume methods.

3.5.1   Numerical solution of hydrodynamic governing equations

The solution of hydrodynamic governing equations gives the prediction of water elevation and velocity (or flowrate) for the computed domain. There are a variety of numerical methods available for the solution approaches. The numerical method employed in this study for solving the 2-D equations is the finite difference method and for solving the 1-D equations is the finite volume method.

For the 2-D governing equations, the finite difference method used in the study is based upon the Alternating Direction Implicit (ADI) scheme which involves the sub-division of each time step into two half time steps. Thus a two-dimensional problem can be solved implicitly but considering only one-dimensional for each half time step, without the need of solving a full two-dimensional matrix.

A space-staggered grid is used, with the variables ζ(water elevation) being located at the centre of grid cell and with U, V and h (water bed depth) being located at the centre of the sides of grid cell.

On the first half time step the water elevation and the U velocity (or Q_x discharge) is solved implicitly in the x-direction, whilst the other variables are represented explicitly. For the second half time step, the water elevation and V velocity (or Q_y discharge) is solved implicitly in the y-direction with the other variables being represented explicitly.

For example, in the first half time step the continuity equation 3.1 and x-direction momentum equation 3.2 are discretized with the respect to time and space, and the discrete form of the equations can be obtained as the following tri-diagonal equations (Falconer, 1986):

$$a_i Q_{x\ i-1/2,j}^{n+1/2} + b_i \varsigma_{i,j}^{n+1/2} + c_i Q_{x\ i+1/2,j}^{n+1/2} = A_i \qquad\qquad 3.19$$

$$d_i \varsigma_{i,j}^{n+1/2} + e_i Q_{x\ i+1/2,j}^{n+1/2} + f_i \varsigma_{i+1,j}^{n+1/2} = B_i \qquad\qquad 3.20$$

where: i, j is the grid number in x, y directions;

n is the time step number.

With appropriate boundary conditions these finite difference equations are solved by using the Thomas algorithm to determine the values of ζ and Q_x. Similarly the discrete form of equation 3.1 and 3.3 are solved in the second half time step to get ζ and Q_y.

The scheme is basically second order accurate both in time and space with no stability constrains due to the time centred implicit character of the ADI technique. However, it has been recognised that the time step needs to be restricted so that a reasonable computational accuracy can be achieved (Chen, Y. 1992). A maximum Courant number (C_f) with an average total water depth (H) being used, has been suggested (Stelling, G.S. 1986) as:

$$C_f = 2\Delta t \sqrt{gH\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)} \leq 4\sqrt{2} \qquad 3.21$$

When the 2-D ADE is also solved for each half time step, the choice of the time step should also consider the stability requirements for the Courant number.

To solve the 1-D governing equations 3.4 and 3.5, the finite volume method is used by integrating with respect to time and volume over the control volume and the tri-diagonal equation system is obtained. Then the discretized equations can be solved using the Thomas algorithm with appropriate boundary conditions. In the finite volume approach a space-staggered varying-size grid is also used, with the stream flowrates being located at the side of the control volume and the water elevation located at the centre of the control volume.

3.5.2   Numerical solution of advective diffusion equation

The ULTIMATE QUICKEST scheme (Lin and Falconer, 1997) is used for solving both 1-D and 2-D advective diffusion equations. Early attempts in numerically modelling the ADE were always plagued by either large amount of numerical diffusion being associated with first-order upwinding schemes or by oscillations associated with high-order central schemes. For example, negative concentrations are frequently encountered in the vicinity of the outfalls as a result of such oscillations. A number of schemes have been developed

to remove spurious oscillations near discontinuities for solving the ADE. Cahyono (1993) carried out a detailed study in which he compared 36 of the most popular finite difference schemes for solving the advective problem both in 1-D and 2-D ADEs and it was shown that the ULTIMATE scheme which was firstly introduced by Leonard (1979) was particularly attractive since it was more general than the others and was easier to apply. The ULTIMATE algorithm plus the third-order accurate QUICKEST scheme used in solving the advective term in the equation can effectively reduce the oscillations even for sharp local changes (discontinuities). The ULTIMATE QUICKEST scheme having third-order accuracy both in time and space is therefore the key scheme in this study to achieve the accurate and numerical oscillation-free solution of ADEs.

In the study, the numerical solution of 2-D ADE (for details, see Lin and Falconer 1997) is based upon finite difference method similar to the ADI technique which involves the sub-division of each time step into two half time steps. Thus the two-dimensional vectors are considered to be only one-dimension for each half time step. So the numerical solution of 2-D ADE becomes to simulate the ADE in one-direction.

In solving the one-direction ADE the staggered grid is used with the computed depth-averaged concentration S being located at the centre of the grid cell, among which in the computation process the solute fluxes located at two sides of the grid for left and right need to be carried out for each half time step.

In solving ADE, the ULTIMATE QUICKEST scheme is used to represent the advective term; the explicit second-order accurate central scheme is used for solving the diffusion/dispersion term and finally the sources and sink terms is solved using the Euler method.

3.6   Summary

This chapter describes the general fundamentals of surface water quality modelling, which is divided into five sections.

Section 3.1 discribes the general process of water quality numerical modelling, which is composed of six steps as follows: (i) analyze the physical phenomenon; (ii) build up the mathematical equation; (iii) solve the equation for numerical solution; (iv) develop the model using programming language; (v) calibrate or validate the model by field or experimental data; and (vi) use the calibrated model for assessment in application of real case study.

Section 3.2 introduces the basic concept of the numerical method, by which engineers solve problems using computer. The derivative equations of higher-order finite difference algorithm are presented.

Section 3.3 presents the standard 1-D and 2-D governing equations for the hydrodynamic process in the water quality modelling.

Section 3.4 shows the standard 1-D and 2-D advective diffusion equations which are the governing equations for describing water quality indicator (pollutant) transport processes.

Section 3.5 describes a space-staggered alternative direction implicit (ADI) finite difference scheme, that is used to solve 2-D hydrodynamic governing equations and a space-staggered finite volume method is used to solve 1-D hydrodynamic governing equations. In solving 1-D and 2-D advective diffusion equations the ULTIMATE QUICKEST scheme is used to achieve accurate and numerical oscillation-free solutions.

Chapter 4

ENTERIC BACTERIA TRANSPORT MODELLING

4.1   Introduction

Survival of enteric bacteria such as total coliforms (TC), faecal coliforms (FC), and faecal streptococci (FS) has been a very important subject in the research field of natural water quality control for many years. The research field covers many topics including the survival in seawater, survival in fresh water, survival in bed sediments and under other different environmental conditions. One issue rising in recent years is that the water quality studies relating to bacterial survival should address the potential pollution risk from the sediments, which can serve as reservoirs for the microbial pollution. Many research studies have been carried out but most of them are field and laboratory experimental studies. How can the microbial pollution derived from the entrainment of bed sediments be monitored and estimated? How can the theory of microbial deposition due to SS settling be applied to modelling? How can the pollution be monitored over larger spatial and temporal areas even in immeasurable fields?

However, indeed there is a need of a modelling tool which could deal with the links between the individual phenomena, such as, the bacterial exchange between the water column and the bed sediments and the links between the theory explanation of the phenomenon and the phenomenon itself, such as, the bacterial mathematical resuspension equation. The modelling tool should be able to cope with the comprehensive variability of

different natural environmental factors, such as, solar radiation and turbidity, etc. This chapter is going to build the theoretical foundation for such a modelling tool.

Once bacteria indicators are released into the water environment, they are transported and kinetically react (die or grow) in the environment. In this modelling study, the physical loss of bacteria due to SS deposition is modelled separately from the bacteria die-off due to bacteriological decay, which is the basis of the new theory for predicting the total bacterial disappearance. Another important consideration is to model the bacteria entering the water column due to the bottom sediment resuspension. Sediment resuspension will bring a significant amount of bacteria from bottom sediments to the water column. Many studies report that bacteria population in bed sediments is generally much higher, on average 100-2000 times higher, than that in the overlying water (Sanfrod et al., 1991; Doyle et al., 1992; Crabill et al., 1999; Obiri-Danso and Johns, 2000). Therefore the bacteria transport modelling should also include the bacteria re-appearance processes.

4.2   Concept of Total Disappearance of Bacteria

A first order decay model (Chamberlin and Mitchell, 1978) for enteric bacterial concentration in natural waters has been assumed to follow the Chick's law (1908):

$$\frac{dC}{dt} = -KC \qquad\qquad 4.1.1$$

where: C = concentration of bacteria, counts/100ml;

   K = specific decay rate, s^{-1};

   t = sampling time, s.

As a tool for engineers, the decay rate is usually expressed in the form of T90, which is the time for 90% bacteria to die (or inactivation). It has the relationship with K, as:

   $$T90 = \ln 10/K \qquad\qquad 4.1.2$$

where: T90 is in hours; K is in h^{-1}.

From the literature, investigations on the decay rate *k* have been consequently studied by many researchers (Alkan et al., 1995; Guilland et al., 1997; Serrano et al., 1998; Wait and Sobsey, 2001; etc). Results show that the k value is affected by many interacting factors including sunlight, salinity, temperature, algal toxins, chemical toxins (heavy metals), physicochemical factors (pH), protozoa, predation, organic matter and nutrients, and sedimentation etc.

Although the effects of sedimentation on the disappearance of bacteria have been reported in some papers (Waksmann and Vartiovaara, 1938; Weiss, 1951; Milne et al., 1986), which might lead a large amount of bacteria disappearing from the water column to the bottom sediment, unfortunately, there is little detailed method for describing the effects, particularly in quantitative way. Till now there is still no other mathematical model except the first order decay equation for modelling the disappearance of bacteria due to sedimentation, thus the only way used to consider the sedimentation effect to date is to add a settling coefficient into the first order decay model's overall die-off rate. For example, equation 2.15 described in Chapter 2; and in <<theory and practice of water and wastewater treatment>> (Droste, 1997, page 172) the decay rate *k* of the first-order decay model is explained as below:

"*K* is overall disappearance or die-off rate constant:

$$K = (k_d + k_r + k_s + k_p)\, \theta^{(T-20)} \qquad\qquad 4.2$$

where: k_r is the dieoff coefficient resulting from radiation;

k_d is the die-off coefficient in the dark;

k_s is the settling coefficient, $k_s = v/H$; v is the particle fall velocity; H is the water depth;

k_p is a predation coefficient;

θ is an Arrhenius constant; T is temperature °C."

Previous studies (Waksmann and Vartiovaara, 1938; Weiss, 1951; Milne et al., 1986) have demonstrated that the settling coefficient k_s is one of the controlling factors which highly affect the bacteria appearance in the water column. But, for practical studies (Canale et al., 1993; Alkan et al., 1995; Droste, 1997) this factor is normally treated as one part of the overall first order decay rate to have a combined decay coefficient.

However, in the view of the auther, the quantitative expression of the decline in bacteria population due to the settling process is differ from the die-off first order decay model and should be described in terms of a different function. Two different representations should be used to represent the total disappearance of bacteria in the water column. One is bacteria die-off based on the first order decay and another is bacteria disappearance due to sedimentation. Thus, the settling coefficient k_s should be omitted from equation 4.2, and the expression of the overall die-off rate K becomes:

$$K = (k_d + k_r + k_p)\, \theta^{(T-20)} \qquad\qquad 4.3$$

where K is namely specific modified decay rate, being used by combining with equation 4.1.1, that will be used in later sections for equation derivation.

Sedimentation is the physical separation of suspended solids (SS) from the water column to the bottom sediment by the action of gravity. Similarly, SS can re-suspend to get into the overlying water column by turbulence. It is well known that the settling rate depends on both the flow regime and the characteristics of the particular deposition including the particle size, the density of particle and the particle concentration. Thus the bacteria disappearance rate due to sedimentation should not simply follow the first-order decay equation. It should follow a settling equation involving the effects of flow and settling characteristics.

4.3   Existence of Enteric Bacteria in Natural Waters

Bacteria in natural waters exist in two types. One is the type of free-living bacteria. The other is the type of attached bacteria, which are absorbed onto the surface of suspended particles. The free-living bacteria move with the flow flux. The attached bacteria move with the suspended particles, which could settle down onto the bottom sediment surface when the suspended particles deposit and turbulence flow can also carry the particles with the attached bacteria to re-suspend into the overlying water column. The free-living bacteria are also called free swimming bacteria.

As in natural waters, 70%-99% bacteria exist in the form of attached bacteria and the remaining 30%-1% bacteria in the form of free swimming bacteria, it becomes clear that the particular deposition brings the attached bacteria to the bottom sediments which have populations of faecal bacteria, that are on average 100-2000 times greater than the water counts.

Since rapid development and urbanisation has made natural waters become more and more turbid, recently high SS concentration often occurs in polluted natural waters. This provides huge amount of suspended particles with enough living surfaces for bacteria. Marshall (1978) indicated that bacteria readily sorb on to different kinds of interfaces such as liquid-solid, liquid-liquid, liquid-gas etc. He also quoted the results from Jannasch who found that only 0.02% of the microbial population in the Nile River was planktonic (free living), the remainder being attached to mineral particular materials. In an aquifer contaminated by treated sewage, 96.8-100% of the bacteria were particle bound when enumerated by direct counting methods (acridine orange direct counting, AODC), as Harvey et al. (1984) Reported. Also Albrechtsen's research (1994) showed that most of the bacteria were attached to small particles and only 0.01% of the total bacteria number was counted to be free-living in the pore-water.

Therefore, when necessary it is reasonable to assume that all the bacteria exist in the type of attached bacteria in polluted turbid natural waters, which is often the case in the water resources around urban areas.

4.4 Conceptual Model of Bacteria Transport

Enteric bacteria in coastal waters derive from:

1. Direct sewage disposals via sea outfalls of wastewater treatment plant, e.g. point source pollution from SSOs or CSOs.

2. Indirect disposals via river inflows, e.g. diffuse pollution from livestock delivered via river systems which may also contain anthropogenic inputs from inland settlements.

3. Direct or indirect disposals from wildlife populations such as water birds who forage in the sea or river water and some on the intertidal beaches.

4. Sediment re-suspension which can also be considered as a bacterial source.

These are depicted in Figure 4.1.

Figure 4.1 shows that the reduction of bacteria in natural waters can be divided into two categories, namely die-off (or inactivation) and deposition. The die-off rate is a first order decay process. The deposition rate (that is, the bacteria disappearance due to sedimentation) is a function of the settling process for the suspended solids (SS). It also shows that sediment resuspension is regarded as one input of bacterial sources.

A water column

Die-off and
Deposition
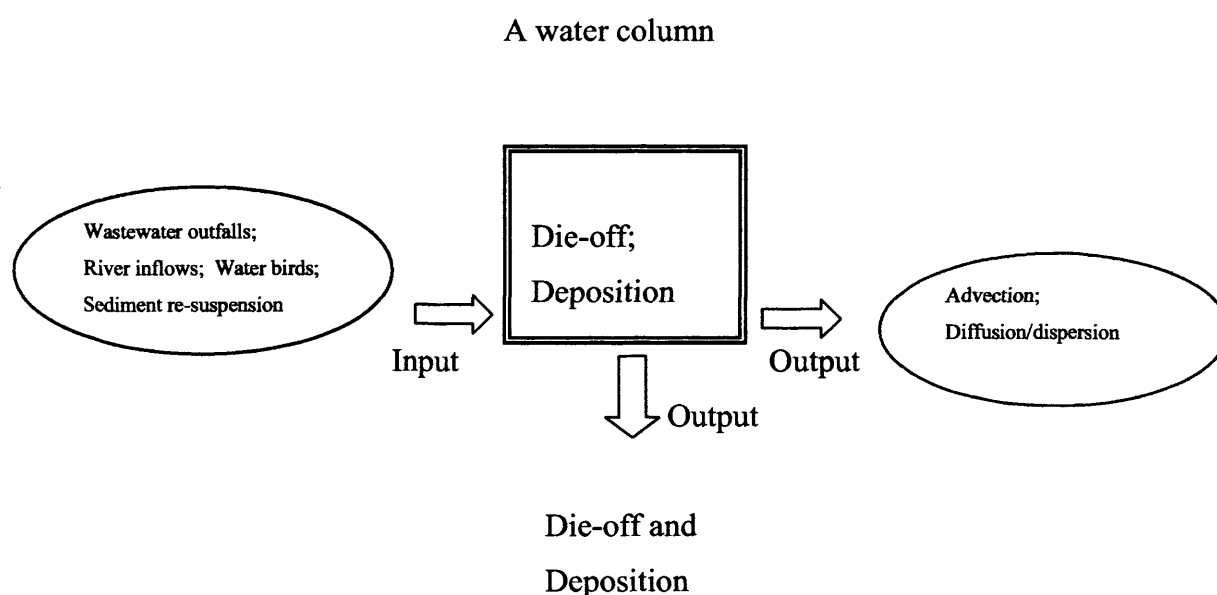
Figure 4.1   Concept model of enteric bacteria transport in natural waters

The above resuspension source of faecal indicators was proved to be the dominated factor for bathing waters to fail the bathing water quality standards when the first two sources become less quantity during some special period in a year. For example, Obiri-Danso and Jones (2000) found that resuspension of indicator bacteria from the sediments is likely to contribute significantly to the microbial content of the overlying seawater only during windy weather. Similarly Valiela et al. (1991) reported that resuspension has been shown to be a contributory factor in bathing water failing the EU Directive on Bathing Water Quality.

In recent years, more and more studies have found that generally the sediments contains a much larger bacterial population and heterotrophic activity, which will be potentially additional sources for the bacterial pollution.

Although many studies (Milne et al., 1986; Burton et al., 1987; Davies et al., 1995; Crabill et al., 1999; Obiri-Danso and Jones, 2000) have focused their research on how the sediments as a bacteria reservoir affect the overlying seawaters for the purpose of investigating the sediments resuspension's influence on the overlying water quality, there is still no quantitative relationship, so far to our knowledge, being established between the bacteria indicators population and the sediment re-suspension concentration. Also there is no computer program to model the link between the water quality of bacteria indicators and the sediments reservoir.

However it is noted in the literature that just like the simulation on the above mentioned bacteria counts coming from sediment re-suspension is a research dearth, there is a gap between the knowledge and the phenomenon of the effect of the SS deposition on bacteria population decrease in the water column as well.

Therefore the goal of this research is to develop the relevant mathematical equations representing both the bacteria disappearance rate based SS deposition and the bacteria increase rate that from the re-suspension of the bed sediments. Then a numerical modelling tool based on these mathematical equations will be developed to predict the enteric bacteria transport associated with sediment transport.

4.5   Sediment Transport in Natural Waters

Sediment transport in natural waters is controlled by the sediment characteristics and the flow motion. Once suspended in the water, sediments are transported with the flow flux and always tend to settling down due to gravity. The settled bottom sediments later could be re-suspended by disturbance, namely resuspension or entrainment. The settling process and the resuspension will be dealt with in this section.

From Figure 4.2, it is clearly seen that the uniformly distributed SS with the uniform size (V_d) can move a maximum vertical distance (h) in the time of Δt ($\Delta t = t2-t1$) by settling. That is, the distance $h = V_d$ (t2-t1). Therefore the particles, if they are under the height h from bottom, will be removed from the water volume (A·h) to the bottom sediment by the settling process during the time of Δt. So the total quantity of the removed particles is $S1 \cdot (A \cdot h)$, or, $S1 \cdot (A \cdot V_d \cdot \Delta t)$.

Therefore the SS concentration at time t2, namely S2, can be worked out as:

$$S2 = S1 - \frac{S1 \cdot (A \cdot V_d \cdot \Delta t)}{A \cdot H} \qquad 4.4$$

Move term S1 to the left side:

$$S2 - S1 = -\frac{S1 \cdot V_d \cdot \Delta t}{H}$$

Apply ΔS_d as the reduction of SS concentration caused by the settling process:

$$\Delta S_d = S2 - S1 = -\frac{S1 \cdot V_d \cdot \Delta t}{H}$$

In the case of the limit of $\Delta t \rightarrow 0$, considering the original SS concentration S as the SS concentration at time t1, that is $S1=S$, we get:

$$dS_d = -S \times \frac{V_d \cdot dt}{H} \qquad 4.5$$

Therefore, the settling loss rate of SS concentration is given as:

$$\frac{dS_d}{dt} = -\frac{V_d}{H} \cdot S \qquad 4.6$$

In equation 4.6 the decrease of SS concentration due to settling is expressed as the function of settling velocity, SS concentration and the water depth. It has to be mentioned that equation 4.6 is derived under the condition of ideal uniform sized particles settling in static water.

The analysis of settling process will be introduced in two types: the particles settling in static water and in flowing water. Only the particles' settling mechanism in flowing water will be implemented to develop the new modelling tool. However the settling process analysis on particles in static water enables us a better understanding of the theory of bacteria population loss due to SS deposition.

The re-suspension of bed sediments will only occur in flowing water while there is disturbance bringing the bed sediments into the water column. Once the sediment characteristics have been defined, the bottom shear stress at the sediment-water interface is the controlling factor for the resuspension.

4.5.1   Settling process of uniform size particles in static water

Consider an elemental volume of water with uniformly distributed SS concentration showing in Figure 4.2, it is assumed that the particles have a uniform size and they do not interact with each other during the settling process in this volume. That is, the particles are idealised simple uniform size, non-cohesive sandy sediments. The change of the SS concentration in this elemental volume from time t1 to time t2 due to settling process is illustrated in Figure 4.2.
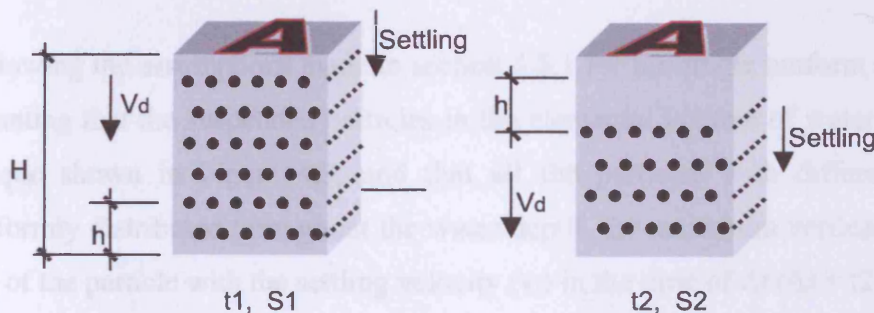
Figure 4.2   Settling process of uniform distributed SS in an elemental water volume

(The settling velocity V_d applies to the uniform particles; S1 and S2 apply to the SS concentration of the water volume at the time t1 and t2 respectively; H is the depth of the water volume and A is the plan area - the settling cross section.)

4.5.2   Settling process of particles with multiple size in static water

In real case study the particles in sediment samples are usually fine-grained sediments which would have a gradual size distribution, usually represented by a distributed settling velocity curve, such as that shown in Figure 4.3.
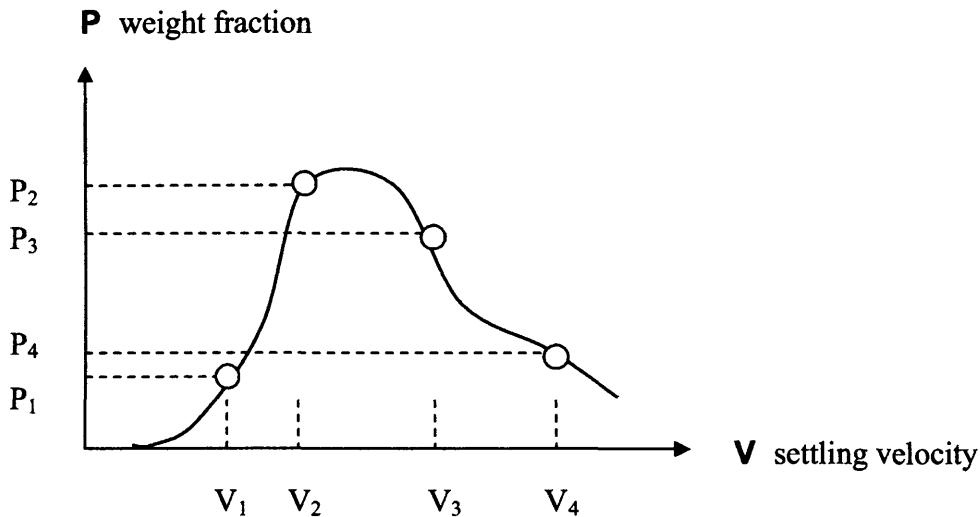
P weight fraction

Figure 4.3   Settling velocity curve for a sediment sample

(v is the settling velocity, P is the weight fraction;

v_i is a particle velocity, P_i is the weight fraction of the particle with the stated velocity v_i.)

Following the assumptions made in section 4.5.1 for the single uniform particle size, now assuming that the suspended particles in the elemental volume of water has the sediment sample shown in Figure 4.3, and that all the particles with different velocities are uniformly distributed throughout the water depth, the maximum vertical settling distance (h_i) of the particle with the settling velocity (v_i) in the time of Δt ($\Delta t = t2-t1$) thus is:

$$h_i = v_i * \Delta t \tag{4.7}$$

Therefore those particles, which are distributed under the height (h_i) measured from the bottom, will be removed from the water volume to the bottom sediments by its settling process during a time period of Δt. The removal weight is:

$(S1*P_i)*(A*h_i) =$

$$S1 \cdot P_i \cdot A \cdot v_i \cdot \Delta t \qquad\qquad 4.8$$

Substituting all the different size particles, the total loss of particles' weight during the time of Δt will be:

$$S1 \cdot P_1 \cdot A \cdot v_1 \cdot \Delta t + S1 \cdot P_2 \cdot A \cdot v_2 \cdot \Delta t + S1 \cdot P_3 \cdot A \cdot v_3 \cdot \Delta t + S1 \cdot P_4 \cdot A \cdot v_4 \cdot \Delta t =$$

$$S1 \cdot A \cdot \Delta t \cdot \sum_{i=1}^{4} Pi \cdot Vi \qquad\qquad 4.9$$

where the weight fraction P_i (P_1 P_2 P_3 and P_4) is shown in Figure 4.3.

Applying the average SS concentration S1 and S2 at the time t1 and t2 respectively to the total loss of particles' weight, we have:

$$S2 = S1 - \frac{1}{A \cdot H} \cdot \left(S1 \cdot A \cdot \Delta t \cdot \sum_{i=1}^{4} Pi \cdot Vi \right) \qquad\qquad 4.10$$

Applying ΔS_d as the total change of SS concentration caused by settling process, equation 4.10 comes to:

$$\Delta S_d = S2 - S1 \;=\; -\frac{S1}{H} \{\sum_{i=1}^{4} Pi \cdot Vi\} \cdot \Delta t \qquad\qquad 4.11$$

In the limit of $\Delta t \rightarrow 0$, considering the SS concentration at time t1 as the original SS concentration S and taking number n to record all sizes of the particles in the suspension sample, the total loss rate of SS concentration results in:

$$\frac{dS_d}{dt} \;=\; -\frac{S}{H} \{\sum_{i=1}^{n} Pi \cdot Vi\} \qquad\qquad 4.12$$

Thus, in the settling process of the particles with multiple sizes, equation 4.12 shows that the total SS loss rate due to settling is the function of weight fraction weighted settling velocity, SS concentration and the water depth.

4.5.3   Cohesive sediment transport equations

It is more common in some cases to consider cohesive sediments for sediment transport modelling along coastal lines as the sewage discharged from WwTW outfalls normally contain flocculated particles. Many studies (Krone, 1962; Parthenaides, 1965; Lick, 1986; Ziegler and Lick, 1988; Sanford et al, 1991; Sanford and Halka, 1993; Sanford and Maa, 2001) focused on investigating the deposition and resuspension rates of cohesive sediments.

A necessary parameter in the quantitative numerical modelling of sediment transport is the sediment flux q_s at the sediment-water interface. The cohesive sediment net flux q_s can be written as:

$$q_s = E - D \qquad\qquad 4.13$$

Where:

> E = resuspension rate;
>
> D = deposition rate.

In equation 4.13 an assumption has been made that entrainment and deposition are independent processes, i.e., E is the sediment flux when no suspended sediment deposition is present, while D is the sediment flux in the absence of entrainment. In the steady state, $q_s = 0$, and the equation indicates that there is a dynamic equilibrium at the sediment-water interface between entrainment and deposition.

4.5.3.1   Cohesive sediment resuspension rate

A linear mathematical formulation for resuspension rate E (in equation 4.13) is widely employed in many studies (Kandiah, 1974; Mclean, 1985; Odd, 1988; Kuijper et al., 1989; Lang et al., 1989; Perillo and Sequeira, 1989; Uncles and Stephens, 1989; Sanford et al., 1991; Hawley and Lesht, 1992; Sanford and Halka, 1993; Mei et al., 1997), which is adopted in this study:

$$E = \begin{cases} M\left(\dfrac{\tau_b}{\tau_c} - 1\right), & \tau_b > \tau_c \\ 0, & \tau_b \le \tau_c \end{cases} \qquad\qquad 4.14$$

Where:

E = erosion rate, $\text{kg m}^{-2}\text{ s}^{-1}$;

τ_b = effective bottom shear stress, N m^{-2} ;

τ_c = critical shear stress for the initiation of sediment resuspension from the bed, N m^{-2}. Jing and Ridd (1996) found τ_c is about 2.0 N/m^2 in Cleveland Bay, Australia.

M = empirical constant in appropriate unit, here $\text{kg m}^{-2}\text{ s}^{-1}$, (M = $\tau_c \times$ the slope of the plot of E vs. τ_b). Sanford et al. (1991) found $M \approx 1.4 \times 10^{-6}$ $\text{kg/m}^2\text{/s}$ and τ_c = 0.016 Pa in northern Chesapeake Bay.

By defining ΔS_r as the amount of increase in SS concentration caused by resuspension within a computed time interval Δt, the resuspension rate can be expressed as $\Delta S_r/\Delta t$. Let $\Delta t \rightarrow 0$, and consider that the total amount of entrainment E per unit bed distributes uniformly over the water depth H, the instantaneous resuspension rate then becomes:

$$\frac{dS_r}{dt} = \frac{E}{H} = \frac{M}{H}\left(\frac{\tau_b}{\tau_c} - 1\right) \Bigg|_{\tau_b > \tau_c} \qquad \qquad 4.15$$

There is a general agreement that the bottom shear stresses exerted per unit area of the bed by waves and currents are the dominant forces causing resuspension (or erosion). These flow-induced forces act on the grains on the bed to cause the motion of bottom sediment. There is a critical shear stress (τ_c) associated with the initiation of sediment resuspension whose value depends on the bed material characteristics (mineral composition, organic materials, salinity, density etc.) and bed structure (water content of the bed sediments). When the effective shear stress (τ_b) exceeds the critical shear stress (τ_c) the bottom sediments start to re-suspend into the water column.

The effective bed shear stress due to currents given by Soulsby (1997) is as below:

$$\tau_b = \rho C_D \bar{U}^2 \qquad \qquad 4.16$$

Where:

$\bar{U}$ = depth-averaged current speed, m/s;

C_D = drag coefficient applicable to depth-averaged current speed;

ρ = density of sea water, typically 1027 kg/m^3.

Either of the following relationships related to Darcy-Weisbach resistance coefficient f or the Chezy coefficient C or the Manning's roughness n can be used to calculate the drag coefficient:

$$C_D = \frac{f}{8} \qquad\qquad 4.17$$

$$= \frac{g}{C^2} \qquad\qquad 4.18$$

$$= \frac{g \cdot n^2}{h^{1/3}} \qquad\qquad 4.19$$

$$= \alpha \left(\frac{z_0}{h}\right)^\beta \qquad\qquad 4.20$$

Where:

h = water depth (m);

g = gravity acceleration (m/s^2) ;

z_0 = bed roughness length (m), for hydrodynamically rough flows z_0 can be obtained by $z_0 = D_{50}/12$;

D_{50} = median particle size of bed material;

The values of empirical constant α and β are proposed as:

Manning-Strickler law: $\alpha = 0.0474$, $\beta = 1/3$;

Dawson et al. (1983): $\alpha = 0.0190$, $\beta = 0.208$.

The selection of the above formulas depends on the type of application. Where no information is available, or only a rough estimate is needed, a default value of $C_D = 0.0025$ can be taken.

The critical bed shear stress according to the Shields diagram is given (van Rijn, 1984a, 1984b) as:

$$D_* = D_{50} \left[\frac{(s-1)g}{v^2}\right]^{1/3} \qquad\qquad 4.21$$

And:

$$D_* \leq 4 \qquad \theta_{cr} = 0.24(D_*)^{-1}$$

$$4 < D_* \leq 10 \qquad \theta_{cr} = 0.14(D_*)^{-0.64}$$

$$10 < D_* \leq 20 \qquad \theta_{cr} = 0.04(D_*)^{-0.10} \Biggr\} \quad Shields \quad curve$$

$$20 < D_* \leq 150 \qquad \theta_{cr} = 0.013(D_*)^{0.29}$$

$$150 < D_* \qquad \theta_{cr} = 0.055$$

In which:

$$\theta_{cr} = \frac{\tau_c / \rho}{(s-1)gD_{50}} \qquad\qquad 4.22$$

Or:

$$\tau_c = \rho \ (\theta_{cr} \ (s-1) \ g \ D_{50}) \qquad\qquad 4.23$$

Where:

s is the specific density, $s = \rho_s / \rho$;

ρ_s is the sediment density, kg/m^3;

v is the fluid kinematic viscosity, m^2/s;

D_* is dimensionless particle diameter.

For investigating only the initial suspension directly from the bed material but not from the top boundary of the bed load layer, Celik and Rodi (1991) used the following empirical relationship to determine the critical shear stress:

$$\tau_c = 0.25 \qquad R_* > 0.6 \qquad\qquad 4.24$$

$$\tau_c = \frac{0.15}{R_*} \qquad R_* \leq 0.6 \qquad\qquad 4.25$$

where: R_* is the hydraulic radius, $R_* = u_* d / v$, u_* is the shear velocity and d is the diameter of particles.

4.5.3.2   Cohesive sediment deposition rate

In equation 4.13, the deposition rate D can be written as (Sanford and Halka, 1993):

$$D = p \cdot w_d \cdot S_b \qquad\qquad 4.26$$

where: p is the probability that a sediment particle will stick to the bed;

S_b is the near bed sediment concentration;

w_d is the deposition velocity, different from the sediment fall velocity w_s defined by the Stock's law.

For very small particles, w_d may be larger than w_s because of Brownian motion diffusion (Lick, 1986; Sheng, 1986); for particle diameters greater than about 1um, approximately $w_d = w_s$ (Lick, 1982). The probability of deposition is usually written (Einstein and Krone, 1962; Dyer, 1986; Mehta, 1989; Self et al., 1989) in the form:

$$\left. \begin{array}{ll} p = 1 - \dfrac{\tau_b}{\tau_d} & \tau_b < \tau_d \\[2mm] p = 0 & \tau_b \geq \tau_d \end{array} \right| \qquad 4.27$$

where: τ_d is the critical shear stress for deposition. Integrating these into equation 4.26, one comes:

$$D = \left\{ \begin{array}{ll} w_s S_b \left(1 - \dfrac{\tau_b}{\tau_d} \right) & \tau_b < \tau_d \\[3mm] 0 & \tau_b \geq \tau_d \end{array} \right. \qquad 4.28$$

where:

D is the deposition rate, $kg\ m^{-2}s^{-1}$.

w_s is the apparent sediment settling velocity, $m\ s^{-1}$.

S_b is the near bed cohesive sediment concentration, $kg\ m^{-3}$.

τ_b is the effective bottom shear stress, $N\ m^{-2}$.

τ_d is the critical shear stress beyond which there is no further deposition, $N\ m^{-2}$

As a uniform distribution is applied to the SS concentration, the change of SS concentration due to cohesive sediment deposition is:

$$\frac{dS_d}{dt} = \frac{D}{H} = \frac{w_s S_b}{H} \left(1 - \frac{\tau_b}{\tau_d} \right) \bigg|_{\tau_b < \tau_d} \qquad 4.29$$

where: H is the depth of the water column, m.

Lick (1986) indicated that in usual fine-grained sediment samples found in lakes or oceanic waters, particle sizes and hence settling velocities varied over orders of magnitude and the deposition rate in equation 4.26 could be approximated as D =

$\Sigma p \cdot w_d \cdot S_b$, where the sediments are separated into different components each with its own average particle size, settling velocity and relatively deposition velocity.

4.5.4 Non-cohesive sediments transport equations

The paradigm of cohesive sediment transport research is that erosion and deposition are mutually exclusive and many laboratory studies have shown that there is a velocity/stress threshold below which erosion does not occur and a lower threshold above which deposition does not occur. In contrast, a deposition threshold is not included in non-cohesive sediment transport models, allowing erosion and deposition to occur simultaneously (Smith, 1977; Dyer, 1986; Glenn and Grant, 1987).

Under this scenario, sediments are transported initially as bedload, which implies a continual exchange between deposited and moving particles. This bedload layer, which is considered to be always in equilibrium with the bottom shear stress, serves as the source layer for suspended sediment when the shear stress is high enough. Net erosion or deposition occurs as the suspended load adjusts to a increase or a decrease in bedload concentration.

Mathematically, this approach amounts to specifying a boundary condition – a concentration at some reference height a, near the top of the bedload layer as (Smith, 1977; Glenn and Grant, 1987):

$$\begin{cases} S_a = \dfrac{S_b \gamma_o \left(\dfrac{\tau_b}{\tau_c} - 1 \right)}{1 + \gamma_o \left(\dfrac{\tau_b}{\tau_c} - 1 \right)} & \tau_b \geq \tau_c \\[4ex] S_a = 0 & \tau_b < \tau_c \end{cases} \qquad 4.30$$

where: S_a = sediment concentration at reference height a;

S_b = sediment concentration in the bed;

γ_o = an empirical constant.

As mentioned in the above for real case of multiple size particles, boundary condition (4.30) may be written for a range of sediment classes, each with its own set of values for

S_b and τ_c. The total distribution of suspended sediment is then expressed as the sum over all of the classes (Sanford and Halka, 1993).

The implementation of these concepts for non-cohesive sediment transport modelling in this study follows van Rijn's (1984a, b) formulae, which are described below.

The non-cohesive sediment net erosion or deposition rate E can be expressed as (Carcia and Parker, 1991; Lin and Falconer, 1995):

$$E = w_s(S_{ae} - S_a) \qquad\qquad 4.31$$

where: w_s = particle settling velocity;

S_a = sediment concentration at reference level a;

S_{ae} = equilibrium sediment concentration at the reference level a; a is assumed to be equal to the equivalent roughness height (k_s), with a minimum value being giving by a = 0.01H.

For the cases:

1) $S_{ae} < S_a$, E < 0 , deposition,

2) $S_{ae} > S_a$, E > 0 , erosion,

3) $S_{ae} = S_a$, E = 0 , equilibrium resuspension, for the case of suspended sediment fluxes that are steady in time and uniform in space.

The expression of S_{ae} was given as (van Rijn,1984a):

$$S_{ae} = 0.015 \frac{D_{50}T^{1.5}}{aD_*^{0.3}} \qquad\qquad 4.32$$

where: D_{50} = sediment diameter of which 50% of the bed material is finer;

T = transport stage parameter (van Rijn,1984a);

D_* = particle parameter shown in equation 4.21.

In a depth-averaged 2D model only the depth mean sediment concentration S is available. Hence the value of the reference concentration S_a must therefore be related to the depth mean concentration S, with this relationship being assumed to be of the form (Falconer and Owens, 1990) as:

$$S_a/S = S_{ae}/S_e \qquad\qquad 4.33$$

where: S_e = depth mean equilibrium concentration;

Substituting equation 4.33 into 4.31:

$$E = w_s \frac{S_{ae}}{S_e}(S_e - S) \qquad 4.34$$

The depth mean equilibrium concentration S_e can be calculated from the ratio (Lin and Falconer, 1995):

$$S_e = \alpha \frac{q_s}{q} \qquad 4.35$$

in which α is a profile factor, and assumed to be 1.13 after Celik and Rodi (1991); q is the fluid flux; q_s is the suspended sediment flux (van Rijn, 1884b).

In summary, by agreement with the other expressions of the SS loss or increase, the final change rate of SS concentration caused by the non-cohesive sediment net erosion or deposition can be expressed as:

$$\frac{dS}{dt} = \frac{E}{H} = \frac{w_s}{H} \frac{S_{ae}}{S_e}(S_e - S) \qquad 4.36$$

When $S_e > S$, net resuspension will occur and then dS/dt = dS_r/dt; when $S_e < S$, net deposition will occur and dS/dt = dS_d/dt.

4.6 Development of Mathematical Equations

4.6.1 Relationship between bacteria and SS deposition

In order to develop new mathematical expressions, the following three assumptions are regarding on the relationship between bacteria and suspended solids in natural waters:

1) Once a bacterium enters the water column, it immediately sorbs to a suspended solid's surface.

2) There are enough SS in the water column, which provide the living places for bacteria. Bacteria are all attached.

3) Within the water column the distribution of SS concentrations and bacterial populations are uniform along the water depth. Therefore, the bacterial populations sorbed onto the SS surfaces are the same as that for each unit of SS concentration.

Under these assumptions, the bacteria disappearance process causing by SS settling can be described by the following expression, in which N/S is the uniform distribution population of bacteria:

$$dN = \frac{N}{S}dS_d \qquad\qquad 4.37$$

where: N = number of bacteria, counts.

S = SS concentration, kg m^{-3}.

dS_d = amount of change of SS concentration causing by settling process during a time step, kg m^{-3}.

If a constant percentage of attached bacteria is applied, then:

$$dN = \alpha_s \frac{N}{S}dS_d \qquad\qquad 4.38$$

where: α_s = population ratio of attached bacteria to total bacteria existed in the water column. In turbid natural waters α_s can be regarded as unity.

Change the unit of bacteria population and divide by the time interval dt, we get the bacterial disappearance rate due to the SS deposition:

$$\frac{dC_d}{dt} = \alpha_s \frac{C}{S}\frac{dS_d}{dt} \qquad\qquad 4.39$$

where: C = bacterial population in water column, counts/100ml.

dC_d = loss of bacteria population due to SS deposition during the time interval (dt).

4.6.2   Relationship between bacteria and bed sediment resuspension

In coastal waters the re-suspension of bottom sediments tends to occur periodically as there is significant turbulent flow due to tides and waves, the amount of increased bacteria caused by this re-suspension can be expressed as:

$$dC_r = 0.1 C_b\, dS_r \qquad\qquad 4.40$$

where:

C_b = bacteria concentration on bed sediments, counts/g.

dS_r = amount of increased SS concentration, coming into the water column by resuspension, kg/m^3.

dC_r = increased bacteria population due to the sediment resuspension, counts/100ml.

0.1 = constant coefficient of the unit change between C_b and C_r.

Divide the time interval *dt* on two sides of equation 4.40, we get the bacterial resuspension rate due to entrainment from the bed sediment:

$$\frac{dC_r}{dt} = 0.1C_b \frac{dS_r}{dt} \qquad 4.41$$

The mechanics of the survival of bacteria in bed sediments employed here is a first order decay equation:

$$C_b = C_{b0} \cdot e^{-k_b t} \qquad 4.42$$

where:

C_{b0} = bacteria concentration on bed sediments at the start time, counts/g;

k_b = bacteria's first order decay rate when the bacteria exist in the bottom sediments, s^{-1}. The decay rate k_b is regarded as nil in this study.

4.6.3 New mathematical model I - bacterial deposition

When we combine equation 4.39 with equations 4.6, 4.12, 4.29 and 4.36, the mathematical models expressing the bacteria disappearance due to settling process with different kinds of SS characteristics can be obtained:

a. bacterial disappearance caused by simple size particles (equations 4.39 and 4.6)

$$\frac{dC_d}{dt} = -\alpha_s \frac{V_d}{H} C \qquad 4.43$$

b. bacterial disappearance caused by multiple size particles with a distributed settling velocity curve (equations 4.39 and 4.12)

$$\frac{dC_d}{dt} = -\alpha_s \frac{1}{H} \cdot \{\sum_{i=1}^{n} Pi \cdot Vi\} \cdot C \qquad 4.44$$

c. bacterial disappearance by cohesive sediments deposition (equations 4.39 and 4.29)

$$\frac{dC_d}{dt} = -\alpha_s \frac{w_s}{H} \cdot \frac{S_b}{S} \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_d}\right) , \qquad \tau_b < \tau_d \qquad 4.45$$

d. bacterial disappearance by non-cohesive sediment deposition (equations 4.39 and 4.36)

$$\frac{dC_d}{dt} = \alpha_s \frac{w_s}{H} \frac{S_{ae}}{S_e} \frac{C}{S} (S_e - S) , \qquad S_e < S \qquad 4.46$$

As described in section 4.4, the total disappearance of bacteria is composed of two parts: the first-order decay die-off and the disappearance due to deposition. Integrating equation 4.1.1 with equations 4.43, 4.44, 4.45, 4.46 the new mathematical model which describing the **total disappearance** of bacteria from water column is obtained and given by the following equations:

1. uniform size particle in static water for SS

$$\frac{dC_T}{dt} = -\left(kC + \alpha_s \frac{V_d}{H} C\right) \qquad 4.47$$

2. multiple size particles in static water for SS

$$\frac{dC_T}{dt} = -\left(kC + \alpha_s \frac{1}{H} \cdot \{\sum_{i=1}^{n} Pi \cdot Vi\} \cdot C\right) \qquad 4.48$$

3. cohesive sediment in natural water for SS

$$\frac{dC_T}{dt} = -\left\{kC + \alpha_s \frac{w_s}{H} \cdot \frac{S_b}{S} \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_d}\right)\right\} , \qquad \tau_b < \tau_d \qquad 4.49$$

4.   non-cohesive sediment in natural water for SS

$$\frac{dC_T}{dt} = -kC + \alpha_s \frac{W_s}{H} \frac{S_{ae}}{S_e} \frac{C}{S}(S_e - S) \ , \qquad S_e < S \qquad 4.50$$

where: dC_T = amount of total disappearance of bacteria during a computational time step dt, counts/100ml. dC_T/dt means instantaneous rate of change.

Equation 4.47 can be applied for modelling idealised, single uniform size particles' deposition process, such as some laboratory studies. It is interesting to note that Equation 4.43, representing the bacterial loss rate due to settling of uniform size particles in static water, is derived to be the same as the formula reported in the literature for representing the setting coefficient k_s, $k_s = V_d/H$ (see Canale et al., 1993 and Droste, 1997).

Therefore, it is concluded that the settling coefficient ($k_s = V_d/H$) used in past studies (see equation 2.18 and equation 4.2) is only a specific case for representing the settling of idealised, uniform size particles in static water.

For a realistic case study where most suspended sediments are extremely fine, particle diameters less than 1 um, the cohesive sediment equation 4.49 should be used.

Equations 4.47 – 4.50 show that when the SS settling process dominates SS vertical movements the bacteria concentration in water column will significantly decrease as the decay and deposition take place at the same time.

For many cases that equations 4.49 and 4.50 can be combined so that the suspended sediments include both cohesive and non-cohesive sediments. In this case the total bacterial disappearance rate is given as:

$$\frac{dC_T}{dt} = -\left\{ kC + \alpha_s \frac{w_s}{H} \cdot \frac{S_b}{S} \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_d}\right) - \alpha_s \frac{W_s}{H} \frac{S_{ae}}{S_e} \frac{C}{S}(S_e - S) \right\} \ , \begin{array}{c} \tau_b < \tau_d \\ S_e < S \end{array} \qquad 4.51$$

4.6.4 New mathematical model II - bacterial resuspension

Substituting equation 4.15(cohesive) and 4.36(non-cohesive) into equation 4.41, the mathematical expressions for describing the bacteria reappearance from bottom sediments to the overlying water column can be derived:

1. bacterial increase due to cohesive sediment resuspension (equations 4.15 and 4.41):

$$\frac{dC_r}{dt} = 0.1 C_{b0} \cdot \frac{e^{-k_b t}}{H} \cdot M\left(\frac{\tau_b}{\tau_c} - 1\right) , \qquad \tau_b > \tau_c \qquad 4.52$$

2. bacterial increase due to non-cohesive sediment resuspension (equations 4.36 and 4.41):

$$\frac{dC_r}{dt} = 0.1 C_{b0} \cdot \frac{e^{-k_b t}}{H} \cdot \frac{w_s S_{ae}}{S_e}(S_e - S) , \qquad S_e > S \qquad 4.53$$

Equations 4.52 and 4.53 describe the increase of bacterial concentration in the water column caused by the sediment resuspension. In a no-entertainment season and without enteric bacteria disposals some coastal waters could still get bacterial pollution when the area's bed bacteria concentration C_{b0} has a very high value. Equations 4.52 and 4.53 clearly show these cases that the total bacteria population could increase linearly with C_{b0} value due to the re-suspension of bed sediment from the bottom sediments.

4.7 Enteric Bacteria Transport Modelling Associated With Sediment Transport

Sediment transported in natural waters may deposit in any local areas, and these deposited particles will act as a temporary or long-term sink for the pollutants they are associated with. When turbid water is considered, water quality modelling has to involve the particles' impaction. Here, the impact is regarded in two parts: deposition and resuspension. In summary, in this section the equations governing the enteric bacteria transport processes which are associated with sediment transport are produced.

4.7.1　Two-dimensional bacteria transport governing equation

The general depth averaged two-dimensional governing equation describing the enteric bacteria transport including advective-diffusion processes can be written as:

$$\frac{\partial C}{\partial t}+\frac{\partial CU}{\partial x}+\frac{\partial CV}{\partial y}-\frac{\partial}{\partial x}\left[D_x\frac{\partial C}{\partial x}\right]-\frac{\partial}{\partial y}\left[D_y\frac{\partial C}{\partial y}\right]=\sum\Phi_s \qquad 4.54$$

where

C　= depth averaged bacteria concentration, counts/100ml.

$\sum\Phi_s$　= sources and sink terms, representing the sources and all kinetic principles of the bacteria transformation in water environment. Here it includes the processes of bacteria decay, deposition disappearance, entrainments from bed, discharge from disposals and river inputs.

$$\sum\Phi_s=\frac{dC_T}{dt}+\frac{dC_r}{dt}+\sum_{n=1}^{n}\frac{Q_oC_o}{A_oH} \qquad 4.55$$

where

Q_o　= outfall discharge rate, m^3/s;

C_o　= outfall discharge concentration, counts/100ml;

A_o　= horizontal outfall discharge area, m^2;

H　= water depth, m;

n　= number of outfalls.

4.7.2　One-dimensional bacteria transport governing equation

The general cross-sectional averaged one-dimensional governing equation describing the advective-diffusion processes in rivers can be written as:

$$\frac{\partial C}{\partial t}+\frac{\partial CU}{\partial x}-\frac{\partial}{\partial x}\left[D_x\frac{\partial C}{\partial x}\right]=\sum\Phi_s \qquad 4.56$$

where

C　= cross-sectional averaged bacteria concentration, counts/100ml.

$\sum\Phi_s$　= sources and sink terms.

4.7.3   Mathematical expression of the sources and sink terms

$\Sigma\Phi_S$ summarises all the biological, chemical and physical transformations including bacteria decay, deposition disappearance, entrainments from bed, discharge from disposals and river inputs etc.

4.7.3.1   2D governing equation

♦ Bacterial sources or sink terms associated with cohesive sediments

By integrating equations 4.49 and 4.52 with equation 4.55, we obtain for cohesive sediments:

$$\Sigma\Phi_s = -kC - \alpha_s \frac{w_s}{H} \cdot \frac{S_b}{S} \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_d}\right)\Bigg|_{\tau_b < \tau_d} + 0.1 C_{b0} \cdot \frac{e^{-k_b t}}{H} \cdot M\left(\frac{\tau_b}{\tau_c} - 1\right)\Bigg|_{\tau_b > \tau_c} + \sum_{n=1}^{n} \frac{Q_o C_o}{A_o H}$$

<div align="right">4.57</div>

♦ Bacterial sources or sink terms associated with non-cohesive sediments

By integrating equations 4.50 and 4.53 with equation 4.55, we obtain for non-cohesive sediments:

$$\Sigma\Phi_s = -kC + \alpha_s \frac{C}{SH} \frac{w_s S_{ae}}{S_e}(S_e - S)\Bigg|_{S_e < S} + 0.1 C_{b0} \cdot \frac{e^{-k_b t}}{H} \cdot \frac{w_s S_{ae}}{S_e}(S_e - S)\Bigg|_{S_e > S} + \sum_{n=1}^{n} \frac{Q_o C_o}{A_o H}$$

<div align="right">4.58</div>

Equations 4.57 and 4.58 are used in the general depth-averaged solute transport governing equation (Equation 4.54) to describe the bacteria transport associated with sediment transport in natural waters. Comparing with the other researches, these expressions not only include the bacteria die-off rate but also the bacteria disappearance by SS deposition to the bottom sediment and also the bacteria entrainment due to the sediment resuspension.

4.7.3.2   1D governing equation

For the cross-sectional averaged one-dimensional governing equation, the sources and sink terms are:

♦ 1D bacterial sources and sink terms associated with cohesive sediments

$$\sum \Phi_s = -kC - \alpha_s \frac{w_s}{A} \cdot \frac{S_b}{S} \cdot C \cdot \left(1 - \frac{\tau_b}{\tau_d}\right)\bigg|_{\tau_b < \tau_d} + 0.1C_{b0} \cdot \frac{e^{-k_b t}}{A} \cdot M\left(\frac{\tau_b}{\tau_c} - 1\right)\bigg|_{\tau_b > \tau_c} + \sum_{n=1}^{n} \frac{Q_l C_l}{A \, \delta x}$$

4.59

♦ 1D bacterial sources and sink terms associated with non-cohesive sediments

$$\sum \Phi_s = -kC + \alpha_s \frac{C}{SA} \frac{w_s S_{ae}}{S_e}(S_e - S)\bigg|_{S_e < S} + 0.1C_{b0} \cdot \frac{e^{-k_b t}}{A} \cdot \frac{w_s S_{ae}}{S_e}(S_e - S)\bigg|_{S_e > S} + \sum_{n=1}^{n} \frac{Q_l C_l}{A \, \delta x}$$

4.60

where

Q_l = flow rate of lateral inflow, m^3/s;

C_l = bacterial concentration, counts/100ml;

A = wetted cross-sectional area, m^2;

δx = segment length in streamwise direction, m.

4.7.3.3   The combined expression of the sources or sink terms

In an integrated modelling tool such as DIVAST and FASTER, there are multiple sub-models for different modelling processes where both cohesive and non-cohesive sediment sub-model are included. In such a modelling tool the sediments sub-model computation results can be used straight away in its following bacteria transport calculation. In these cases, the combined expression of the source or sink term that is derived based on both the cohesive and non-cohesive sediment results can be written as:

In 2-D model

$$\sum \Phi_s = -KC - \alpha_s \frac{Q_{dep}}{S}C + 0.1 * Q_{ero}C_b + \sum_{n=1}^{n} \frac{Q_o C_o}{A_o H}$$

4.61

In 1-D model

$$\sum \Phi_s = -KC - \alpha_s \frac{Q_{dep}}{S} C + 0.1 * Q_{ero} C_b + \sum_{n=1}^{n} \frac{Q_l C_l}{A \, \delta x} \qquad 4.62$$

where

Q_{dep} = predicted total deposited SS rate that includes both non-cohesive and cohesive sediments, $kg/m^3/s$;

Q_{ero} = predicted total suspended sediments from bed that include both non-cohesive and cohesive sediments, $kg/m^3/s$;

S = suspended solid concentration for both coarse and fine particles, kg/m^3;

C = bacteria counts in water column, counts/100ml;

C_b = bacteria counts on bed sediments, counts/gm;

The constant 0.1 is the coefficient for the unit change.

4.8   Summary

This chapter describes the concept model of enteric bacteria transport in natural waters and based on this, the theory of enteric bacteria transport modelling associated with sediment transport is introduced. The new mathematical equations applied in this enteric bacteria transport modelling are derived from the concept model, which are equations 4.43-4.53. The sources and sink terms represented in the standard 2D and 1D governing equations are generated, in equations 4.57-4.62.

In section 4.6.3, it is conducted that the settling coefficient (k_s =V_d/H) used in past studies (in equation 2.18, after Canale et al., 1993 and equation 4.2, after Droste, 1997) is only a specific case for representing the idealised, uniform size particles settling in static water.

Chapter 5

INTEGRATION OF SIMULATION MODELS

As we move into the new millennium we have begun to realise that science or research is being used in solving problems of global importance. Hydroinformatics software tool is a kind of modelling system developed by integrating the state of the art of information technology with the specific methods used in the water-related engineering disciplines to face the high level of complexity of water problems worldwide.

The integrated simulation model to be developed in the present study belongs to this kind of hydroinformatics tool, which is capable of predicting water elevations, velocities, cohesive and non-cohesive sediment concentration distributions, and the bacterial contaminations associated with suspended sediments. The model comprises modules for hydrodynamic modelling, bacterial transport modelling, cohesive sediment transport modelling, non-cohesive sediment transport modelling, and bacterial decay and transformation modelling. It also provides data storage tools and output reporting facilities. In this modelling system, the integration between disparate modules is implemented by using object-oriented design methods and in this chapter particular emphasis is placed on the construction of the object-oriented multi-process modelling tool.

5.1 Object Oriented Design

Object oriented design is a method encompassing the processes of object-oriented decomposing (Booch, 1994). During the process of object oriented design, the complexity of a system is decomposed into a number of objects which are instantiated from their corresponding classes. An object, as defined by Booch (1994), is a tangible entity which exhibits some well defined behaviour, and a class is a set of objects that share a common structure and a common behaviour. Object oriented design is being widely applied in computer software engineering to implement complex codes which possess good maintainability, reusability and extensibility (Qiang, 2000). This technique makes it possible for complex environmental problems to be solved by large team work from disparate sources. Also, re-use of existing models and their reliability in new software development can greatly reduce the cost of a project and provide benefits in terms of working/research efficiency. Object oriented methodology provides the foundation for building integrated modelling software tools. This is done by applying an object oriented framework equipped with advanced numerical computation modules and the state of the art data handling tools. The simulation model developed in this study has its object oriented structure detailed in the following section.

5.2 Structure of the Simulation Model

With object oriented design, after analysis of the complex water modelling processes system, the simulation model is first decomposed into two major parts: 1-D model and 2-D model. Each contains different modelling facilities which are named submodels, such as hydrodynamic submodel, bacteriological decay submodel etc. These submodels are classes abstracted from their individual modules (objects). Then relationships are built up among these classes and objects. Fortran 90 is the programming language for writing the numerical computation components with parallel implementation of Visual Basic 6.0. These programming languages present the objects linking and provide submodels with Graphical User Interface (GUI) to make the model friendly facing the outside communication.

The structure of the objectives in this model system is presented in Figure 5.1. The submodels are tested separately before they are integrated into the simulation model system, which has the capability of handling the input data. The modelling objectives are the job targets that the modeller wants to perform. To perform different modelling processes, selected submodels should be executed. For example, when carrying out hydrodynamic modelling only the hydrodynamic submodel is executed. The other modelling processes need two or more submodels to be run (as shown in figure 5.1). When performing "decay with SS" bacterial modelling six submodels need to be executed
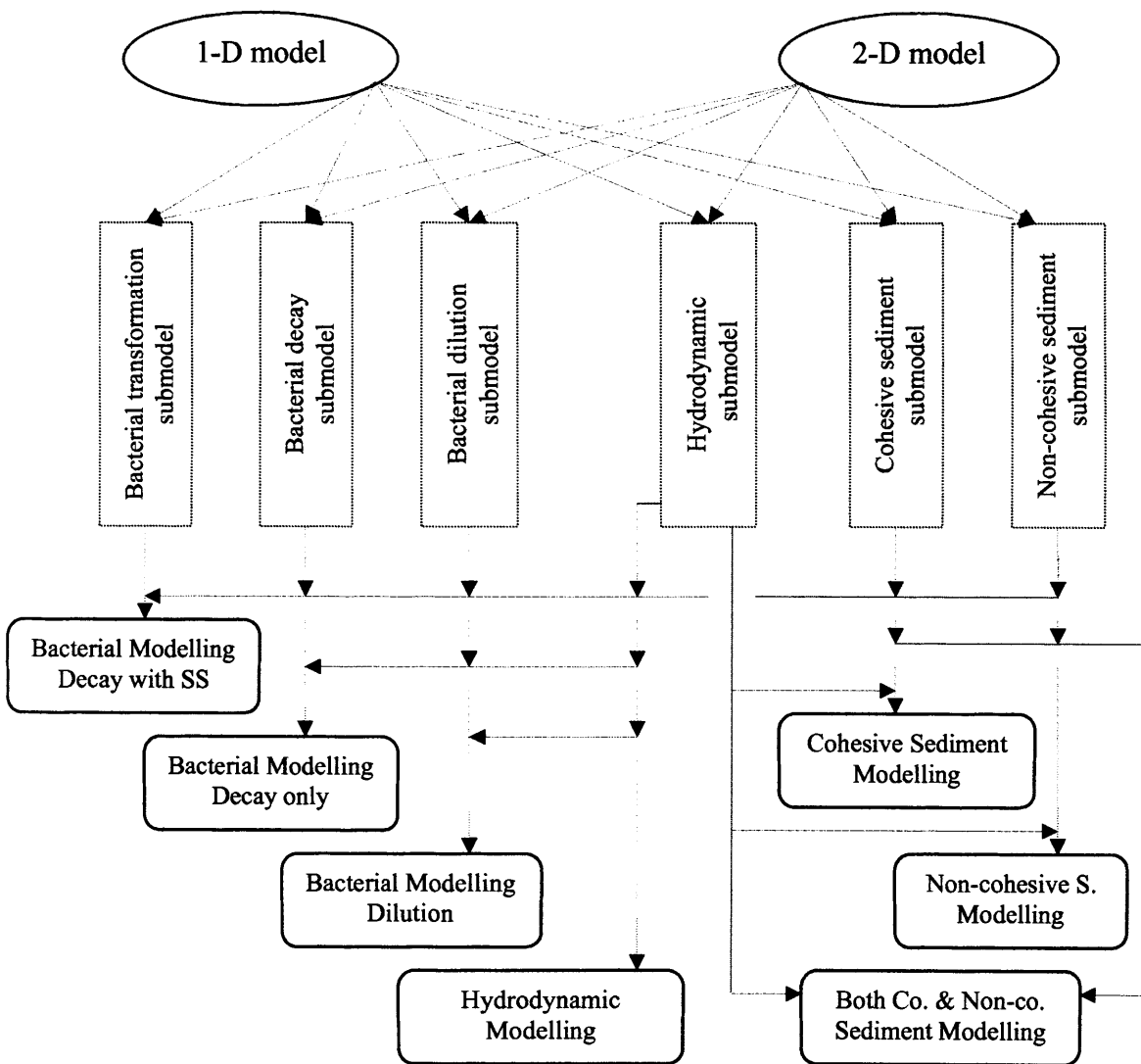
Figure 5.1   Structure of objectives in the simulation model

in turn. Output data can be easily retrieved after the running is finished. The output module is separately defined, which has the user-controlled dimensions corresponding to the modelling objectives for handling the relative output data.

♦ Hydrodynamic submodel

The hydrodynamic submodel solves for flows, which are unsteady, non-uniform, turbulent flow with the consideration of bottom friction, wind shear and the earth's rotation in 2-D part. There are two hydrodynamic submodels contained in each of the 1-D and 2-D part respectively. For 1-D part the submodel is based on the solution of the St. Venant equations for mass and momentum conservation (equation 3.10 and 3.11), solving for a well-mixed river or estuarine system with an arbitrary cross-section.

In the 2-D part the submodel is based on the standard 2-D governing equations consisting the momentum and continuity equation (equation 3.1-3.3), solving for a well-mixed horizontal, unsteady flow such as the shallow water body in estuarine and coastal area.

The hydrodynamic submodels are used to compute the tidal flow for tidal water elevation, speed and direction of the tidal currents in 2-D and 1-D areas. These hydrodynamic modelling results when presented graphically can have the water elevation contour and the current field drawing.

♦ Cohesive sediment submodel

Cohesive sediment submodel solve for the cohesive sediment transport fluxes, which is based on the governing equation of the advective-diffusion equation 3.13 (for 2-D part) or equation 3.14 (for 1-D part) with the sources and sink terms represented in equation 4.13.

This submodel contains separate erosion and deposition modules. The erosion module represents the independent resuspension process described in the equation 4.14; and the deposition module represents the settling process described in the equation 4.28.

Same as having two hydrodynamic submodels there are also two submodels sited in each of the 1-D and 2-D parts respectively for the cohesive sediment computation in the different flow fields. As shown in equation 3.13 and 3.14, the flow velocity and water

depth are requested to perform the ADE computation so the hydrodynamic submodel is executed before any indicators are calculated.

♦ Non-cohesive sediment submodel

Non-cohesive sediment submodel solves for the non-cohesive sediment transport fluxes, which is based on the governing equation of the advective-diffusion equation 3.13 (for 2-D part) or equation 3.14 (for 1-D part) with the sources and sink terms represented in the net erosion or deposition equation 4.31.

For non-cohesive sediment study it is regarded that the deposition and erosion could happen simultaneously and the net movement will be net erosion or net deposition or the equilibrium balance of a net zero sediment transport between the water column and the bottom.

♦ Bacterial dilution submodel

The dilution submodels solve for the bacterial transport with pure advective/diffusion effect. It is based on the standard governing equation of the advective diffusion equation (equation 4.54 in 2-D submodel or equation 4.56 in 1-D submodel) except setting a zero decay rate for the sources and sink terms.

♦ Bacterial decay submodel

The decay submodel solves for the bacterial concentration levels in water under the first order decay model (equation 4.1). In this submodel the specific decay rate, k, is modified as a function of SS concentration. So the sediment predictions must be executed before running decay submodel in this modelling system.

Empirical T90-SS equations are obtained from experiments conducted under a certain sunlight radiation (I*) in Lab-scale, representing separately under dark and light conditions. These equations will be detailed in chapter 6.

For bacterial decay modelling, the dilution submodel needs to be connected with the decay submodel in both 1-D and 2-D regions.

♦ **Bacterial transformation submodel**

This submodel solves for the bacterial transformation to simulate bacterial concentration levels which are associated with the sediment transport, representing the bacterial resuspension and deposition processes due to the movement of suspended sediments in the water system.

In this submodel bacteria are assumed to be attached bacteria which are absorbed onto the surface of the suspended sediments. Numerical solution is applied to equation 4.39 to carry out the bacterial resuspension computation; and applied to equation 4.41 to carry out the bacterial deposition computation. Both cohesive and non-cohesive sediments can be counted into the suspended sediments concentration levels.

5.3 Dimension of the Simulation Model

When modelling a large water resource system, the modelling domain often covers areas of different physical natures, e.g. large water basin with 3-D or 2-D flow structures and narrow meandering cannels with 1-D flow structure. If a 1-D model is used for the whole system, it would be incapable of predicting the lateral and vertical variations of the hydrodynamic as well as morphological characteristics. If a 3-D model is used for the system, it would fit the system's physical nature by dividing the modelling domain into different grid size systems. However, as the computer's speed has its limits the running of a 3-D model in large water resource system would be unacceptably slow, thus it would sometimes be too expensive to be applied to practical engineering projects. If a 2-D model is used in such cases, a very fine grid system is often needed for modelling narrow meandering channels which could dramatically increase the computing burden as well.

Therefore for many engineering problems, the optimal choice of the numerical model for hydrodynamic research and engineering design should be a mixed-dimensional model. The concept of applying the mixed-dimensional model to study an entire large water system is a logical compromise, and should be most cost-effective.

In this study, the simulation model combines two compartments: a 1-D cross-section area averaged model for carrying predictions in river systems which is capable of accounting

for the effects of highly irregular cross-section configurations and a 2-D depth-averaged model to perform predictions in shallow coastal and estuarine waters with horizontal hydrodynamic characteristics by using an overlapping area which covers both 1-D and 2-D area in the connecting area between 1-D and 2-D domain, so it is called a dynamically linked 1-D and 2-D modelling software tool. This overlapping area is used to explicitly exchange the data between the 2-D and 1-D models for providing boundary conditions for each other.

The dynamically linked 1-D and 2-D modelling system runs firstly on the 2-D model area from downstream open boundary to upstream open boundary at the starting position of the high water level at seaward boundary. For the first half time step the x-direction velocity and water level are computed and then the second half time step, the y-direction velocity and water level are computed. The computed velocity and water level at the border of the linked area provides the lower boundary water level for the 1-D model. During the 1-D modelling process, the new produced discharge at another border of the linked area will be used as the upper boundary data to 2-D model in next time step. The contaminants calculations are then followed after the hydrodynamic modelling procedure.

5.4 Maintenances in the Simulation Model

The linked 1-D and 2-D modelling system is developed based on the research group's existing two models: the 2-D modelling tool – DIVAST and the 1-D modelling tool – FASTER, which are models thoroughly tested in the previous studies (Falconer, 1986; Falconer and Chen, 1991; Lin and Falconer, 1997; Wu et al., 1999; Kashefipour and Falconer 1999; Lin et al., 2001; Yang et al., 2002, etc). Therefore the programming task for the development of this simulation model includes developing new modules and refining the existing modules. Except the bacteria transformation submodel, the most of the programming work is the maintenance of the existing modules. Some of the major maintenances are listed below.

5.4.1   Using FORTRAN 90

DIVAST model was originally written in Fortran 77. In this study it has been upgraded to Fortran 90, because Fortran 90 contains some features of object-oriented programming

languages with user defined generic data type, pointer and modules, which provide a much better linkage with Visual Basic interfaces than Fortran 77.

5.4.2 Improved data handling objects

In Fortran 77 the *dimension* of an array and also the *subscript bound* for each *dimension* have to be declared in the *common* statements in programs. So Fortran 77 only provides the static storage, which is created at the beginning of program execution, to be taken as a fixed memory space.

In general hydraulic computation mostly deals with huge amount of time series data by using at least 2 dimension arrays for tracing the data. So the fixed-bound arrays declared in Fortran 77 will either waste machine's memory space by declaring too large space at the beginning of running or restrict the model's application by producing error if the array bounds are exceeded.

Fortran 90 offers Allocatable arrays to implement the especially useful user-defined feature, which avoids the waste of memory space and the limited array bound and dimensions. In the new version of DIVAST, the previous fixed-dimension arrays declared in the previous *common* file for handling domain's boundary data and outfalls data have been replaced with Fortran 90 Allocatable arrays located in the array modules, which produce a dynamic storage in machine memory when the array is called by the user during the model simulation.

The dynamic data handling objects enable the new version of DIVAST to automatically fulfil any computation challenge under all different boundary conditions and different situation of outfall disposals with no restricted limits.

5.4.3 Data interpolation methods

For solving the numerical equations the appropriate boundary conditions are always required by interpolating collected relative series of water level, flow discharge, velocity or solute concentration data.

The simplest piecewise linear interpolation is used for interpolating the concentration input data. The disadvantage of linear function approximation is that at each of the

endpoints of the subintervals there is no assurance of differentiability, which, in a geometrical context, means that the interpolating function is not "smooth" at these points. It is clear that such a smoothness condition is not suitable for interpolating some data e.g. the water level data at seaward boundary. An alternative method mostly suitable for the water level change is the cubic spline interpolation.

Therefore in this new version of DIVAST, both linear and cubic spline interpolation methods are used and they are built in separate linear and cubic spline interpolating modules.

5.4.4 Other improvements over the previous version

Comparing with the previous versions of FASTER and DIVAST, the linked model including both 1-D and 2-D parts has been made with some programming improvements to reduce the computational time and save machine's memory space. Apart from the those mentioned above, special effort was made to improve the efficiencies of the computation process on machine. Some of the main improvements are as follows:

◆ The counting method for recording the order of the solutes computation

In the previous versions of FASTER and DIVAST, when some solutes transport simulations were carried out it was always needed to count the order of the solutes computation by counting a number NS (NS=NS+1) and the counting was repeatedly placed in the program for running program, searching information, storing and retrieving data. The statement of NS=NS+1 was written so many times throughout the program, which appeared in hundreds of lines in the previous version.

In the new version, counting variables NNSED, NNCHS, NNSAL, NNTEM, NNTCL, NNFCL, NNFST...etc. have been used to record the solute calculation order for both 1-D and 2-D models. The counting of NS=NS+1 is only needed once at the beginning of the simulation and immediately the counting variables followed are given the correspondent specific number for recording the order, then the counting variable can be used afterwards whenever the solute order is needed to be indicated. Therefore any tasks during the programming such as recording array's values, searching boundary data, performing relative calculations and importing results can be accurately pointed to the correct components by using these counting variables. This counting change not only reduced

hundreds of lines in the program but also avoided possible human errors caused by the repeating of one statement.

◆ **The Tecplot output subroutine**

The new subroutine offers dynamic multi-solute printout with only 50 lines in the program, comparing with the previous subroutine which had 210 lines in the program but could only import printout for one type of solute.

The dynamic multi-solute printout is produced as a file with the extension of ".PLT" under the format requested by the Tecplot software. By opening Tecplot, the multi-solute printout can be easily switched to any of the contents, as the water level, the bed elevation, the sediments concentration and the bacteria population etc. and so presented graphically in the Tecplot drawing.

5.5 Interface Development

Over the past four decades, numerical models have been widely used in all aspects of environmental science and engineering, particularly in the hydro-environmental fields. The rapid increase in the speed and memory of modern personal computers and the development of advanced numerical methods for solving the governing equations more efficiently and accurately have made such modelling tools ideal for solving practical problems in environmental water management to assess water quality in aquatic basins by combing the computational hydraulics and hydrology with bio-chemical processes (e.g. Thomann, 1972; Abbott, 1979; Brebbia and Ferrante, 1983). These developments in this field have led to the establishment of a new research discipline that integrates computational hydraulics, hydrology and water quality with modern computing technology, namely, hydroinformatics. Hydroinformatics is about making better and more appropriate use of advanced information technology to improve the level of technology in water science and engineering (Abbott 1999). It offers computational hydraulics a modern way of presentation by introducing object-oriented methodology to create integrated modelling tools and by using Graphical User Interfaces (GUIs) to

provide an understandable and friendly usage of numerical models for both hydraulic experts and non-specialist users.

As mentioned previously, the FASTER and DIVAST program were originally written in FORTRAN language and run their estimations under the MS-DOS system. In this study the upgrading of the numerical models to become the state-of-the-art hydroinformatics tool has been made by introducing the object-oriented framework to create integrated modelling tool and by adding the easy to use graphical user interfaces. The interface design methods encompass a vast array of visual and physical methods to allow data to be transferred with ease over the shortest possible period of time. It is known that graphical user interface is a dominant tool for exchanging information between computers and people in modern IT. Good user interface can make work much more enjoyable for the user and therefore increasing their productivity due to positive work attitude. Also the GUIs provide the users an easy operation of the data input and output and also an easy control of the modelling processes.

5.5.1   Visual Basic 6.0 programming language

Visual Basic is one of the fourth generation language tools that enable the creation of a graphical user interface much easier. To write Windows programs using Visual Basic is mostly by dragging and dropping graphic objects onto the screen from a toolbox that houses those objects. The program that you build looks the same as the program your users see when they run the program from Windows. Visual Basic is much more than just such a Windows programming language. It is an object oriented programming language. In Visual Basic "control objects" is used to give the best-looking interface to the application that is under building and "code objects" can be created to perform specific tasks to handle data or combine independent model objects (Schneider, 1999). Visual Basic is also a very powerful programming language as it reduces the amount of code which is required to form the interface structure, allowing more time to be spent on how the interface looks and functions. Originally only large specialist software could produce these, due to the large sums of capital investment needed to develop software. However these new languages, such as Visual Basic or Visual C++ etc are allowing more people to program and more successfully, opening up the field of user interfaces to a larger market (Jerke, 1999, McKinney, 1997).

Visual Basic is an enjoyable language. One major advantage with Visual Basic is the way it allows the programmer to run their program at any time during the design process at the touch of a button. This allows the programmer to pick out any bugs far easier than before to identify any physical or numerical instability. The language also creates an executable file when the program is completed, removing the need to know how to compile programs. With all these and new more powerful commands added to the BASIC language allows Visual Basic to be a very simple programming language which can be picked up very quickly, producing very powerful interfaces.

Visual Basic interfaces contain a wide range of the best-looking controls and pre-designed forms which are common to the window-based programmes used today, e.g. Microsoft Word, Excel etc. It is familiar for user to go from one program to another. These interfaces give a considerable amount of convenient operation features, such as tool-tips, popped-up menu, help menu etc, to guide user any specific requirement for data input.

Visual Basic interface design is object orientated. The programmer first designs the visual look of the program then decides what actions each control should respond to and finally writes the code for each action required to be carried out. The programming process of using Visual Basic can be summarised in Figure 5.2.
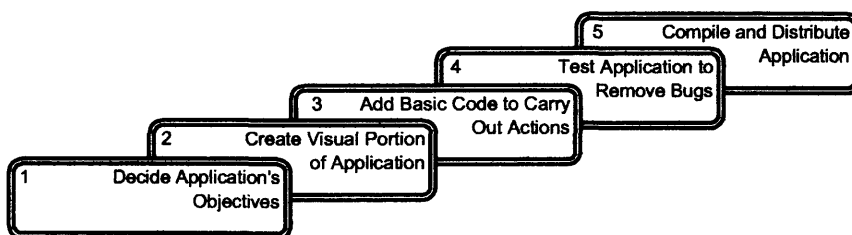
Figure 5.2   Visual Basic Programming Process

The interface development for FASTER model has been published in Journal of Environmental Modelling and Software (Yang et al. 2002) and next section is going to present the DIVAST interfaces.

```
                  ┌─ Geometric Data ──┬── Wet or Dry map
                  │                    └── Bathymetric Data
                  ├─ General Hydraulic parameters
                  ├─ Boundary Data
┌───────────┐     ├─ Outfall Information
│ Data Input│─────┤
└───────────┘     ├─ Solute parameters
                  ├─ Observation Station Data
                  └─ Modelling Process Option

                  ┌─ Hydrodynamic Computation
                  ├─ Sediment Transport Modelling
                  │   ├── Cohesive sediment
┌──────────────┐  │   └── Non-cohesive sediment
│Model Running │──┤
└──────────────┘  ├─ Physical Dilution only modelling
                  ├─ Bacterial Decay Modelling
                  └─ SS Associated Bacterial Decay Modelling

                  ┌─ Calibration at Observation Stations
                  │
┌────────────────────┐ ├─ Plot of 2-D distributions of tidal currents
│Results Presentation│─┤
└────────────────────┘ ├─ Plot of 2-D distributions of water elevations
                  ├─ Plot of 2-D distributions of solute concentrations
                  │
                  └─ Animation Show
```

Figure 5.3   The interface framework of DIVAST

5.5.2   Development of the DIVAST interfaces

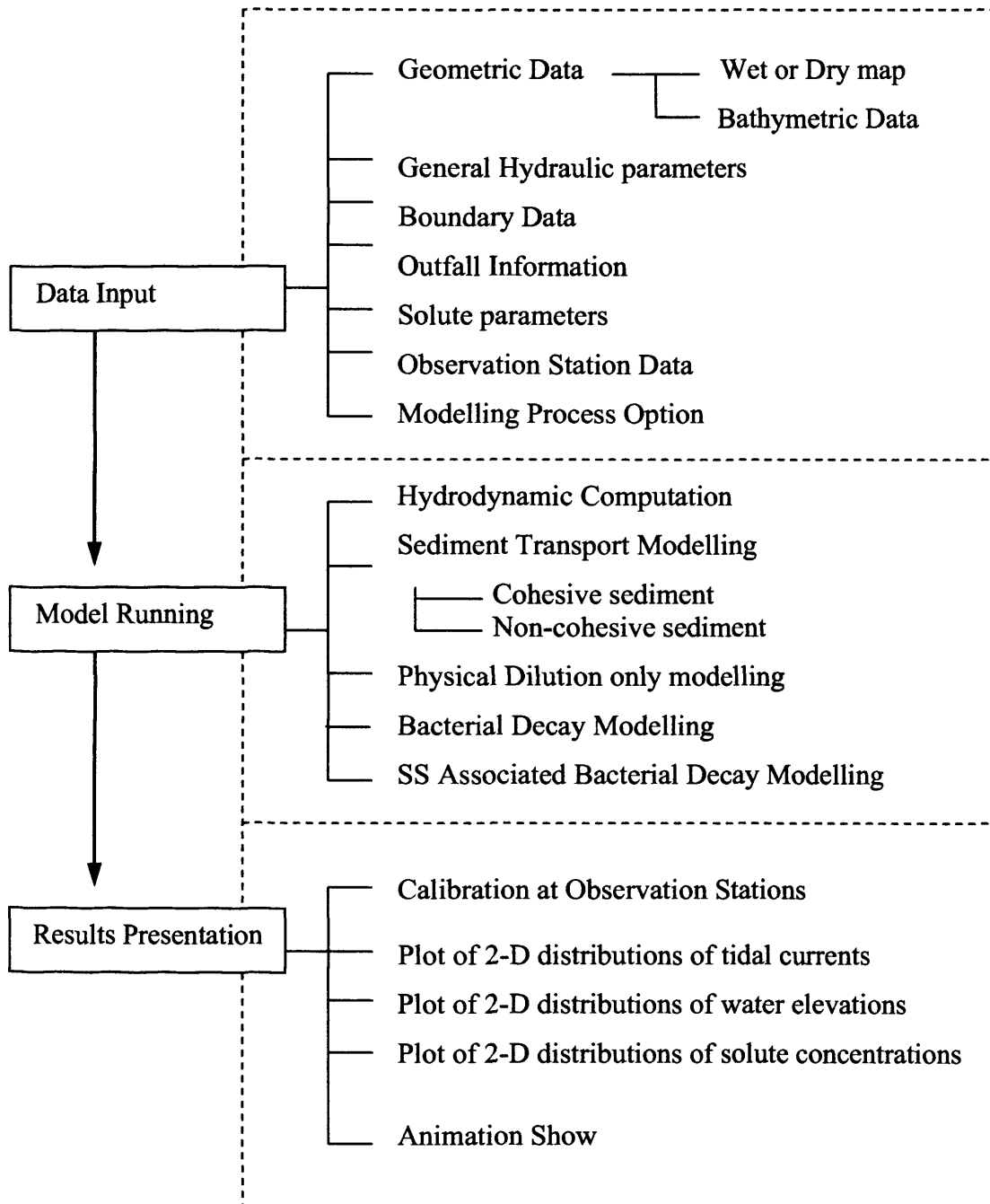The interface design method is object-oriented. The interface framework for the version of DIVAST integrates three main parts which are the data input, the model running and the results presentation. Within every part different interfaces are constructed to facilitate each of their specific functions and these are illustrated in Figure 5.3.

There are a total of 15 interfaces built into the DIVAST model to interconnect or interact with the above mentioned function objectives. The concept of the interface design is to make the interface more usable and flexible, effective and easy to access for information.

Generally speaking, hydrodynamic water quality modelling is data intensive. For the data input part, it includes bathymetric data, boundary data, outfall data, initial conditions and local inputs data etc. For such a huge amount of data inputting, particular formats must be followed when entering the data, however the human inputting mistakes can easily occur. In providing a user-friendly interface for data input, unnecessary human error in the data inputting can be avoided, also time is saved as well as the time cost in the user's needing to learn the particular formats to insert all of the data. The user can easily enter the data through the interface without the need to learn the logical order and formats required for the data to be written in the input data file. The labels, icons and graphics shown on the interface will clearly instruct the user what needs to be done next.

The DIVAST model begins with the interface as illustrated in Figure 5.4, this interface is designed to introduce the model and connect to all the other main windows. Firstly it gives the user the option to choose data input windows from six data input tabs – the **Model Setup** tab, the **Area Map** tab, the **Hydrodynamic Parameters** tab, the **Transport processes** tab, the **Outfall Information** tab, and the **Output Parameter** tab.

Figure 5.5 presents the Model Setup Window for entering general parameters which are the project title, the simulation start and end time, the domain area dry and wet map, the bathymetric data, the grid size and the time step etc. It can be seen that the data are grouped in different frame controls to give the user clear data inputting categories and clear labels. Additional tool-tips also included to assist in entering proper data when some of the input buttons were being clicked.
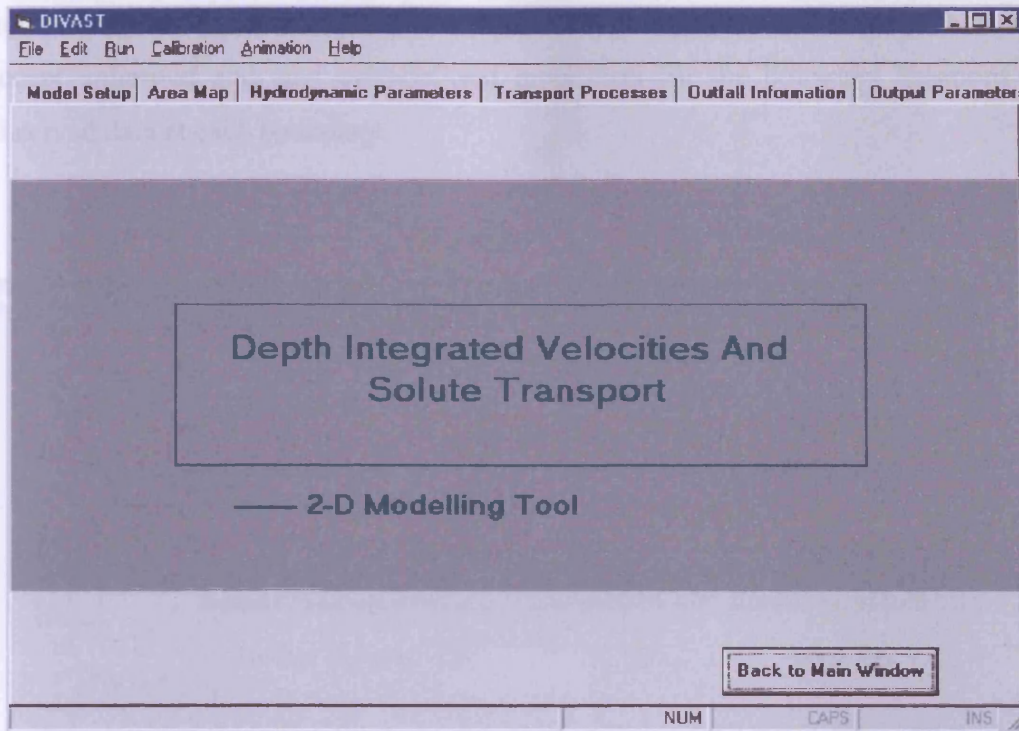
Figure 5.4   Introduction Interface of DIVAST
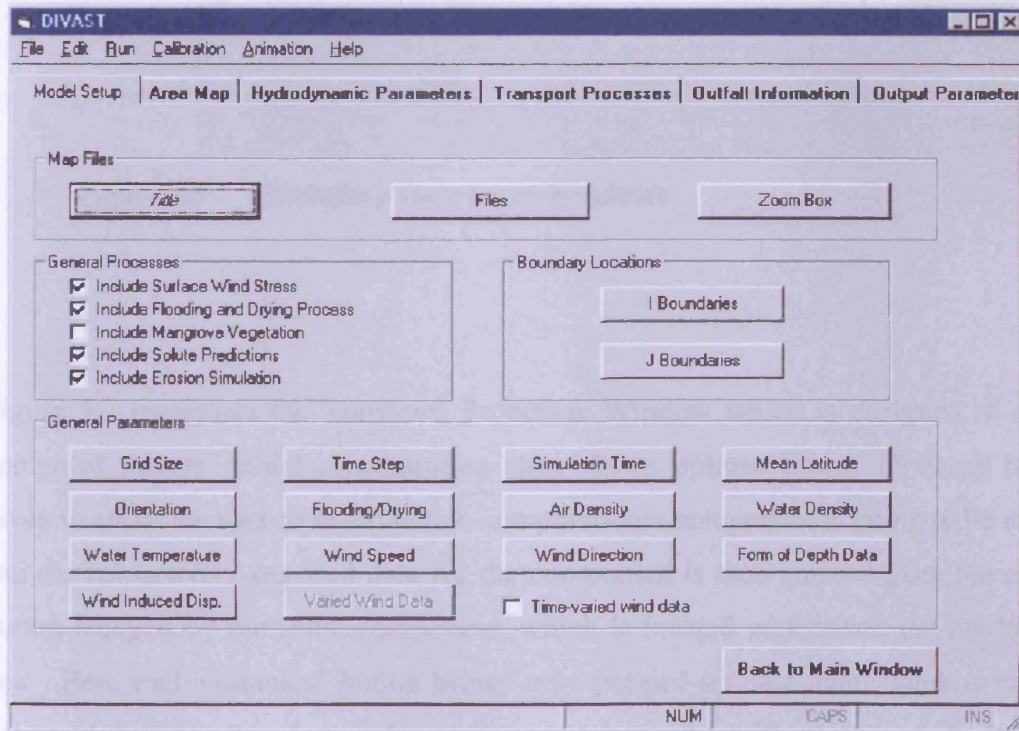

Figure 5.5   Model Setup Window for entering general parameters
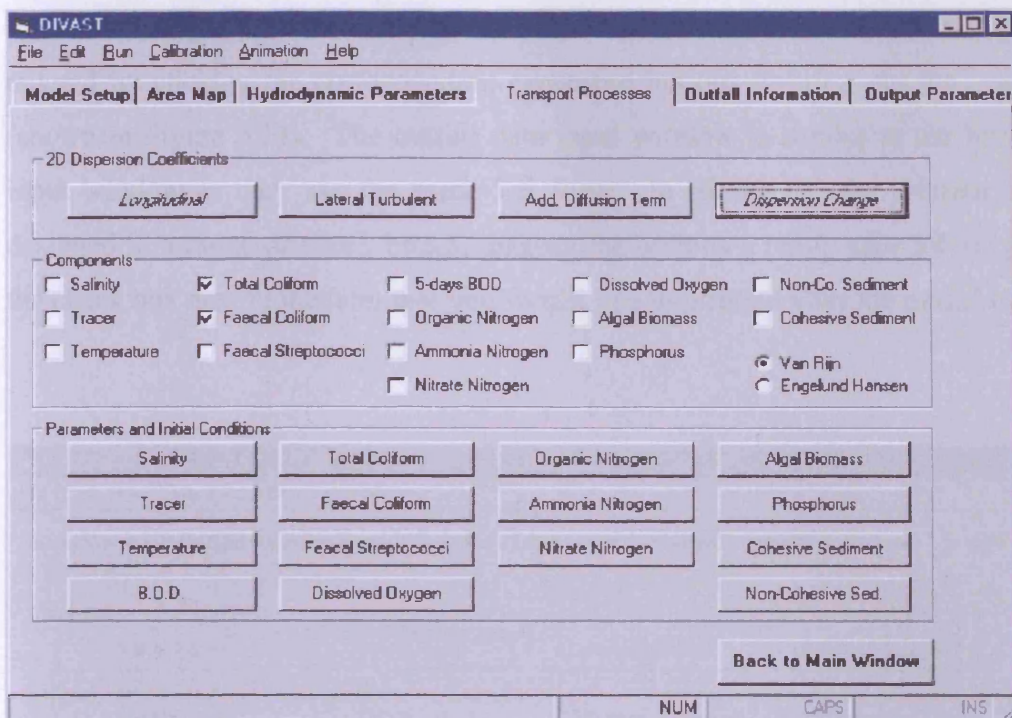
Figure 5.7   Transport Processes Window
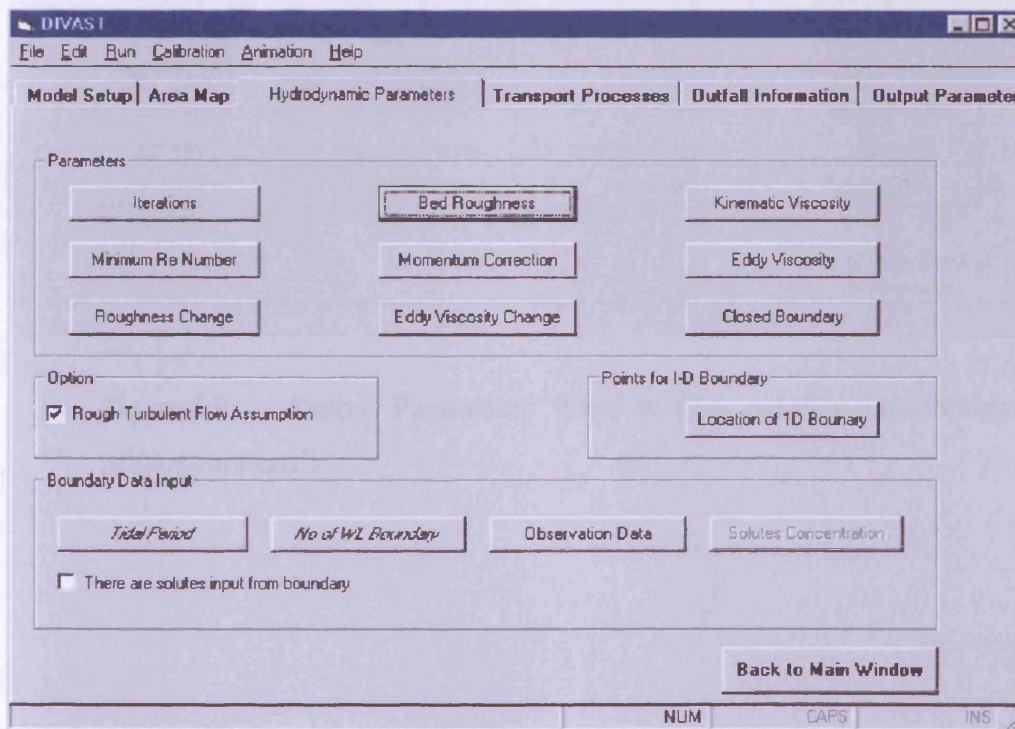
Figure 5.8   Hydrodynamic Parameters Data Input Window

The other three data input windows are presented in Figures 5.8 -5.10 respectively. With the same design idea, from the Outfall Information Window the outfall data can be entered by clicking the correspondent command buttons to bring out the input window (shown in Figure 5.11). The outfall data input window is similar to the boundary data input window as they use the same VB form. In Figure 5.9 the printout options are designed in a range of check boxes, making the options a really easy job by just ticking the check box next to the item that you would like to printout after the model running.
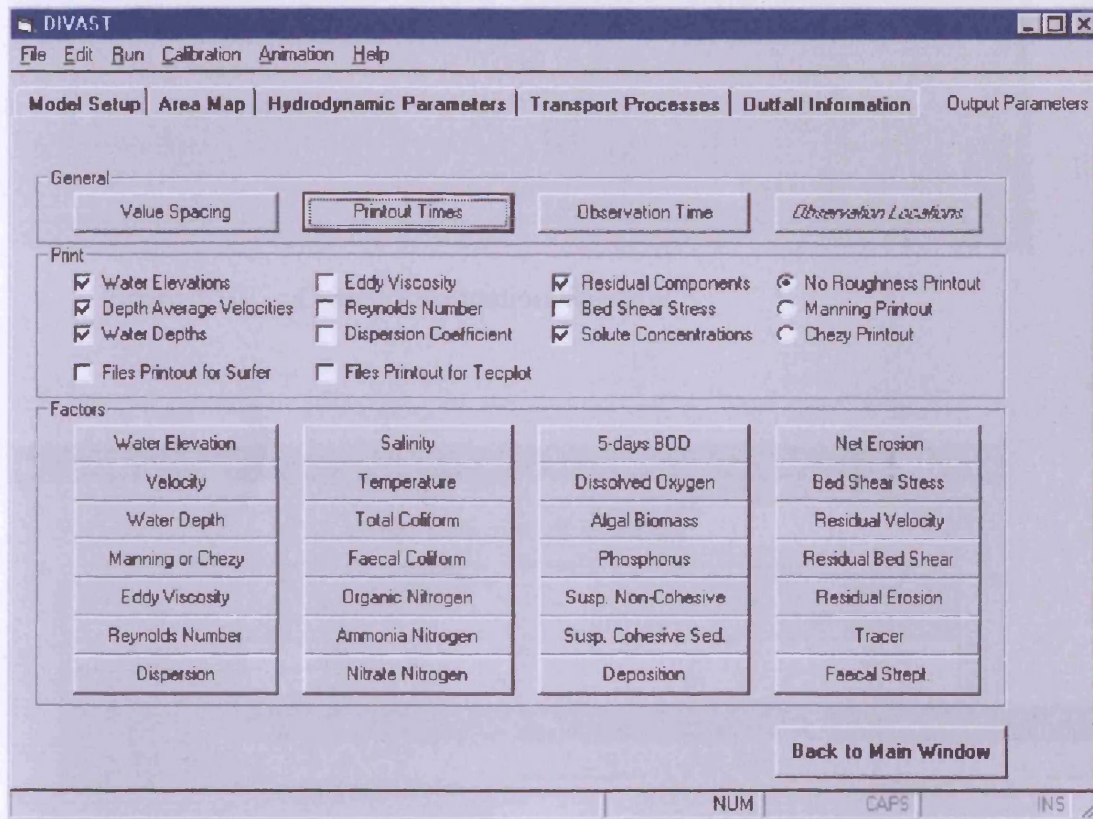
Figure 5.9   Output Parameters Window (For entering information to specify printout options.)
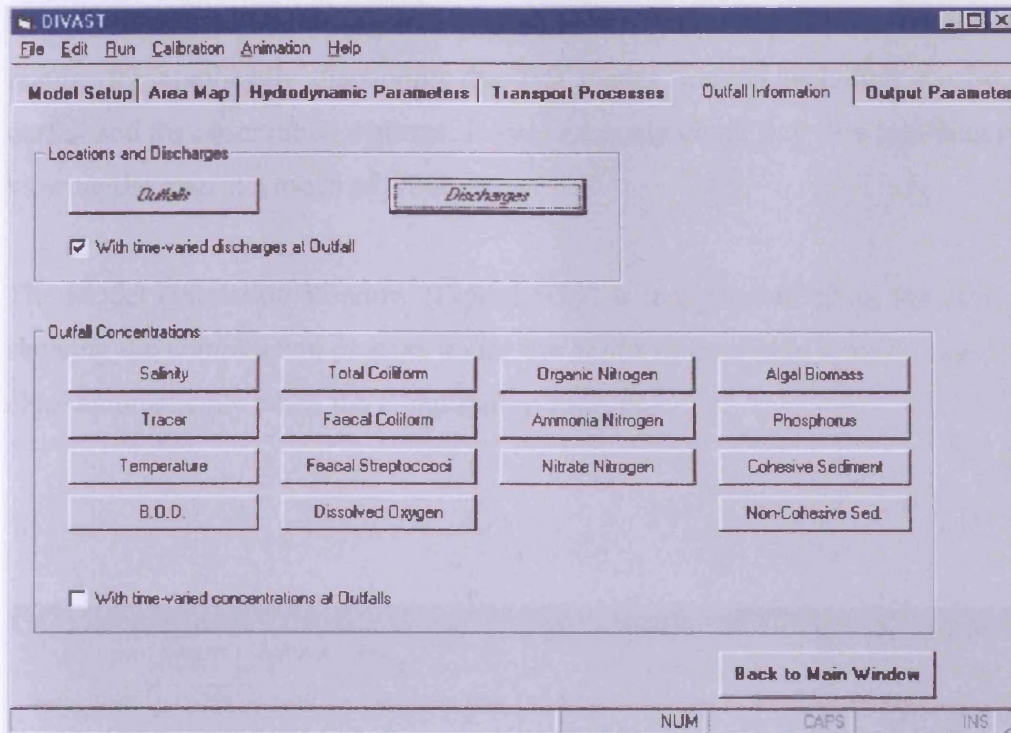
Figure 5.10   Outfall Information Window
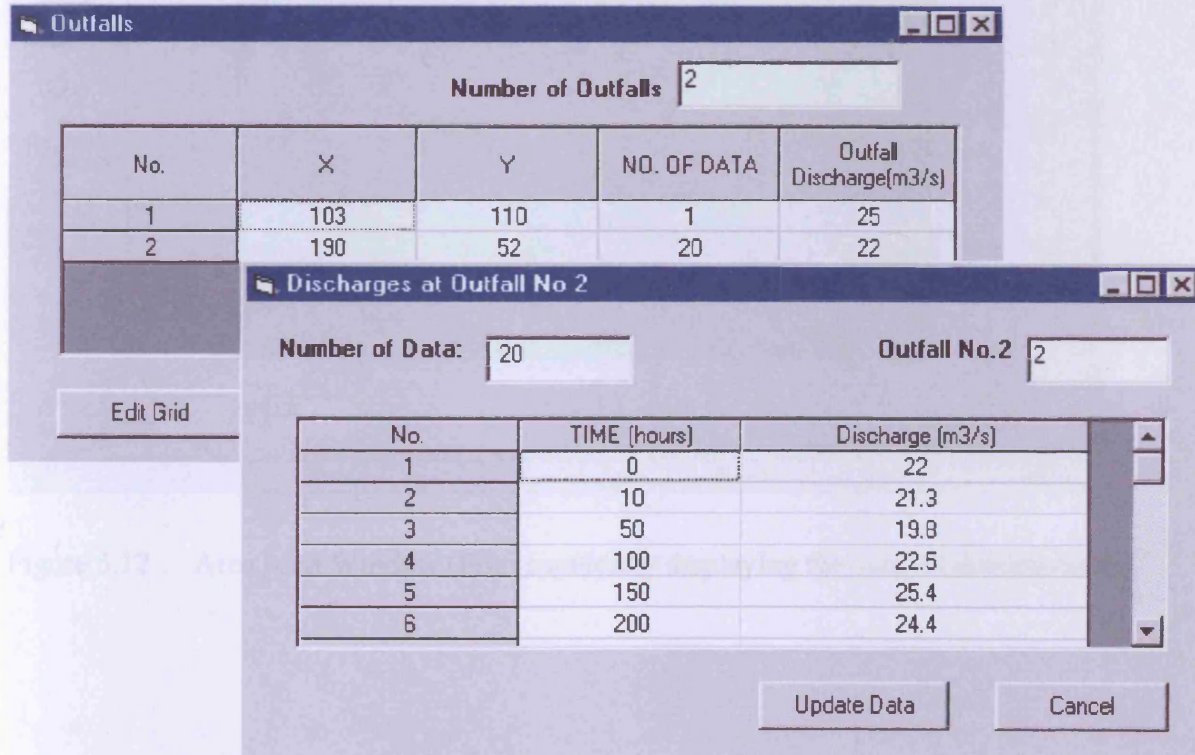
Figure 5.11   Outfall Data Input Windows

In the DIVAST model the Map Area Window (Figure 5.12) is built to facilitate an extra feature for graphically displaying the 2-D model domain including the boundary, the outfall and the observation stations. Users can easily check any data inputting mistakes by viewing the map at a touch of a button.

The Model simulation Window (Figure 5.13) is independent of all the other interfaces, showing the computation process under the MSDOS operation system. The window will close automatically when the computation finishes.
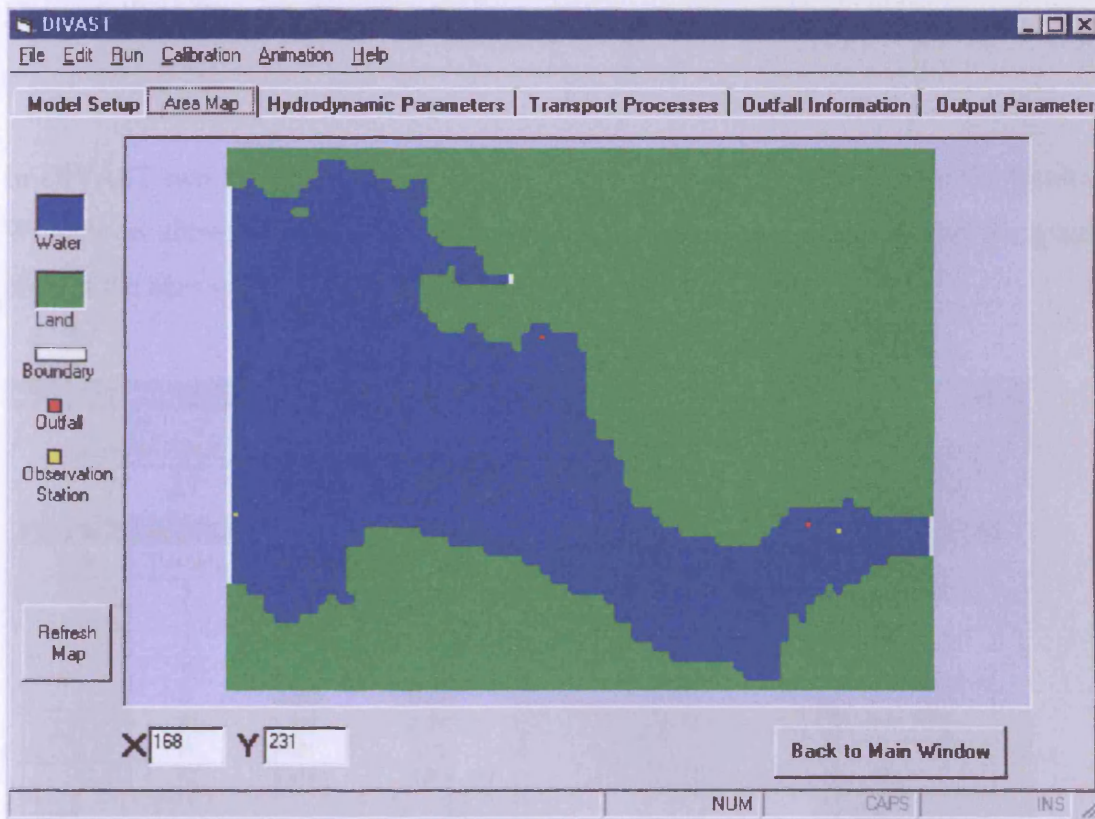
Figure 5.12   Area Map Window (For graphically displaying the entered domain data)
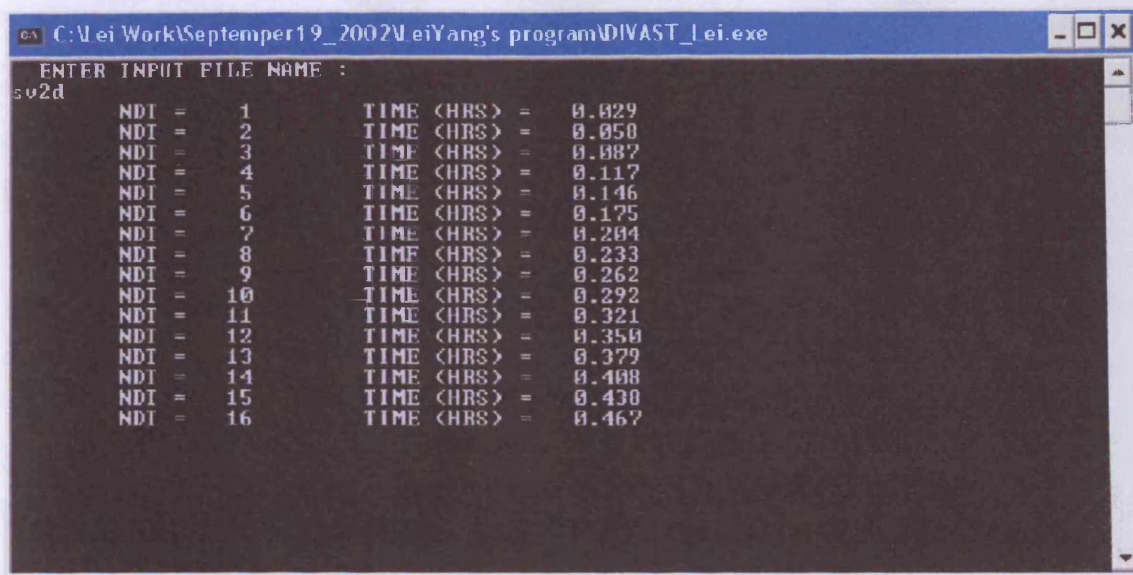
Figure 5.13   Running the program

In DIVAST two kinds of output display interfaces are designed. One is the Calibration Window as shown in Figure 5.14, presenting both the tabular results and the graphical plots at the nominated observation stations.
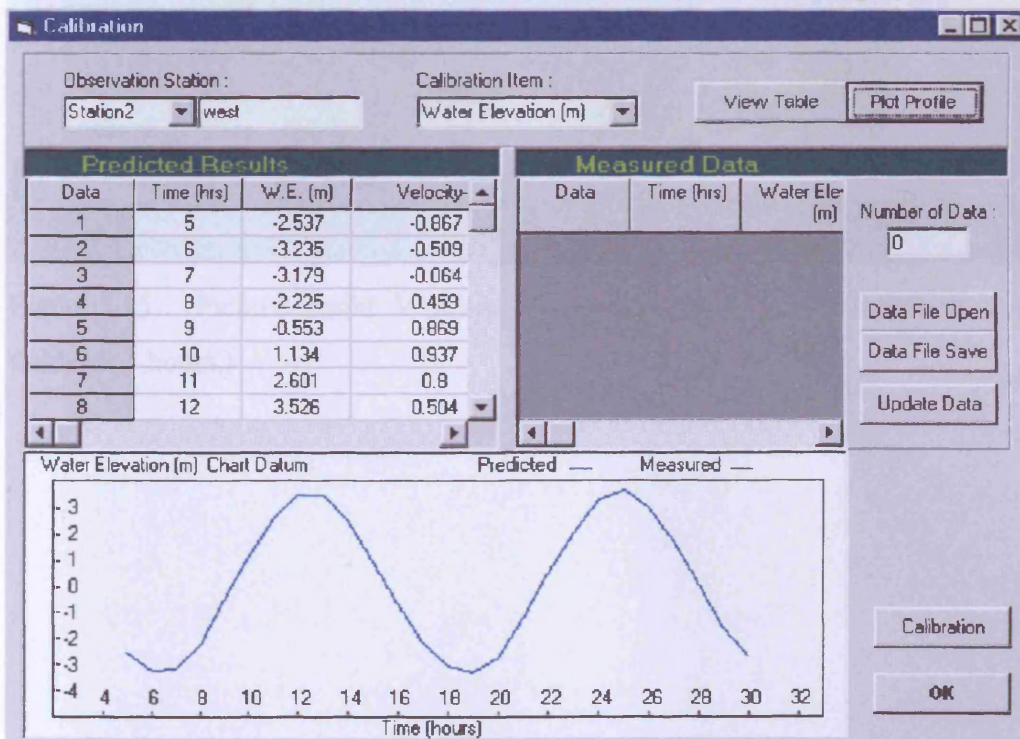
Figure 5.14   Calibration Window

Another is the Picture Building Window (as shown in Figures 5.15 – 5.17), with the arrow distributions showing the 2-D distributions of the current fields and the colour contour map showing the 2-D distributions of the solute concentration within the whole domain at a nominated simulation time.

Animation show is based on the already built Picture Building windows, giving a continuously view of the time series of the simulation results.
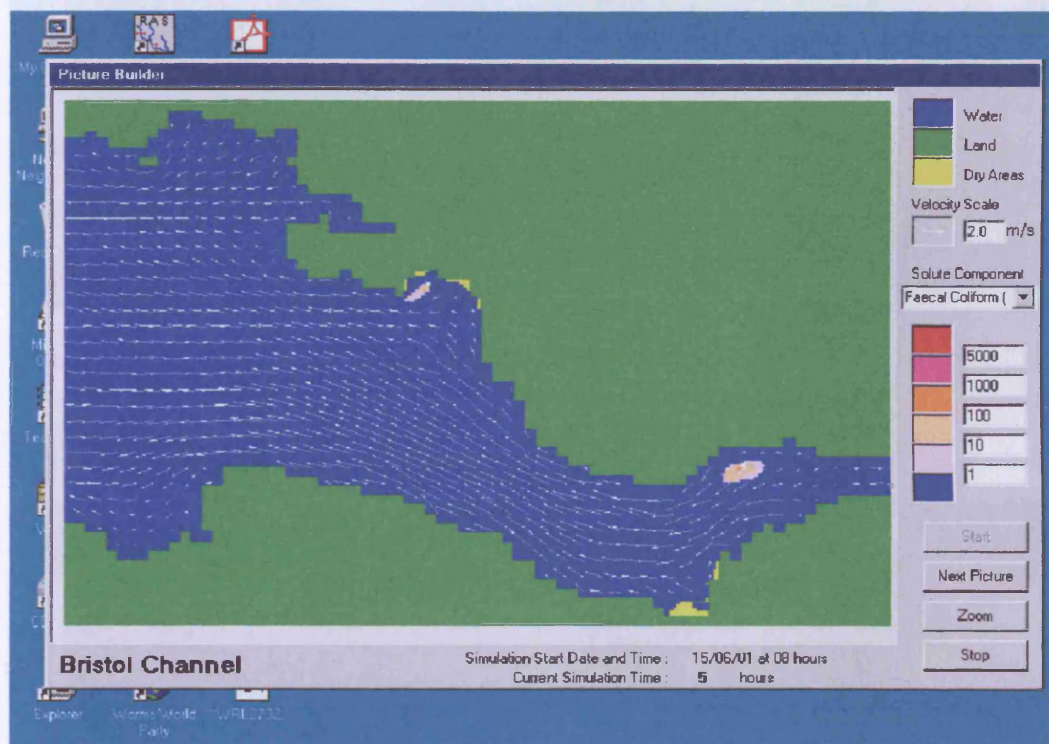
Figure 5.15   Picture Build Window (Showing velocity and coliform concentration fields, at 5 hours.)

Figure 5.16   Picture Building Window (Showing simulation results at 25 hours.)
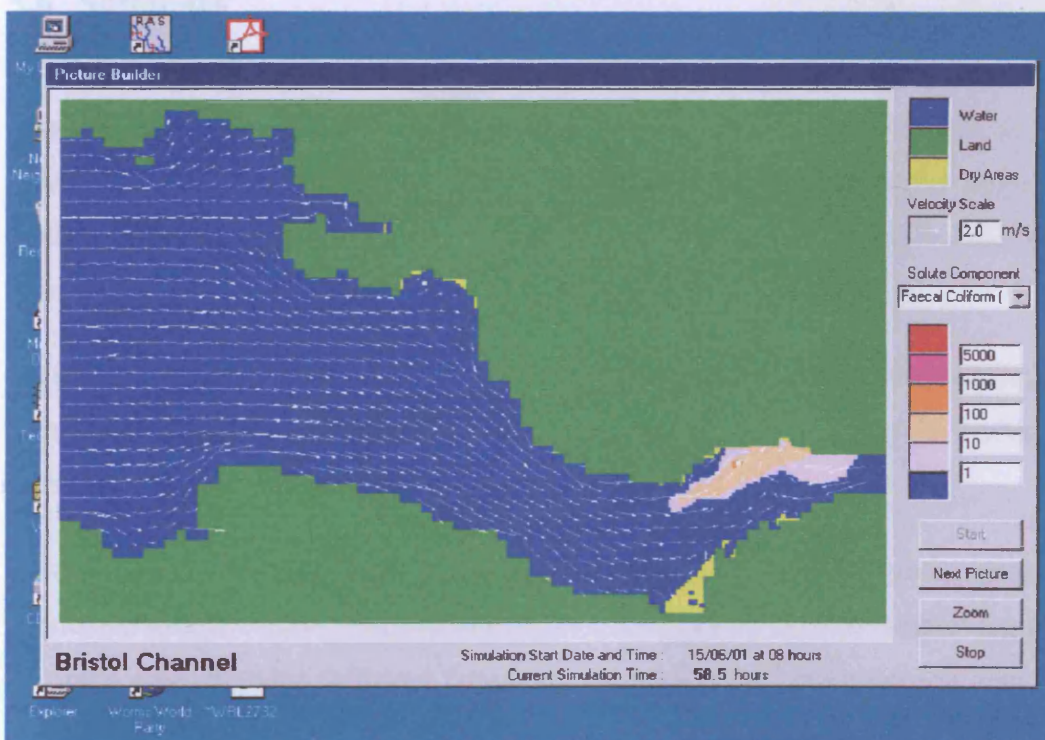
Figure 5.17   Picture Building Window (Showing simulation results at 58.5 hours.)

To summarise, the user-friendly interfaces facilitate the easy use of the software. After entering all the required data through the interfaces, computation of hydrodynamic water quality analysis is performed by clicking a button. The DIVAST interfaces provide the following functions:

- Data entry and edit facilities for: general information, geometric inputs, boundary conditions and outfall data, also the modelling process options and the printout/display options.
- Graphical display of input data.
- Input data file management which is processed from the menu bar.
- Execution of hydrodynamic/sediment transport/water quality computation.
- Tabular report of output data.
- Tabular and graphical reports of calibration results at observation stations.
- Graphical display of computational results and animation show across the whole computation domain.

5.6 Summary

This chapter firstly details the development of the simulation model – the dynamically linked 1-D and 2-D hydroinformatics software tool by employing the object-oriented methodology to integrate both existed and newly developed modules, and this is detailed in sections 5.1 and 5.2.

Section 5.3 describes that the integration of the one-dimension and two-dimension models greatly increases the applicability of the simulation model to a much wider range of problems in real environment.

Section 5.4 addresses the programming maintenance during the integration process of the simulation model. Many enhancements have been made, such as: improving the model accuracy, upgrading the Fortran 77 program language to the latest version, improving the computation speed and saving the memory space to reduce the machine's loads.

Section 5.5 describes how the numerical model is constructed together with the user-friendly interfaces by implementing the Visual Basic 6.0 programming language and the functional objectives of the interfaces. The interfaces' facilities are detailed subsequently.

As far as the hydroinformatics software system is launched, the methodologies of the hydroinformatics enable the numerical modelling to become more practical, more user-controllable and more effective and efficient for decision-making in a wider range of water environmental management issues.

Chapter 6

Model Application to Bristol Channel and Severn Estuary

6.1   Site Description

Bristol Channel and Severn Estuary is located between the coastlines of South Wales and South West England (Figure 6.1). The domain of this study covers a water area up to 15,000 km^2 including a number of bays, rivers and the estuary.

The Bristol Channel is renowned for its strong currents and high tidal range and is a major supply for sand use, so the estuary has very turbid water which transports the load of sediments. This area supports active fishing and tourist industries, a number of large ports and industrial resources. It has been utilised not only for the water-contact recreation and fishery etc but also to receive sewage disposals from the cities on both sides of the estuary also river inputs distributed in its catchment area. There are 29 river inputs with different values of the microbial contaminants and 34 sewage discharges from wastewater treatment works located along the coastal lines on both sides. Moreover many cities situated in its catchment area request the water area to serve for all the water-related activities. All these make the estuary a very complicated situation regarding the microbial contamination.

Therefore for such a complex water environment, the prediction of enteric bacteria contamination has to face the challenge of complexities in the modelling process, to which the integrated simulation model - the dynamically linked 1-D and 2-D hydro-environmental modelling tool - is developed to address.

When microbial pollutants are released into a turbid channel, it is very important to know the behaviour of the pollutants associated with the turbidity as the suspended sediments have a great affinity for bacteria. Thus in this application the focus is the SS linked microbial contamination and enterococci is employed as an indicator.
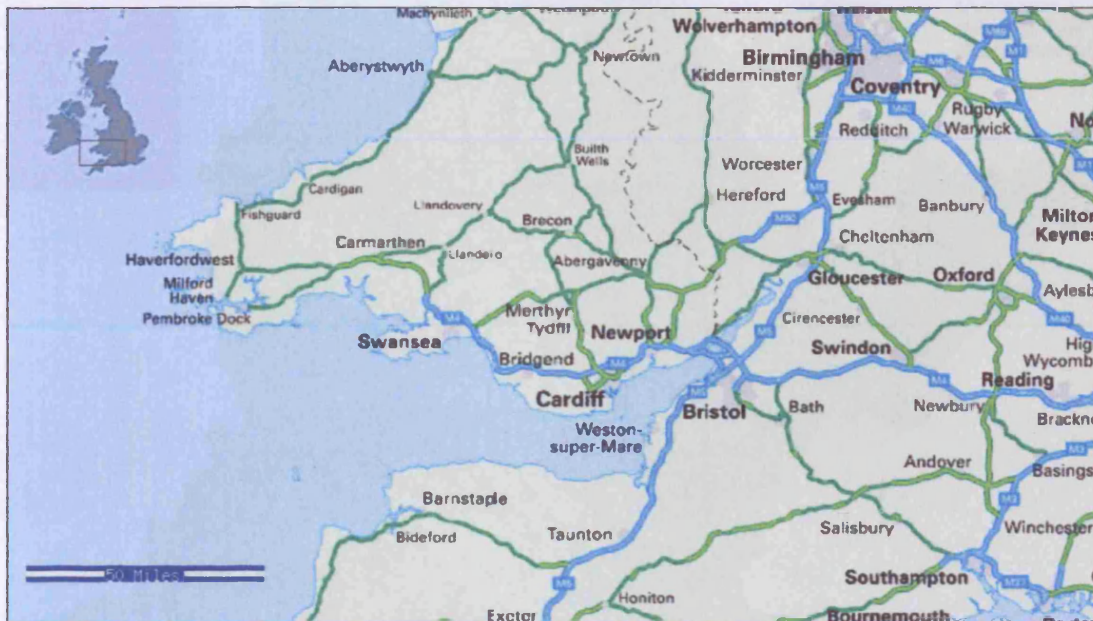

Figure 6.1   The location of Bristol Channel and Severn Estuary

6.1.1   Bathing water compliance locations

The bathing water compliance locations to be investigated are defined in Table 6.1 and shown in Figure 6.2.

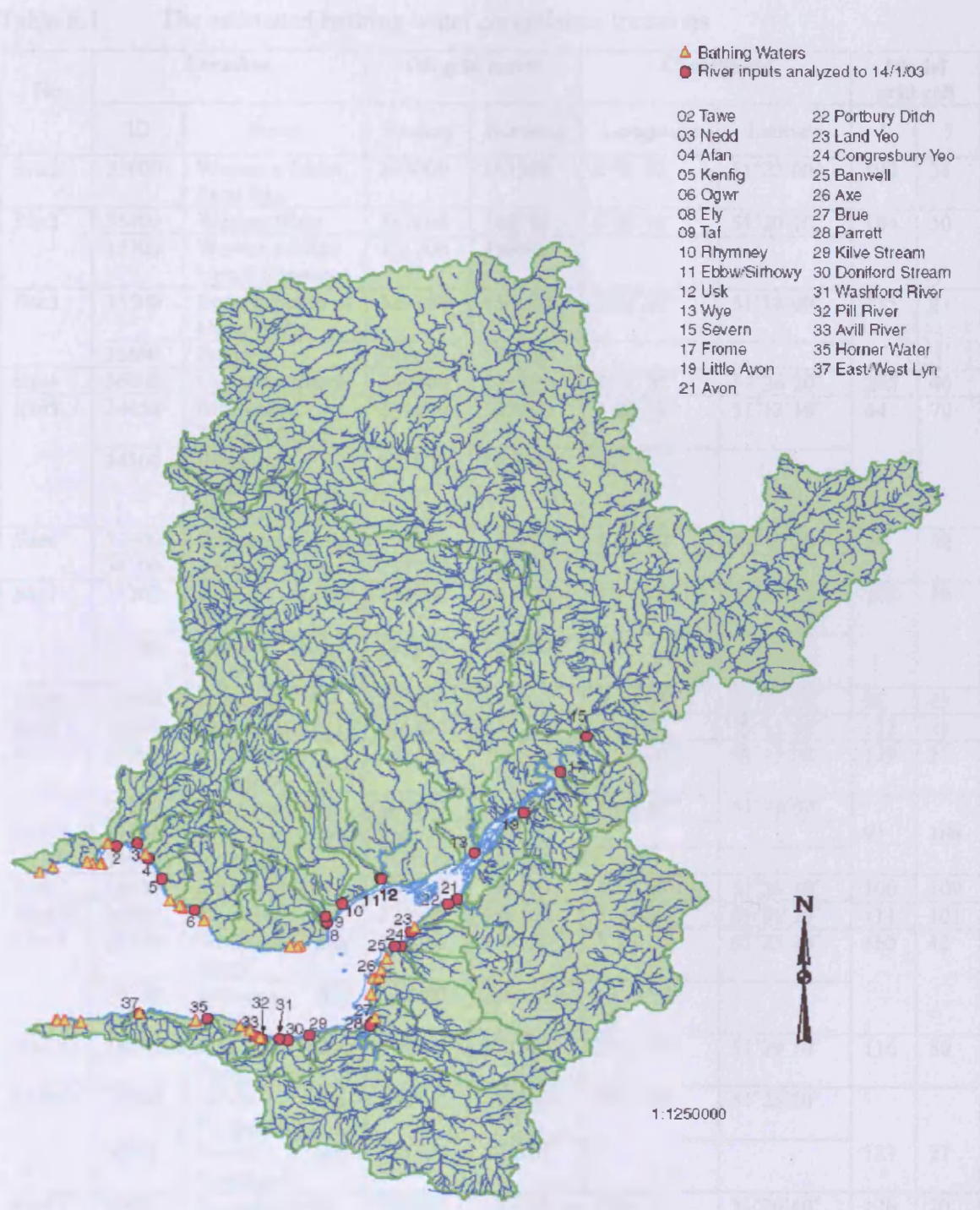Figure 6.2   River inputs and bathing water compliance locations

Table 6.1   The estimated bathing water compliance locations

No	Location		OS grid meter		Coordinate		Model grid cell	
	ID	Beach	Easting	Northing	Longitude	Latitude	I	J
Site1	35900	Weston-s-Mare Sand Bay	333000	163500	2°58'40"	51°22'00"	190	34
Site2	35800	Weston Main	331600	160700	3°00'10"	51°20'20"	184	30
	35700	Weston-s-Mare Uphill Slipway	331200	158800				
Site3	35500	Berrow North of Unity Farm	329300	154500	3°02'20"	51°18'00"	175	21
	35600	Brean	329600	158500				
Site4	36000	Clevedon Beach	339800	171200	2°52'20"	51°26'20"	205	40
Site5	34450	Ilfracombe Tunnels Beach	251450	147800	4°08'10"	51°12'10"	44	70
	34500	Ilfracombe Capstone (Wildersmouth	251820	147900				
Site6	34600	Ilfracombe Hele	253550	147920	4°06'00"	51°12'20"	59	52
	34700	Combe Martin	257720	147320				
Site7	35200	Blue Anchor West	302300	143500	3°24'00"	51°11'30"	140	19
	35100	Dunster North West	299700	145500				
Site8	34800	Lynmouth	272500	149750	3°49'40"	51°14'30"	92	43
Site9	34900	Porlock Weir	286400	147900	3°37'40"	51°13'30"	112	33
Site10	35000	Minehead Terminus	297300	146500	3°29'00"	51°13'00"	129	27
Site11	37200	Langland Bay	260600	187100	4°00'40"	51°33'50"		
	37100	Limeslade Bay	262500	187000			91	104
	37000	Bracelet Bay	263000	187100				
Site12	36900	Swansea Bay	264400	192100	3°57'20"	51°36'10"	100	109
Site13	36800	Aberafan	273900	189600	3°49'00"	51°35'20"	111	101
Site14	36200	Whitmore Bay Barry	311450	166250	3°16'20"	51°23'20"	160	42
	36100	Jacksons Bay Barry	312200	166570				
Site15	36700	Rest Bay Porthcawl	280000	177900	3°43'40"	51°29'10"	116	80
Site16	36600	Sandy Bay Porthcawl	282400	176500	3°41'30"	51°28'20"		
	36500	Trecco Bay Porthcawl	283100	176300			121	77
Site17	36400	Southerndown	288400	172900	3°36'30"	51°26'40"	126	70
Site18	36300	Cold Knap Barry	309650	166400	3°18'00"	51°23'20"	157	44
Site19	37400	Oxwich bay	250700	186200	4°08'30"	51°33'45"	79	108
Site20	37500	Port Eynon Bay	247200	184800	4°11'25"	51°33'	70	106

6.1.2 River inputs and WwTW outfall locations

The river input locations have been defined in both 1-D and 2-D areas. There are 17 river inputs including 25 rivers located in the 2-D model area as cited in Table 6.2 and Figure 6.2. The river inputs in the 1-D model area are River Wye; Severn; Frome; and little Avon, see Table 6.3.

Table 6.2   River inputs locations in 2-D domain

No	Location		OS grid		Coordinate		Model grid cell	
	ID	Catchments	Easting	Northing	Longitude	Latitude	I	J
Input1	2	Tawe	266598	191653	3°55'26"	51°36'20"	101	109
	3	Nedd	271881	192432				
Input2	4	Afan	274556	188667	3°48'28"	51°35'05"	111	107
Input3	5	Kenfig	277919	183473	3°45'35"	51°32'12"	113	94
Input4	6	Ogwr	286123	175787	3°38'50"	51°28'00"	117	78
Input5	8	Ely	318583	172672	3°09'20"	51°26'40"	170	42
	9	Taff	318218	172672				
Input6	10	Rhymney	322282	177474	3°07'20"	51°28'30"	184	52
Input7	11	Ebbw	331480	183805	2°58'30"	51°31'18"	201	55
	12	Usk	331798	183633				
Input8	21	Avon	350115	178583	2°43'20"	51°30'20"	210	40
	22	Portbury Ditch	347817	177420				
Input9	23	Kenn-Blind Yeo-Land Yeo	338862	170310	2°52'40"	51°26'00"	206	39
Input10	24	Congresbury Yeo	336494	166748	2°55'30"	51°23'55"	195	36
	25	Banwell						
Input11	26	Axe	330852	158536	3°01'10"	51°13'20"	184	29
Input12	27	Brue	329428	147527	3°00'15"	51°13'20"	172	20
	28	Parrett	329130	146844				
Input13	29	Kilve Stream	314335	144453	3°13'50"	51°11'50"	153	11
Input14	30	Doniford Stream	309059	143213	3°18'15"	51°11'35"	144	18
	31	Washford River	306997	143524				
Input15	32	Pill River	302706	143520	3°23'25"	51°11'35"	135	17
	33	Avill River	300883	144247				
Input16	35	Aller-Horner Water	289210	148512	3°35'15"	51°13'58"	116	32
Input17	37	East-West Lyn	272291	149678	3°49'45"	51°14'20"	91	43

Table 6.3   River inputs locations in 1-D domain

No	Location		OS grid		Coordinate		Model segment
	ID	Catchments	Easting	Northing	Longitude	Latitude	Node no.
Input 1	13	Wye	354231	190223			3
Input 2	15	Severn	381548	219350			300
Input 3	17	Frome	375173	210497			206
Input 4	19	Little Avon	366257	200314			100

Table 6.4   WwTW outfall locations in 1-D domain

No.	Name	OS grid		Coordinate		Model segment
		Easting	Northing	Longitude	Latitude	Node No.
1	Thornbury STW	359990	193010	2°34'40"	51°38'	4
	Sedbury	353990	193420	2°40'08"	51°38'10"	
2	Blakeney	369110	206040	2°26'50"	51°45'	150
	Frampton	373570	208530	2°23'	51°46'25"	
3	Cheltenham STW	389930	224860	2°09'47"	51°55'10"	335
	Gloucester Longford STW	384730	221180	2°13'20"	51°53'13"	
4	Gloucester Netheridge STW	380900	215900	2°16'40"	51°50'30"	295
5	Longhope STW	369060	217880	2°27'02"	51°51'25"	120
6	Lydney	363760	200550	2°31'40"	51°42'05"	95
	Sharpness	367000	201500	2°29'	51°42'35"	

In total there are 34 WwTW sea outfalls distributed in the whole domain. These have been grouped for modelling purpose into 6 outfall inputs in the 1-D area and 19 outfall inputs in the 2-D area, as shown in Tables 6.4 and 6.5 respectively. The graphical presentation of the outfall locations in the 2-D domain can be seen in Figure 6.4.

Table 6.5   WwTW outfall locations in 2-D domain

No.	Name	OS grid		Coordinate		Model grid cell	
		Easting	Northing	Longitude	Latitude	I	J
1	Afan WWTW	274055	185075	3° 48.9'	51°33'00"	111	97
	Magor Brewery Effluent Plant	343765	184585	3°48'30"	51°33'40"		
2	Bishopston STW	258605	187305	4°1.7'	51°34'55"	89	104
3	Cardiff WWTW	325085	173955	3°4'40"	51°27'40"	186	44
4	Cog Moors STW	319306	167576	3°9'40"	51°24'05"	173	44
5	Llantwit Major WWTW	296355	167145	3°29'25"	51°24'05"	136	53
6	Nash STW	333455	184115	3°57'25"	51°33'10"	96	104
7	Overton STW	246395	184485	4°12'05"	51°33'20"	68	107
8	Penybont STW	287845	176845	3°36'20"	51°29'10"	125	70
9	Ponthir STW	334665	190435	3°56'20"	51°36'40"	101	109
10	Southgate STW	255385	187005	4°4'20"	51°34'40"	82	108
11	Swansea STW	268370	189437	3°53'05"	51°36'05"	103	108
12	The Leys outfall, Aberthaw	302305	165605	3°24'	51°23'00"	145	46
13	Avonmouth STW	351900	180700	2°41'50"	51°31'20"	204	40
	Portbury Wharf STW	348550	178150	2°44'25"	51°29'50"		
14	Bridgewater STW	330340	138810	3°00'05"	51°08'02"	170	20
	West Huntspill STW	329420	146840	3°00'55"	51°12'30"		
15	Doniford Outfall	308740	144010	3°18'30"	51°10'58"	140	18
	Watchet STW	306520	144550	3°20'20"	51°11'20"		
16	Kingston Seymour STW	338400	168660	2°53'10"	51°24'40"	195	36
	Wick St Lawrence STW	336510	166600	2°54'45"	51°23'30"		
17	Minehead STW	299450	146970	3°26'30"	51°12'30"	129	26
18	Porlock STW	288350	148300	3°36'00"	51°13'20"	113	33
19	Weston-Super-Mare STW	330580	158690	3°00'00"	51°19'20"	184	29

6.2   Model Set Up

The dynamically linked 1-D and 2-D model has been set up for the whole of the Bristol Channel and a major part of the Severn Estuary, covering an area from an imaginary line drawn between Hartland Point and Stackpole Head to the tidal limit of the River Severn, see Figure 6.3.
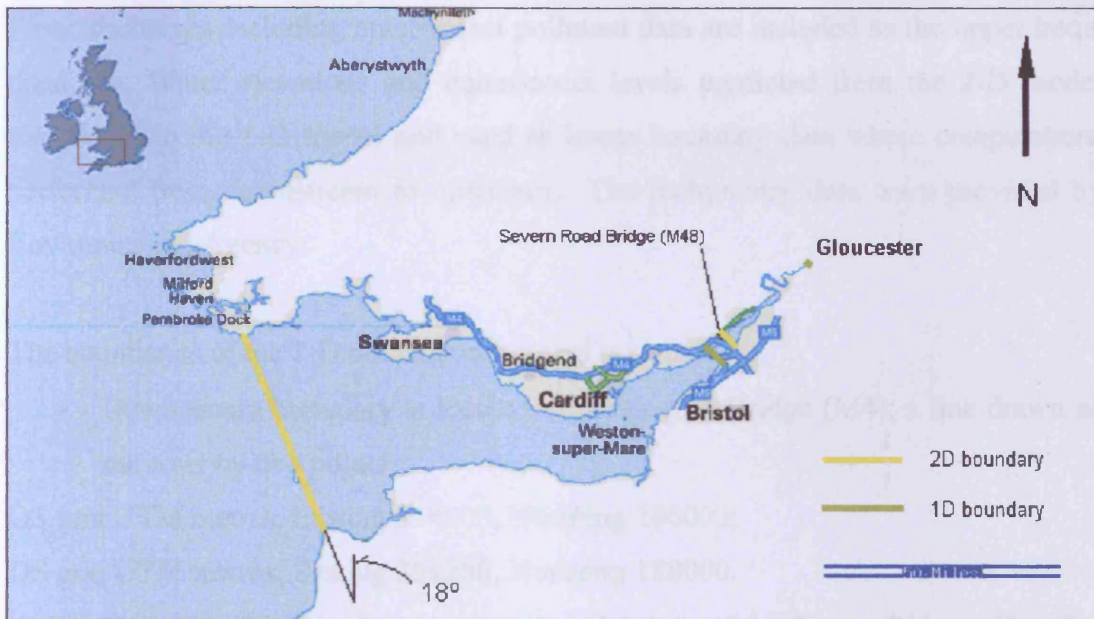

Figure 6.3   Whole modelling domain of the Bristol Channel and Severn Estuary

6.2.1   Model domain

The study area extends from the seaward boundary of the outer Bristol Channel to the tidal limit of the River Severn. It is divided into two modelling domains. The 2-D modelling domain primarily covers the Bristol Channel and the 1-D modelling domain includes the Severn Estuary up to the tidal limit along the River Severn.

There is an area of overlap between the 1-D and 2-D domains, which was from the M4 Severn Bridge (i.e. the new Severn Bridge) to the M48 Severn Bridge (i.e. the old Severn Bridge), see Figure 6.3. The overlapping area is used to provide boundary data between 1-D and 2-D models.

6.2.1.1   1-D model area

The 1-D model area is specified as being from the M4 Severn Bridge (i.e. the downstream boundary) to Haw Bridge (i.e. the upstream boundary). There are four reaches (total length 80km) distributed along the domain, including a total of 351 nodes (i.e. computed cross sections), with the average distance between cross-sections being about 240m. The reach length is 62378m for reach1; 5720m for reach2; 3109m for reach3 and 8920m for reach4.

Flow discharges including enterococci pollutant data are included as the upper boundary condition. Water elevations and enterococci levels predicted from the 2-D model are transferred to the 1-D model and used as lower boundary data where computations are performed from downstream to upstream. The bathymetry data were provided by the Environmental Agency.

The boundaries of the 1-D domain are termed as:

- Downstream boundary is located at the Severn Bridge (M4), a line drawn across the river by two points:

OS grid UTM metres, Easting 354000, Northing 186000;

OS grid UTM metres, Easting 351250, Northing 188000.

- Upstream boundary is located at the tidal limit of the Severn River at Haw Bridge, by the point:

OS grid UTM metres, Easting 384500, Northing 227800.

6.2.1.2   2-D model area

The 2-D model domain covers the Bristol Channel over an area of 14,636.2 km². The domain was divided into a mesh of 242×168 grid squares, with a fixed size of 600 m × 600 m. There are two main boundaries in the 2-D domain, which are: (i) the downstream boundary, which extended from Heartland Point to Stackpole Head - a distance of 74 km, and with the co-ordinates of the two points being 51° 01.5′ N, 4° 31.4′ W; 51° 37.8′ N, 4° 53.0′ W, and (ii) the upstream boundary, being the line drawn across the river, located at the old Severn Road Bridge (M48), of length of 2.8 km and with the two points on the upstream boundary being: OS grid UTM metres, Easting 356300, Northing 190000; and Easting 352250, Northing 190700.

The downstream boundary is specified as a tidal water elevation boundary, while the upstream boundary is specified in the form of a flow boundary. The downstream boundary water level was obtained from the POL (Proudman Oceanographic Laboratory) Irish Sea model. The upstream boundary condition includes the velocities, sediment and enterococci concentrations as computed from the 1-D model, with these data being transferred between the 1-D and 2-D modelling suites to enable dynamically exchange between the 1-D and 2-D models. Figure 6.4 is a Tecplot drawing which covers the 2-D model domain, where the coloured points indicate the WwTW outfall locations.
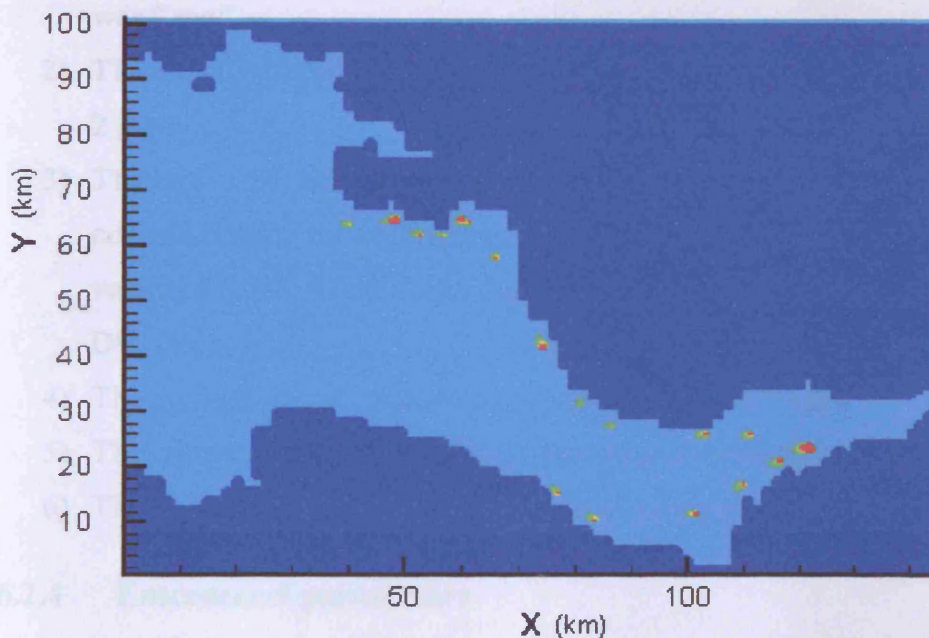

Figure 6.4   2-D model domain with WwTW outfall Locations

6.2.2   Simulation time

The model simulation period was chosen to cover the four field survey dates, they are: 24/07/2001, 26/07/2001, 30/07/2001 and 01/08/2001.

The simulation start time and date are: 17:30pm 20/07/2001. The simulation end time and date are: 5:30am 02/08/2001. The total simulation time is 300 hours.

6.2.3 Sediment parameters

This study is mainly concerned with the behaviour of bacteria which is associated with sediment transport. In order to provide instantaneous concentration distributions of suspended sediments, which are the carrier of enterococci, the computation of sediment transport is completed before the enterococci calculation during a time step.

The sediment parameters and initial values are selected as follows, in which the sizes of the particles were derived from the microcosm and settlement experiments conducted by the CREH team at the University of Wales, Aberystwyth (Stapleton et al., 2004):

1) The initial value of non-cohesive sediment concentration across the whole domain was 2 mg/l.

2) The initial value of cohesive sediment concentration across the whole domain was 2 mg/l.

3) The D16, D50, D84 and D90 of the particles for the non-cohesive sediment were computed using the analysed samples taken at the four sampling sites. The mean values of 0.026, 0.058, 0.126 and 0.15 mm were obtained for D16, D50, D84 and D90 respectively.

4) The average size of cohesive flocs was 0.010 – 0.063 mm.

5) The critical shear stress for the deposition of cohesive particles was 0.100 N/m^2.

6) The critical shear stress for the erosion of cohesive particles was 2.000 N/m^2.

6.2.4 Enterococci parameters

In this application the initial values of the enterococci conditions for the modelling process are selected as follows:

1) The population ratio of attached enterococci to total enterococci was 80% and this is regarded as a constant value during the estimation time. Values of 20% and 50% were also chosen for the sensitivity analysis.

2) The initial value of enterococci on bed sediments was 1000 cts/g. The sensitivity analysis was also carried out using 10 and 100 cts/g concentration levels on beds.

3) Decay rate in bed sediments was assumed to be zero value in this study.

4) The initial value of enterococci in water column was assumed to be 0 cts/100ml.

5) The T90 value in water column is time varying, while the value obtained from the empirical regression equations will be described in the following section 6.2.4.3.

6.2.4.1   *River inputs*

Field data collected from 29 rivers were available for this model calibration and application, which was conducted by the CREH research team. The data included hourly-recorded flow rates and microbial data, shown in the files with the names of "severnin.xls", "inputs2.xls" and "inputs3.xls" (given in attached CD). The numerical model accepts dynamically varying inputs during simulations.

6.2.4.2   *WwTW discharges*

The WwTW discharges (i.e. flow rates and enterococci concentrations) collected by CREH were largely constant during the model simulation period, except at the Minehead WwTW outfall. The discharge at Minehead was tidally controlled and behaved according to the following general rule: from 4 hr after HW to 2 hr before HW the outfall discharge was constant, during the remaining time there was no discharge. These discharge data are stored in the file of "Severn Continuous _2000PE.xls" (given in attached CD).

6.2.4.3   *T90 equations*

6.2.4.3.1   **T90 as a function of turbidity**

The decay rate in water used in this study was predicted based on the empirical regression equations (T90 vs. turbidity) obtained from the laboratory experiments conducted by the CREH research team. Details of the establishment of the equations are given in the documents of Stapleton et al. (2004) and Kay et al. (2005). The experiments used a fixed irradiance equivalent to a sunny day at noon in the Severn Estuary in July 2001. The irradiance values used for the experiments were:

Visible light: 260 ±14 W·m^{-2};

UV-A: 5.2 ±0.4 W·m^{-2};

UV-B: 1.1 ±0.02 W·m^{-2}.

The empirical regression T90 equations adapted in the modelling simulations were:

Light excluding outliers: $\text{Log T90} = 0.0047 \times \text{Turbidity} + 0.677 \pm 0.2070$ 6.1

Dark excluding outliers: $\text{Log T90} = 0.0019 \times \text{Turbidity} + 1.237 \pm 0.199$ 6.2

$\text{Turbidity} = 139.479 \times \text{Log SS} - 244.736 \pm 32.678$ 6.3

where: T90 is in hours; SS concentration is in mg/l.

From the above equations it can be seen that the T90 values predicted from the SS concentrations are time-varying values because the SS concentration is a time-varying parameter. SS concentration also varies specially over the computational domain. Therefore, during modelling the dynamically predicted T90 values are recalculated by a renewed local SS concentration for each grid cell at each time step.

6.2.4.3.2   Refined light T90 equation - Using diurnal irradiation data

Many studies indicated that the sunlight significantly affected the mortality of faecal bacteria. Bellair *et al.* (1977) suggested that faecal coliform die-off rates were inversely related to irradiance intensity as follows:

$$T90 = 3.4 \, I^{-0.42} \qquad\qquad 6.4$$

where: T90 is in hours; I is hourly solar radiation, in $MJ \cdot m^{-2} h^{-1}$.

Pommepuy et al. (1992) reported that a close relationship was found between the light intensity received by bacteria and the T90, which was similar to the finding by Bellair et al. (1977) with the form:

$$T90 = 1.2 \times 10^4 \, I_n^{-0.56} \qquad\qquad 6.5$$

where: T90 is in hours,

I_n is the light energy received by bacteria, $\mu E \, m^{-2} \, h^{-1}$, which is a function of turbidity and water depth.

Alkan et al. (1995) studied the survival of enteric bacteria exposed to a sunlight simulator in varying conditions of light intensity, turbidity, sewage content, degree of mixing and temperature under controlled laboratory conditions, reporting the variability of bacteria die-off due to the effect of light was linearly increased with the light intensity. Taking into account a combined coefficient to include turbidity and sewage content, the relationships discovered were:

$$K_{EC} = A_{EC} + 1.3 \times 10^{-5} \, I_L \qquad\qquad 6.6$$

$$K_E = A_E + 1.1 \times 10^{-5} \, I_L \qquad\qquad 6.7$$

where: K_{EC}, K_E are the die-off rates for E. coli and Enterococci respectively, min^{-1};

A_{EC}, A_E are the combined coefficients for E. coli and enterococci, which are related to three other factors – turbidity, sewage content and mixing effects;

I_L is the surface light intensity, $W \cdot m^{-2}$ (or $J \cdot m^{-2} \cdot s^{-1}$).

Guilland et al. (1997) studied the survival of E. coli in both laboratory and in-situ under sunlight illuminations, with the impact of sewage and SS concentration level also being considered. The relationship between light intensity and T90 was found as below:

$$T90 = 53683\ I_m^{-0.666} \qquad\qquad 6.8$$

where: T90 is in hours;

I_m is the mean light intensity in the vertical water section, $\mu E\ m^{-2}\ h^{-1}$, which is a function related to surface light intensity, water depth and SS concentration.

Among the above four studies, the condition used to derive equation 6.7 (by Alkan, 1995) is most close to the current case study and it is applied to refine the T90 equation 6.1, which has a fixed irradiation. Taking into account the sunlight-dependent term in equation 6.7 with the decay rate presented in the form of T90 = ln10/K_E, we have:

$$T90^1 = \ln10/(1.1\times10^{-5}\ I)/60 = 3.5\times10^3\ I^{-1} \qquad\qquad 6.9$$

where: $T90^1$ is the partial enterococci mortality rate depending on surface sunlight (I) only, in hours. I is the surface light intensity, $W\cdot m^{-2}$.

Hence, by combining equation 6.9 with equation 6.1, the refined T90 equation which takes account of both the time varying sunlight intensity and the impact of turbidity, can be written as:

$$T90 = T90^2 + (T90^1 - T90_*^1) \qquad\qquad 6.10$$

where:

$T90^2$ is the predicted T90 depending on turbidity, see equation 6.1.

$T90^1$ is the predicted T90 depending on surface sunlight (I), in hours.

$T90_*^1$ is the constant of the predicted $T90^1$ value under the fixed irradiance I*, in hours. $T90_*^1 = 3.5\times10^3\ /I*$.

I* is the fixed irradiance operated in the T90 vs. turbidity experiments, $W\cdot m^{-2}$.

To summarise, the refined T90 equation was obtained from the integration of the time-varying SS-dependent equation ($T90^2$ values) and the time-varying sunlight-dependent equation ($T90^1$ values), dynamically representing the real-time decay rate during daytime.

For the real-time T90 predictions the diurnal irradiance data obtained for Swansea Bay and provided by the Environment Agency were used. The diurnal irradiance data are

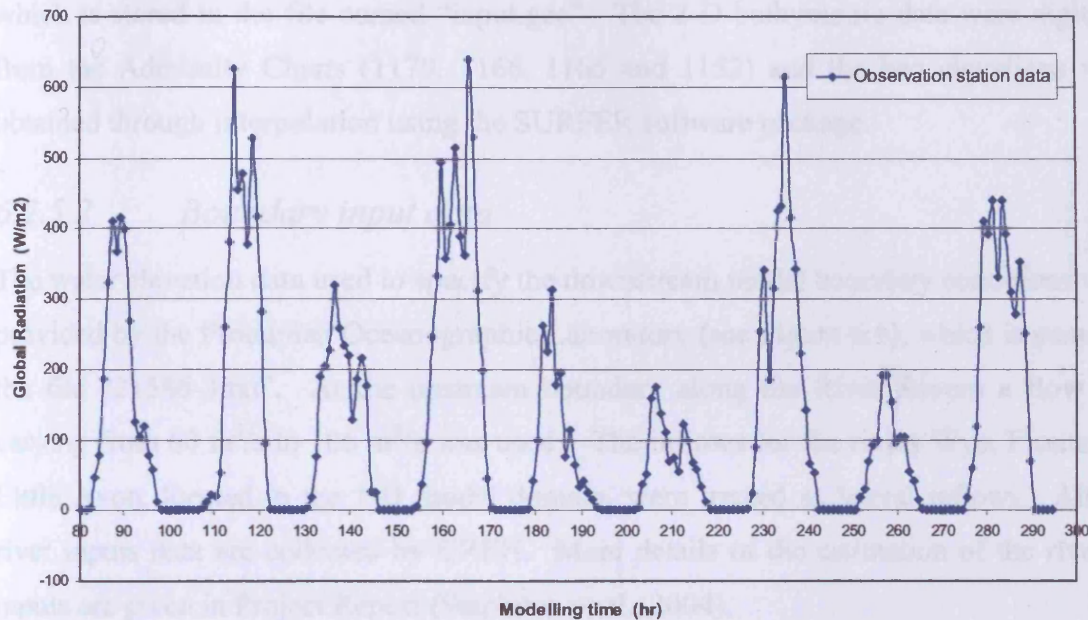stored in the file named "Cardiff Irradiation1.xls" (given in attached CD), and shown in Figure 6.5.

Figure 6.5   Swansea Bay irradiance data (sunlight), 24/07/2001 – 01/08/2001

6.2.4.3.3   T90 in river

The above empirical T_{90} equations were primarily obtained from experiments using seawater samples. From experience gained from a recent study of faecal coliforms in the Ribble Estuary, it was found that for fresh water the T_{90} value was about two times longer than that in seawater. Therefore it was assumed that during the computations the T_{90} values in the 1-D domain were twice the values used in the 2-D domain, otherwise the same representations were applied in both models.

6.2.4.3.4   Limits of the equations

The above empirical T90 equations have their standard error terms and these values are all not small. To reduce the impact from these error terms, the lowest limits for the T90 equations were proposed and some tests on the available survey sites were designed to find the limits. These tests showed that the corrections for the equations were necessary. These limits were found to be: the minimum T90 in light condition was 0.5 hours; the minimum T90 in dark condition was 20 hours.

6.2.5   Hydrodynamic parameters

6.2.5.1   Bathymetry data

The bathymetric data used in the 1-D region were provided by Jeremy Benn Associates, which is stored in the file named "input.geo". The 2-D bathymetric data were digitised from the Admiralty Charts (1179, 1166, 1165 and 1152) and the bed elevations were obtained through interpolation using the SURFER software package.

6.2.5.2   Boundary input data

The water elevation data used to specify the downstream model boundary conditions were provided by the Proudman Oceanographic Laboratory (see Figure 6.6), which is stored in the file "21586-3.txt". At the upstream boundary along the River Severn a flow rate varying from 60 m^3/s to 106 m^3/s was used. The inflows for the rivers Wye, Frome and Little Avon, located in the 1-D model domain, were treated as lateral inflows. All the river inputs data are collected by CREH. More details of the estimation of the riverine inputs are given in Project Report (Stapleton et al., 2004).
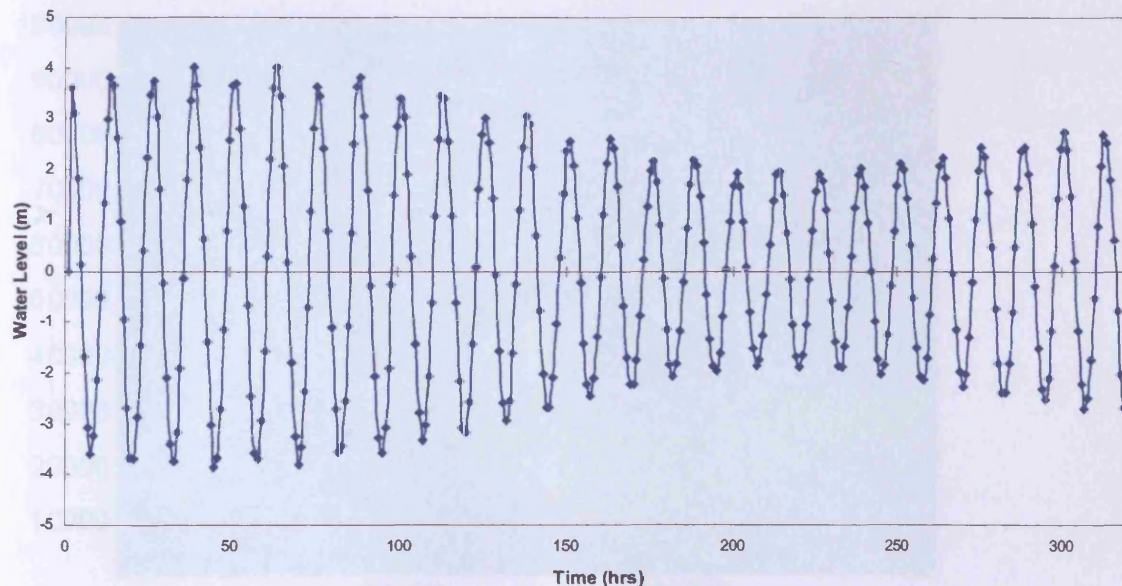

Figure 6.6   Water levels at lower boundary, used as input data

6.2.5.3   *Survey data*

Four sets of survey data were used for calibrating the hydrodynamic and enterococci parameters. The locations of the hydrodynamic surveys were:

S. Wales (24 July 2001, Survey 1), 51° 26.102' N 3° 38.414' W

S. Wales (26 July 2001, Survey 2), 51° 26.103' N 3° 38.375' W

Minehead (30 July 2001, Survey 3), 51° 12.820' N 3° 23.30' W

Minehead (01 August 2001, Survey 4), 51° 12.820' N 3° 23.30' W

There were eight sampling locations for the water quality surveys. These locations are listed in Table 6.6 and represented in Figure 6.7.

Four parallel water quality sampling surveys were carried out on each day, they were as follows:

Survey 1 has four sampling sites 1-4;

Survey 2 has four sampling sites 1-4;

Survey 3 has four sampling sites 5-8;
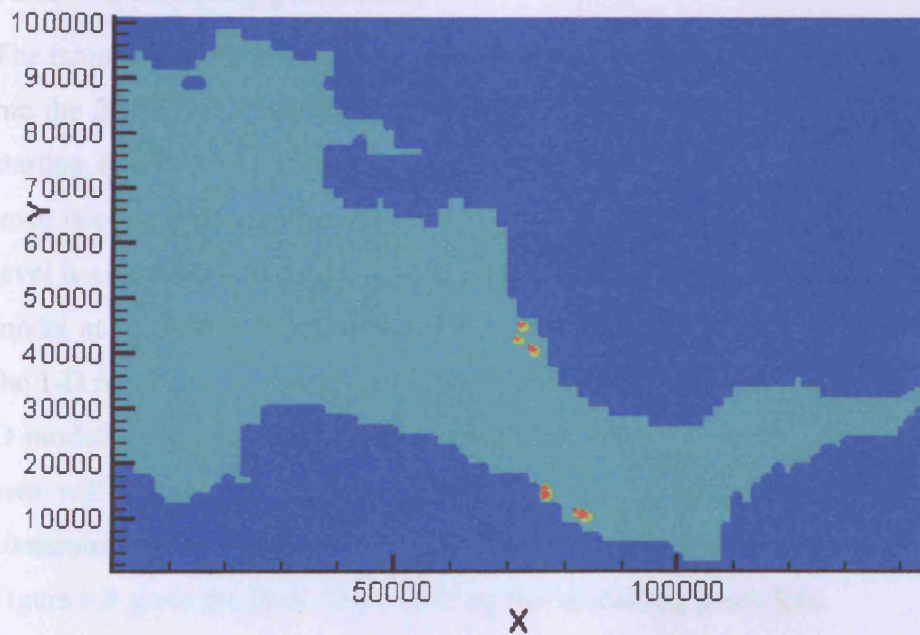
Survey 4 has four sampling sites 5-8.

Figure 6.7   The locations of survey sites (meters)

Table 6.6   Locations of water quality survey sites

No.	Name	On Survey	Location Coordinates	Model grid cell	
				I	J
1	Offshore CSV 1	Survey 1, 2	51° 26.103 N, 3° 38.375 W	124	69
2	Offshore Rib 1	Survey 1, 2	51° 26.796 N, 3° 40.617 W	120	72
3	Trecco Bay BW	Survey 1, 2	NGR: SS 8310 7630	121	77
4	Southerndown BW	Survey 1, 2	NGR: SS 8840 7290	126	70
5	Offshore CSV 2	Survey 3, 4	51° 12.820 N, 3° 23.30 W	137	20
6	Offshore Rib 2	Survey 3, 4	51° 13.534 N, 3° 28.303 W	128	25
7	Minehead Terminus BW	Survey 3, 4	NGR: SS 9730 4650	129	27
8	Dunster North West BW	Survey 3, 4	NGR: SS 9970 4550	140	19

6.3   Hydrodynamic Modelling

6.3.1   Modelling procedure

The main procedure of the dynamically linked 1-D and 2-D modelling system is firstly to run the 2-D model from the downstream open boundary to the upstream open boundary starting from high water. For the first half time step the x-direction velocity and water level is computed and then the second half time step, the y-direction velocity and water level is computed. Secondly, the computed velocity and water level obtained for the 2-D model at the border of the overlapped area provides the lower boundary water level for the 1-D model, which starts its computation from downstream to upstream. During the 1-D modelling process, the new produced discharge at another border of the overlapped area will be used as the upper boundary data to 2-D model in next time step. The contaminants calculations are then followed after the hydrodynamic modelling procedure. Figure 6.8 gives the flow chart showing the modelling procedure.
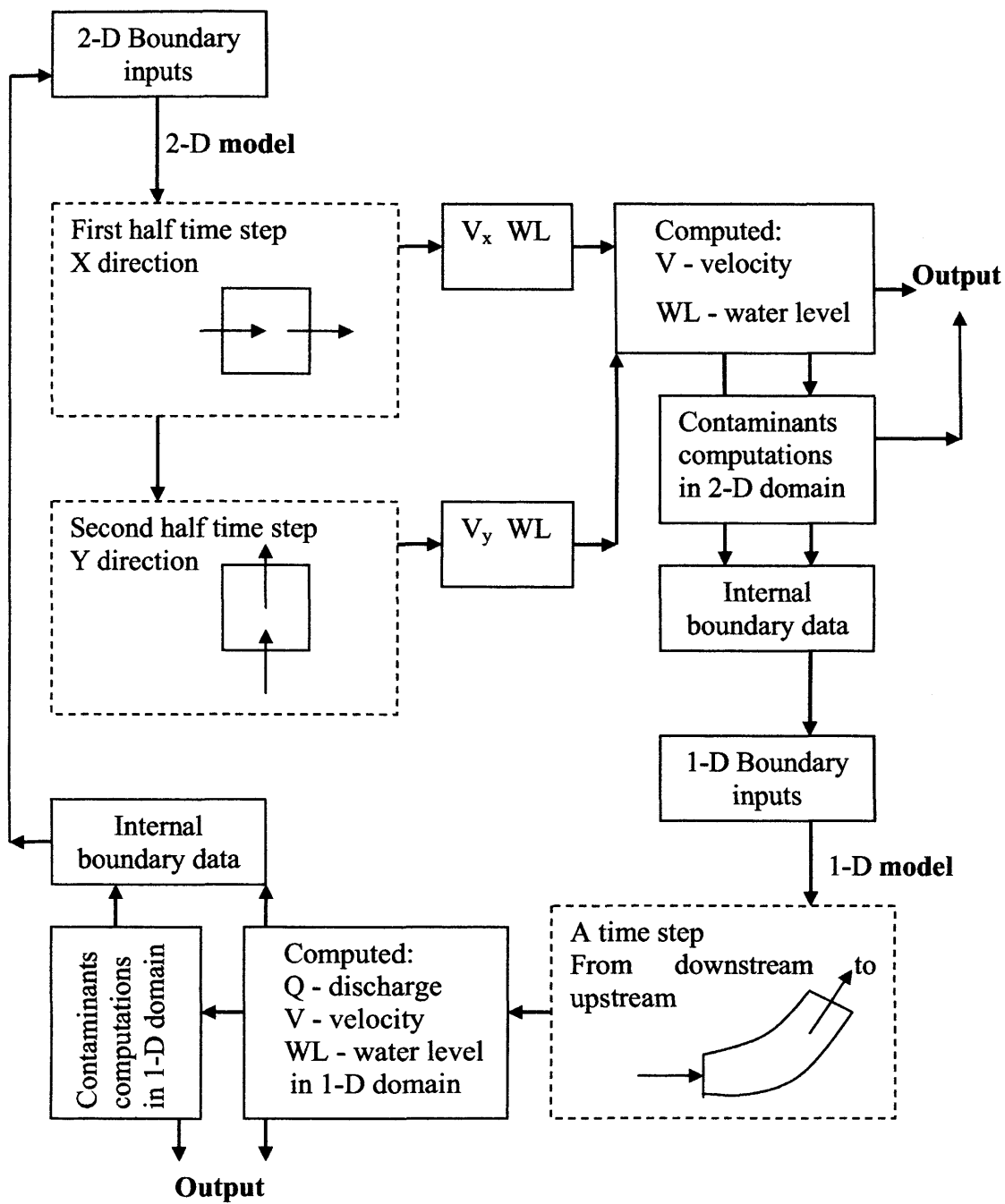
Figure 6.8   Modelling procedure of linked 1-D and 2-D model

The hydrodynamic modelling is based on the standard 1-D and 2-D governing equations, which consist of the momentum and the continuity equations, as used to compute the tidal water elevation changes and the tidal and riverine currents (both speed and direction) in the 2-D and 1-D model domains. These hydrodynamic results, when presented graphically, can provide contours of water elevations and current fields, both for the 2-D and 1-D domains. As the survey data are given in the form of water depth, tidal water elevations are deducted from the bed elevations to give the water depth outputs for the modelling results. Figures 6.9-6.12 show predicted water level and velocity distributions at four stages of a tidal cycle for a spring tide. Figures 6.13-6.16 show predicted water level and velocity distributions at four stages of a tidal cycle for a neap tide.
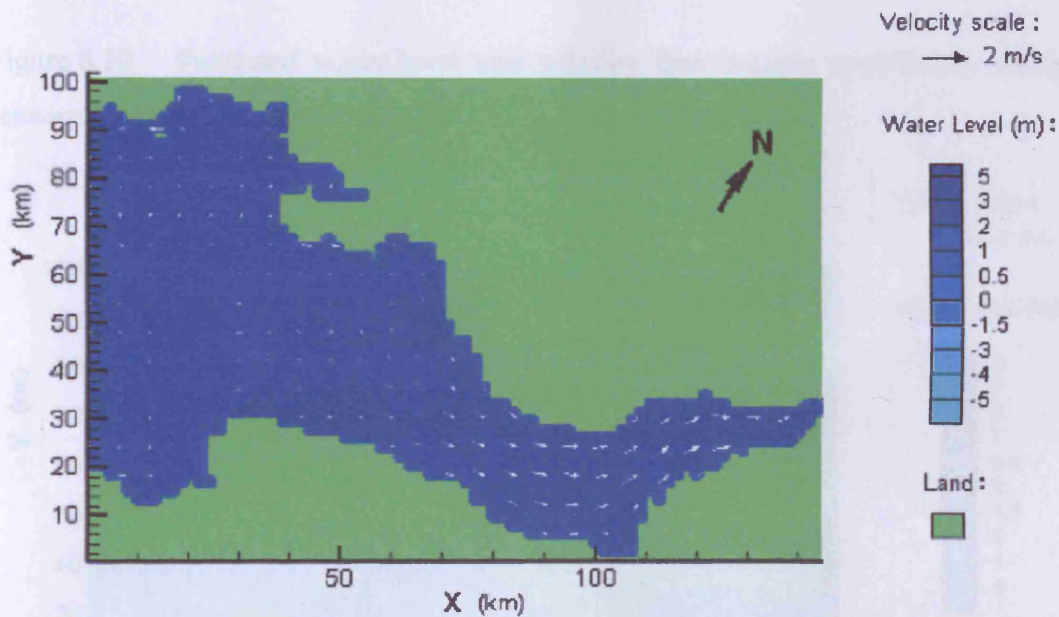
Figure 6.9   Predicted water level and velocity distributions at high water, referring to seaward boundary, for a spring tide
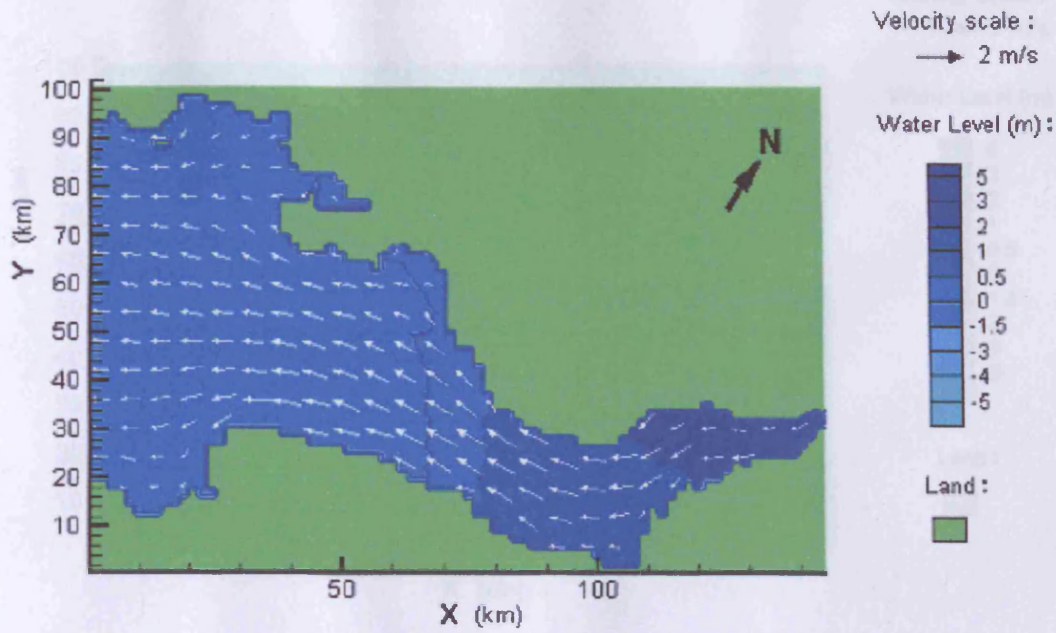
Figure 6.10   Predicted water level and velocity distributions at mid-ebb, referring to seaward boundary, for a spring tide
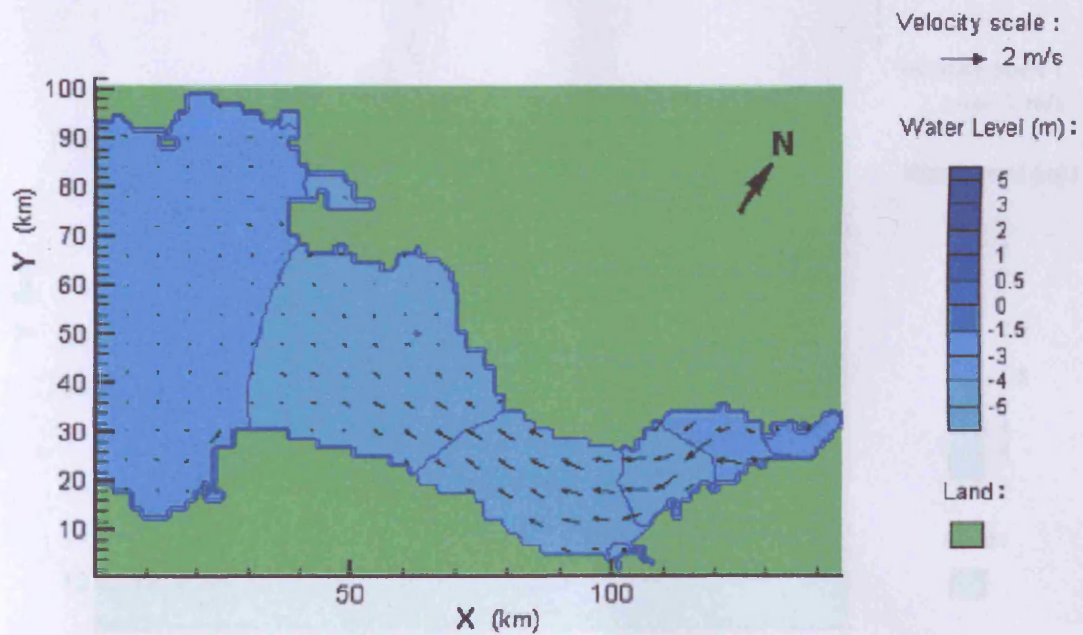

Figure 6.11   Predicted water level and velocity distributions at low water, referring to seaward boundary, for a spring tide
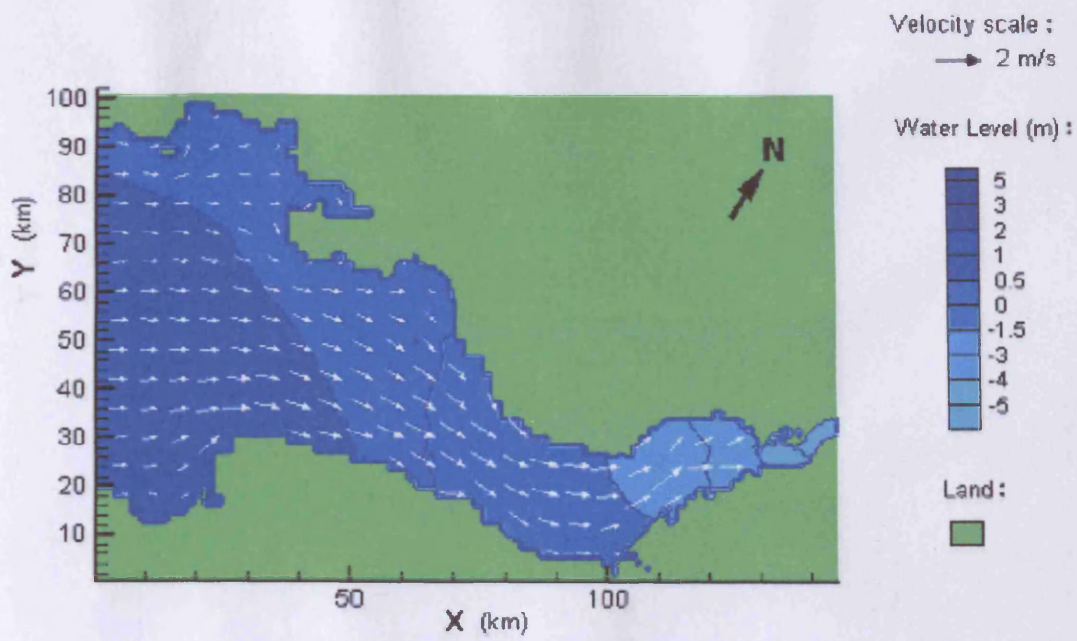
Figure 6.12   Predicted water level and velocity distributions at mid-flood, referring to seaward boundary, for a spring tide
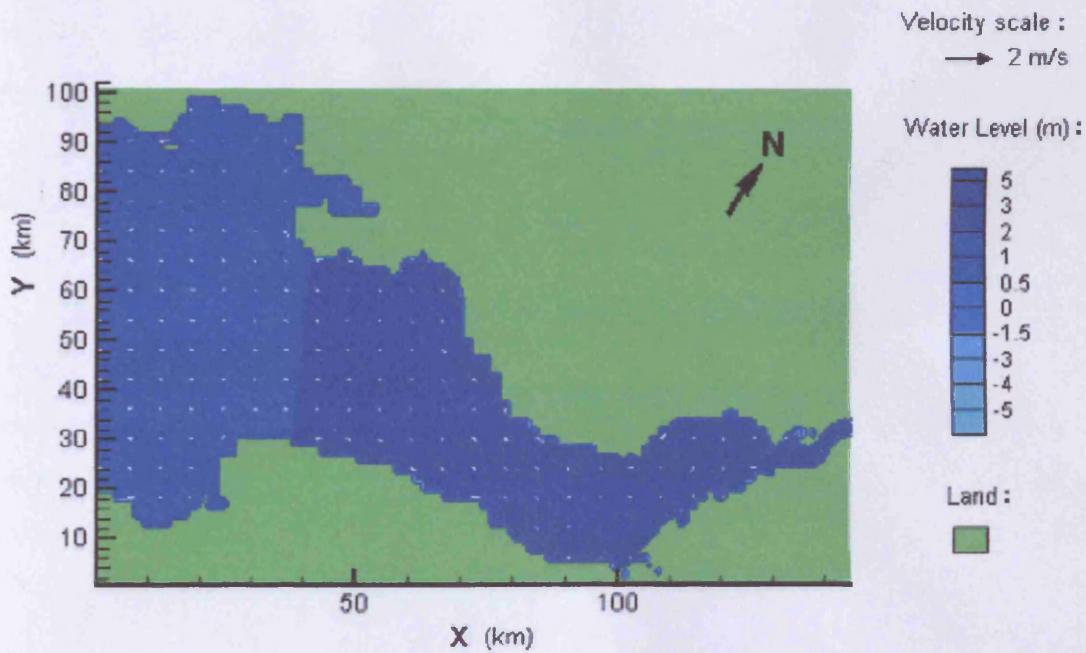

Figure 6.13   Predicted water level and velocity distributions at high water, referring to seaward boundary, for a neap tide
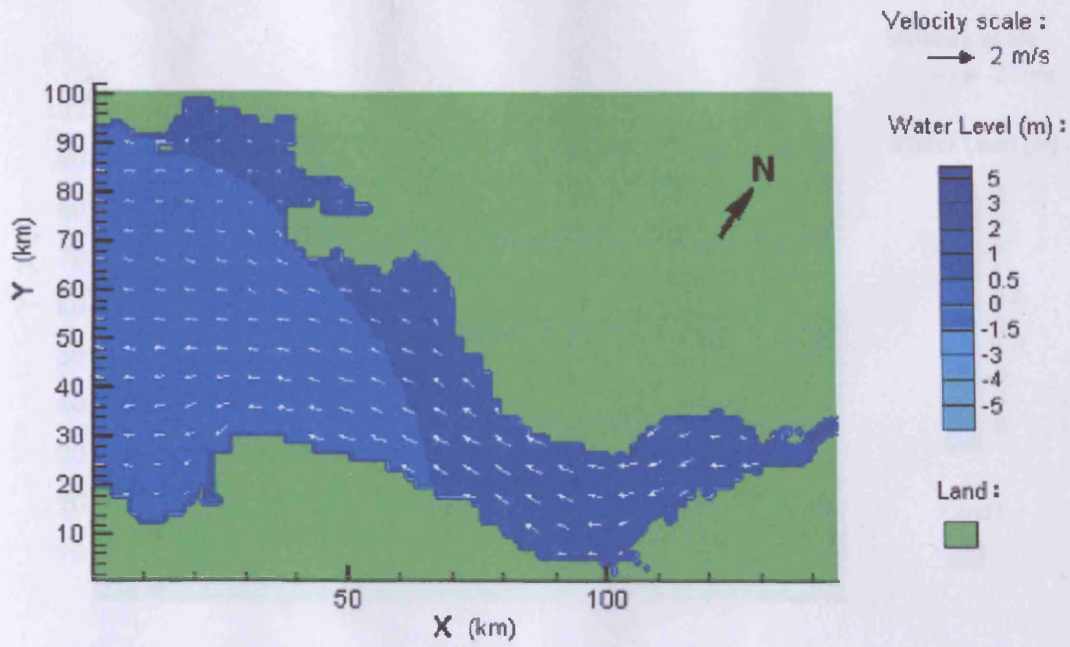
Figure 6.14   Predicted water level and velocity distributions at mid-ebb, referring to seaward boundary, for a neap tide
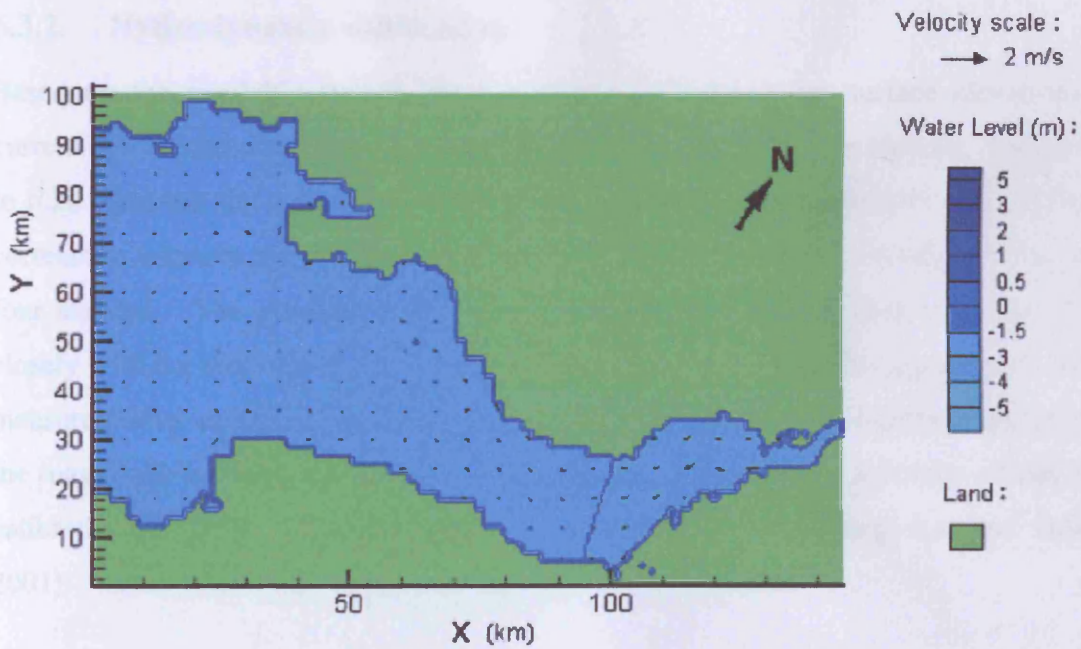

Figure 6.15   Predicted water level and velocity distributions at low water, referring to seaward boundary, for a neap tide
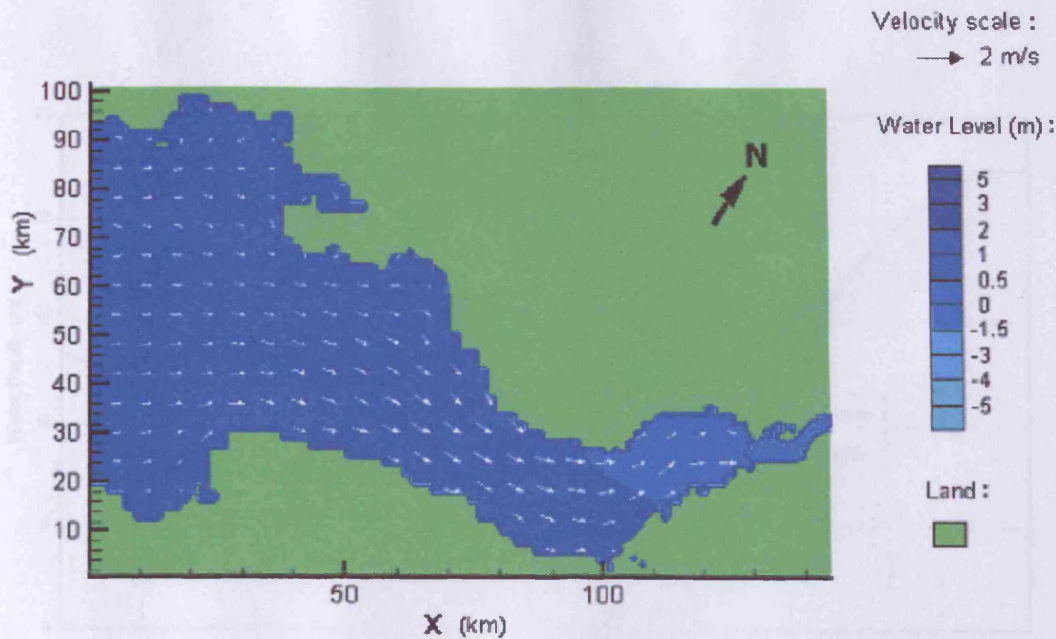
Figure 6.16   Predicted water level and velocity distributions at mid-flood, referring to seaward boundary, for a neap tide

6.3.2   Hydrodynamic calibration

Based on the available survey data, calibration of the water surface elevations, and current speeds and directions were carried out for each of the four surveys. Figures 6.17 to 6.28 illustrate the calibration results. The hydrodynamic calibration showed that the correlation between the predicted and measured data is very good for tidal phasing for all four surveys. The prediction of the water depths and current directions agreed very closely with the site survey data. The current speed predictions also agreed well with the measured data, except at the South Wales site where the model slightly under predicted the magnitude of fluid speed during the ebb tide. The order of accuracy of this model calibration is similar for other studies of the Bristol Channel (e.g. Lin and Falconer, 2001).

These calibration results demonstrate that the model is capable of producing accurate hydrodynamic characteristics. The sediment and enterococci parameter predictions based on this hydrodynamic template therefore can be derived.
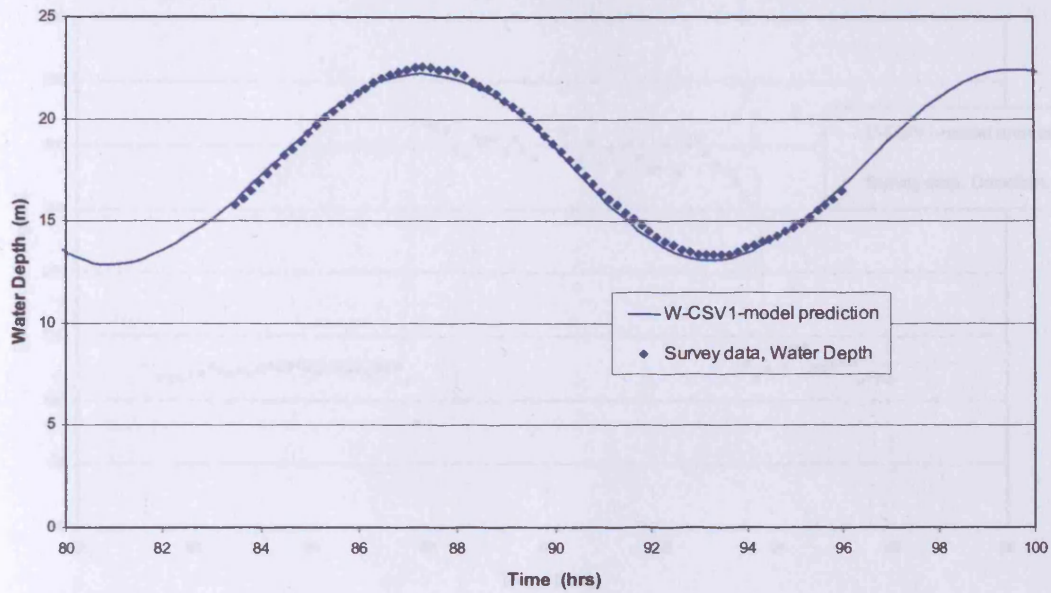
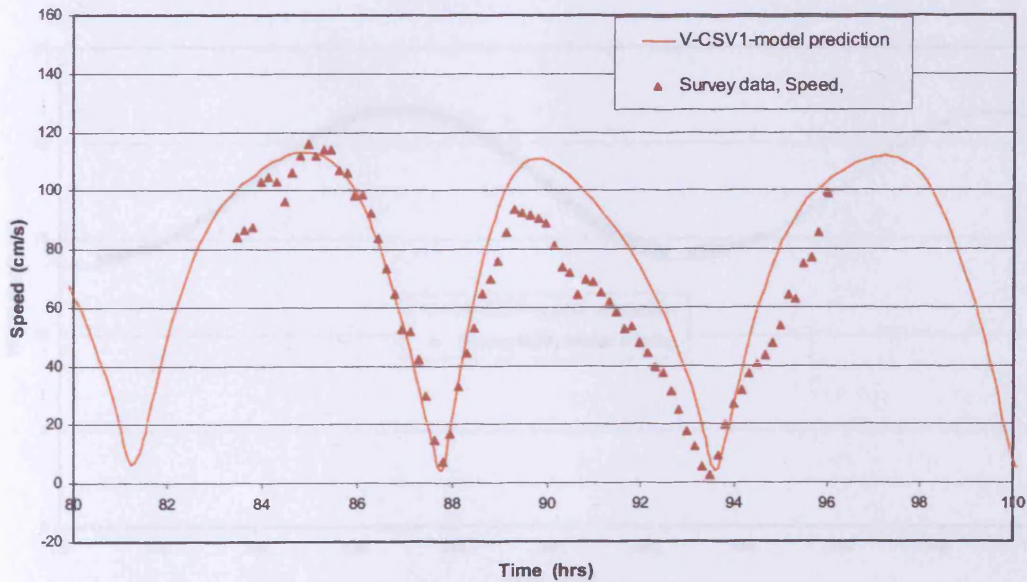Figure 6.17   Comparison of predicted and measured depths at S. Wales site on 24/07/01

Figure 6.18   Comparison of predicted and measured current speeds at S. Wales site on 24/07/01

Figure 6.19   Comparison of predicted and measured current directions at S. Wales site on 24/07/01

Figure 6.20   Comparison of predicted and measured depths at S. Wales site on 26/07/01

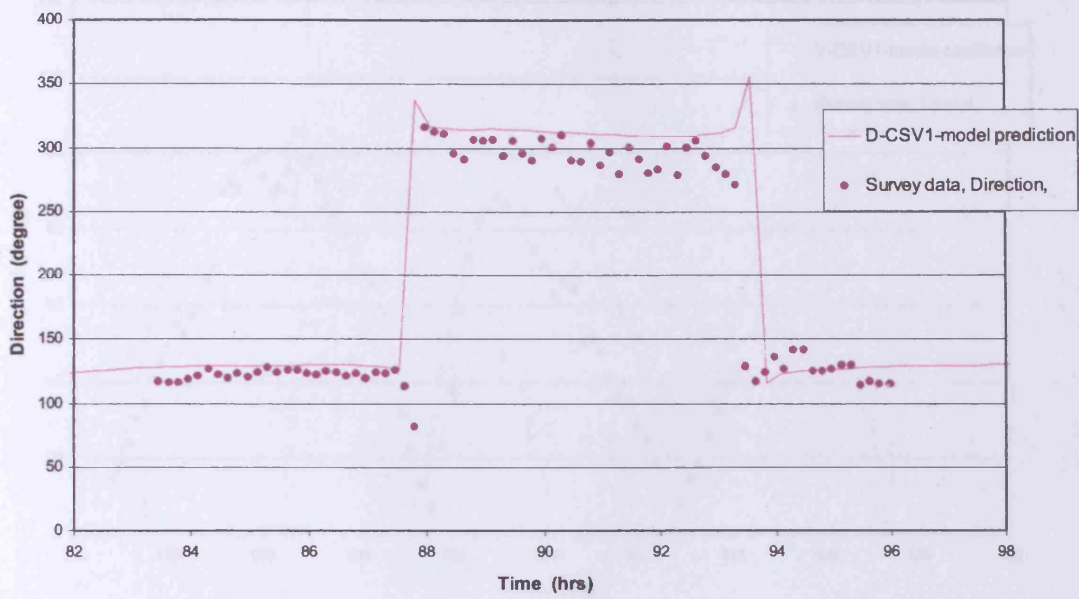Figure 6.21   Comparison of predicted and measured current speeds at S. Wales site on 26/07/01

Figure 6.22   Comparison of predicted and measured current directions at S. Wales site on 26/07/01
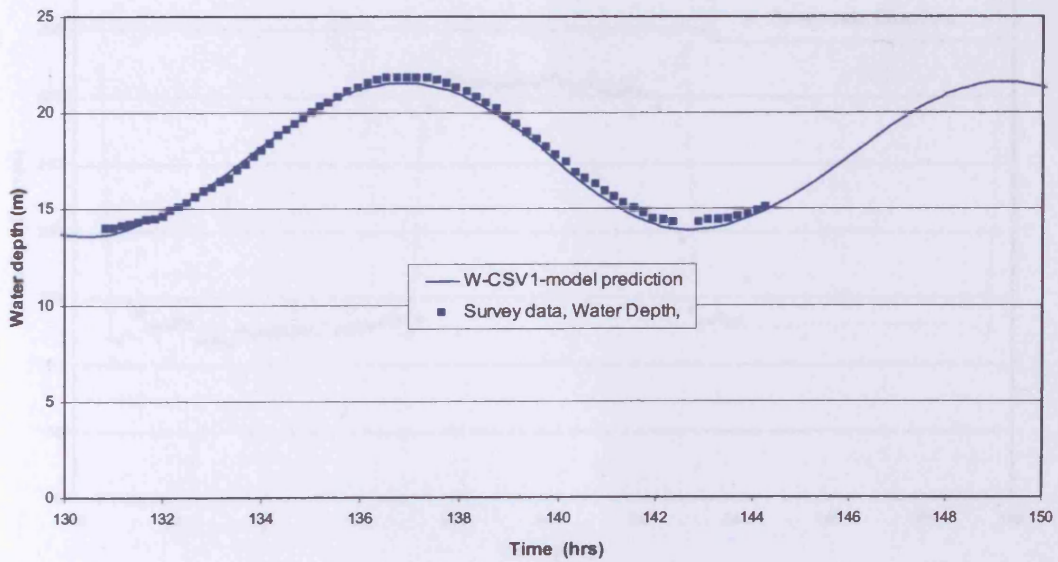
Figure 6.23   Comparison of predicted and measured depths at Minehead on 30/07/01

Figure 6.24   Comparison of predicted and measured Current Speeds at Minehead on 30/07/01

Figure 6.25   Comparison of predicted and measured current directions at Minehead on 30/07/01

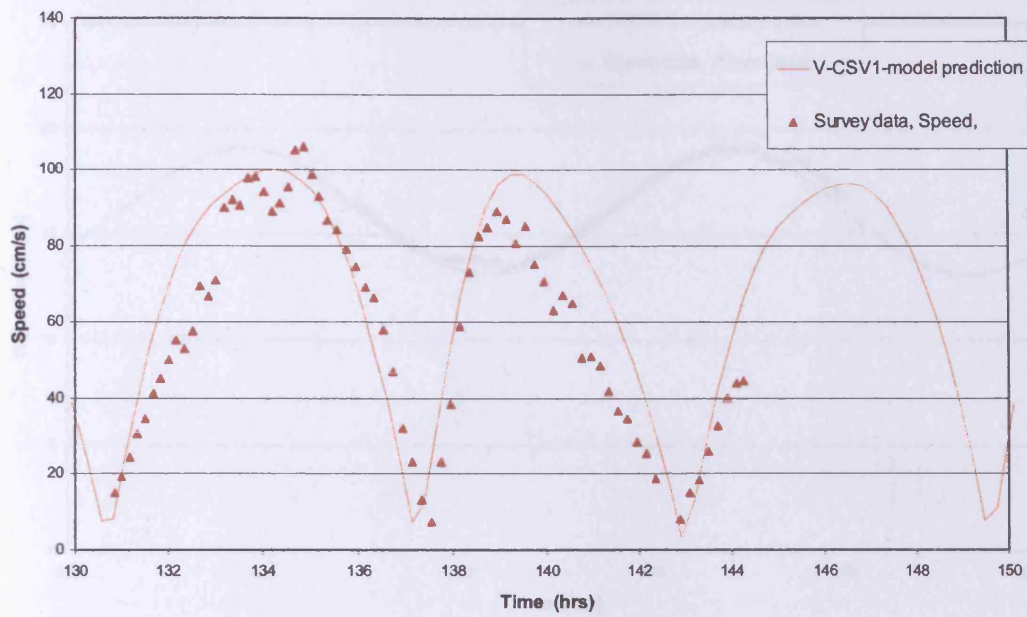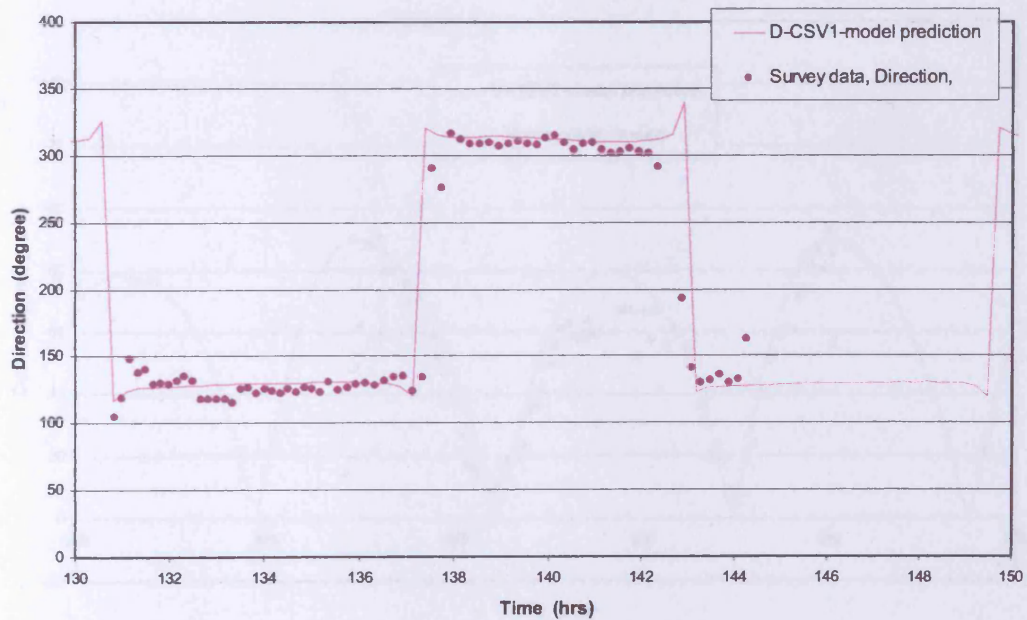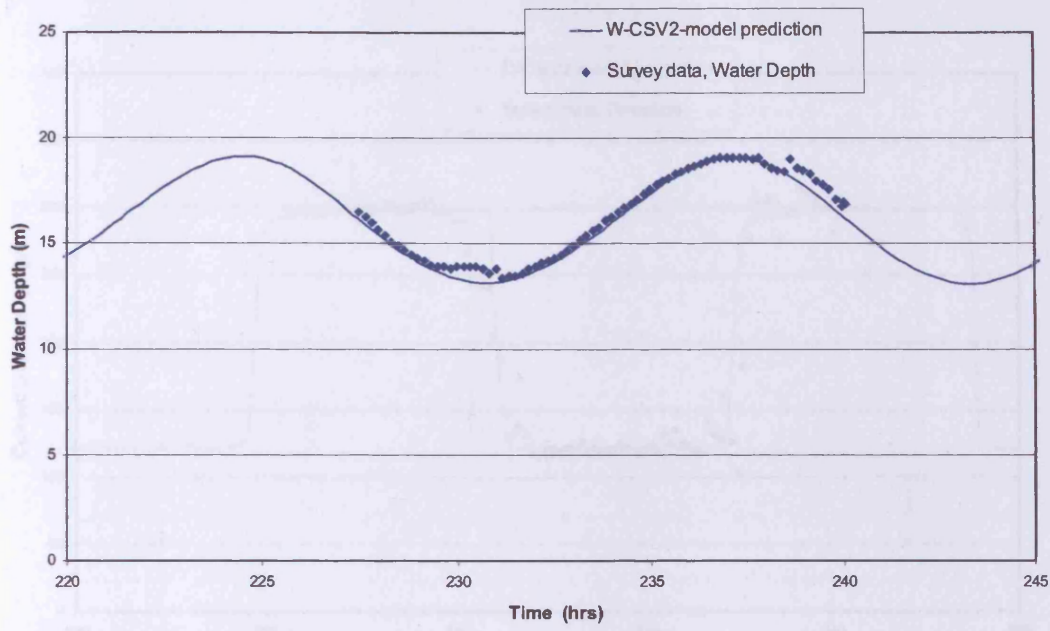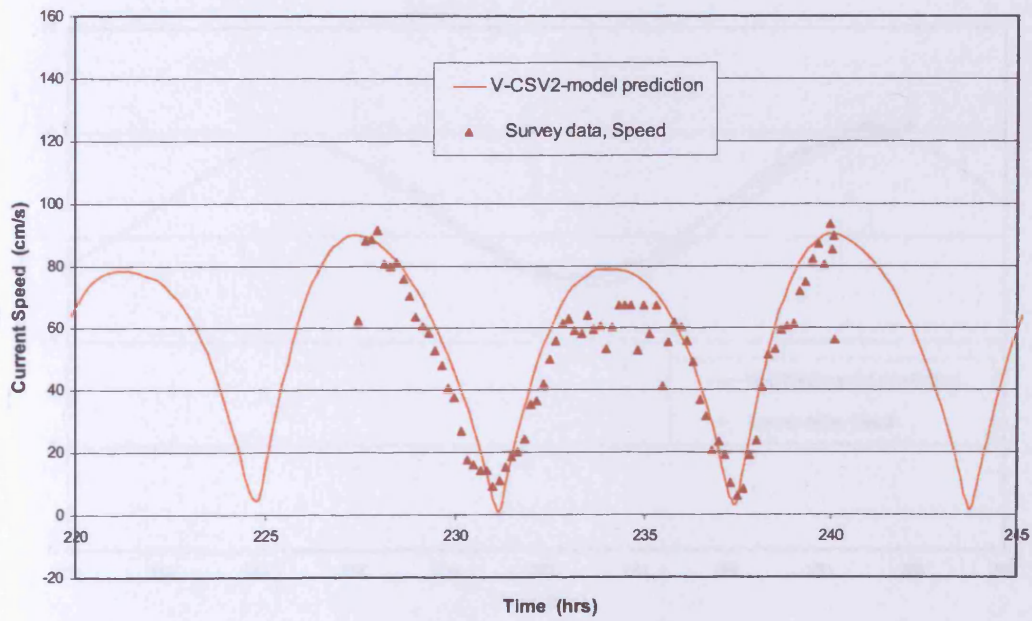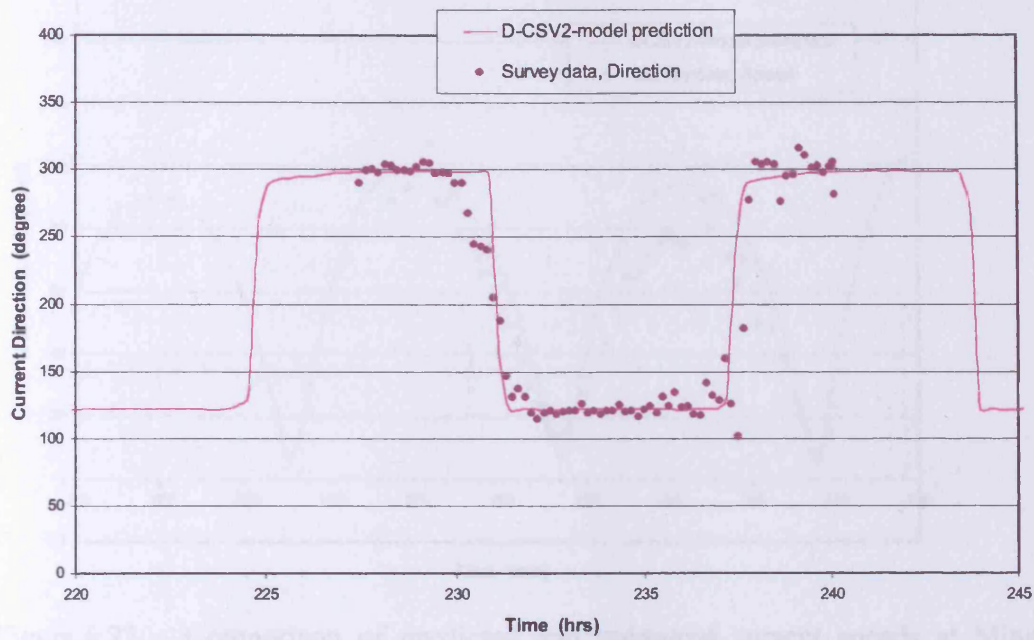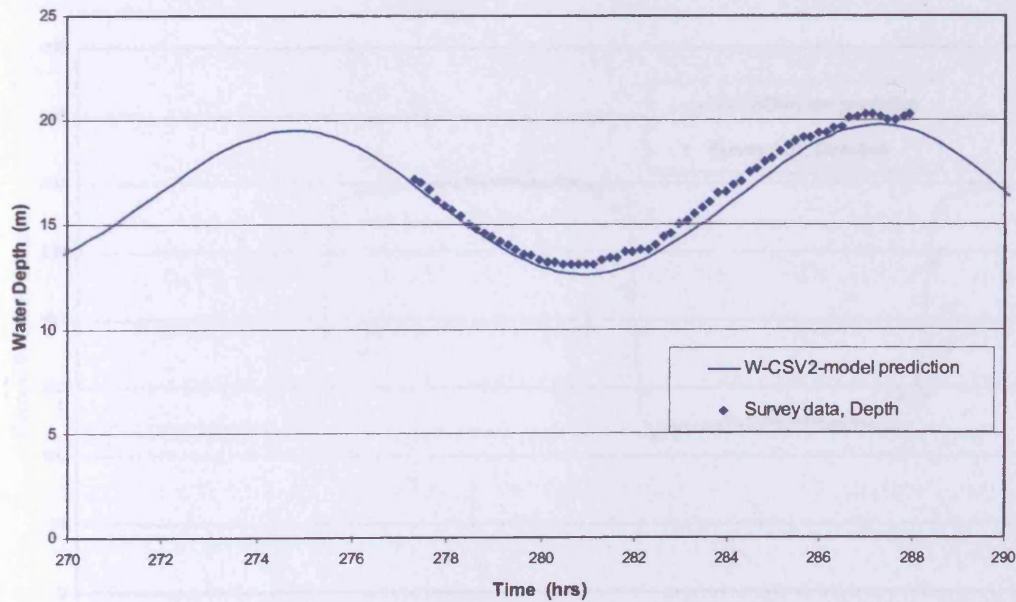Figure 6.26   Comparison of predicted and measured depths at Minehead on 01/08/01
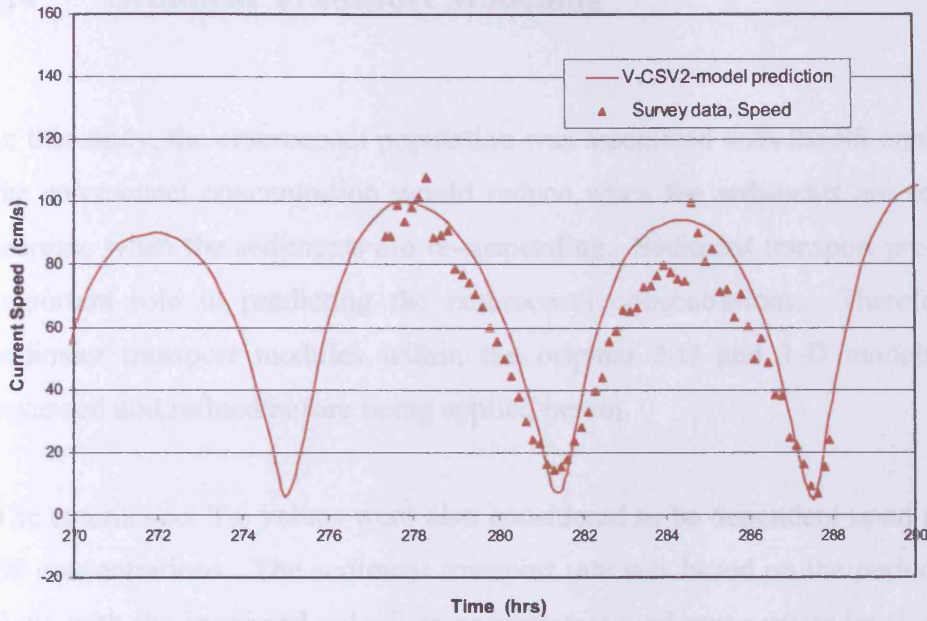
Figure 6.27   Comparison of predicted and measured current speeds at Minehead on 01/08/01
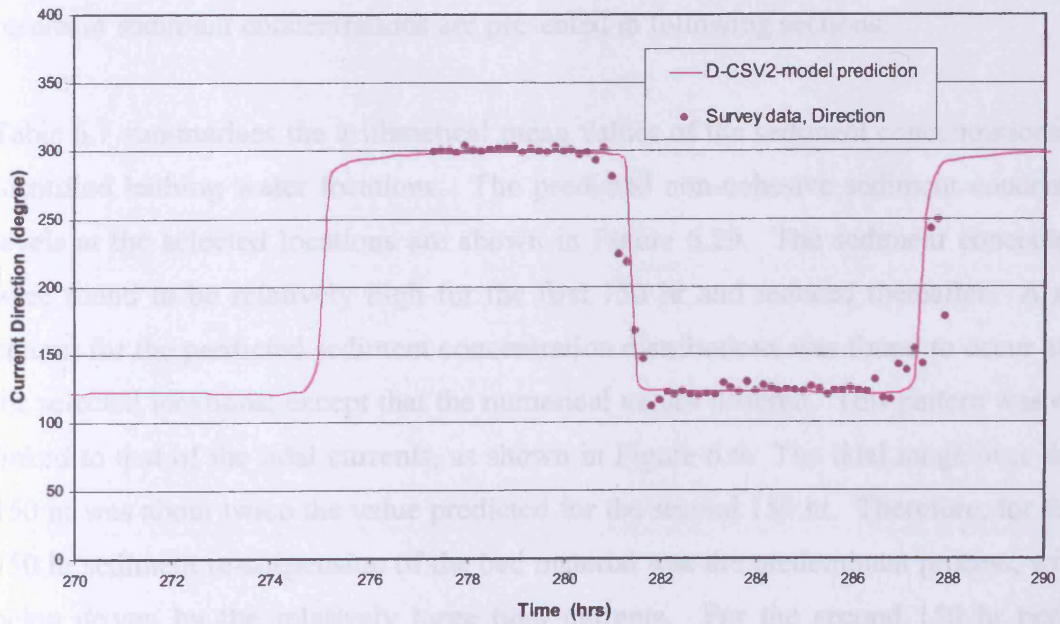

Figure 6.28   Comparison of predicted and measured current speeds at Minehead on 01/08/01

6.4 Sediment Transport Modelling

In this study, the enterococci population was associated with the SS concentration. Thus, the enterococci concentration would reduce when the sediments are settling down and increase when the sediments are re-suspending. Sediment transport processes played an important role in predicting the enterococci concentrations. Therefore, the existing sediment transport modules within the original 2-D and 1-D models were carefully reviewed and refined before being applied herein.

The enterococci T_{90} values were also considered to be dependent upon the instantaneous SS concentrations. The sediment transport rate was based on the periodicity of the tidal flow, with the increased velocities occurring around mean water level causing increased entrainment of the local bed sediments into the water column.

In the sediment transport model, as stated previously, both non-cohesive and cohesive sediments were included, with the suspended solids (SS) concentrations being the sum of non-cohesive and cohesive sediment concentrations. The series plots of the predicted results of sediment concentrations are presented in following sections.

Table 6.7 summarises the arithmetical mean values of the sediment concentrations at the identified bathing water locations. The predicted non-cohesive sediment concentration levels at the selected locations are shown in Figure 6.29. The sediment concentrations were found to be relatively high for the first 150 hr and reduced thereafter. A similar pattern for the predicted sediment concentration distributions was found to occur at all of the selected locations, except that the numerical values differed. This pattern was closely linked to that of the tidal currents, as shown in Figure 6.6. The tidal range over the first 150 hr was about twice the value predicted for the second 150 hr. Therefore, for the first 150 hr sediment re-suspension of the bed material was the predominant process, with this being driven by the relatively large tidal currents. For the second 150 hr period of simulation, sediment settling was the predominant process, based on the smaller tidal currents leading to a higher proportion of the sediments being deposited back onto the

bed. As the sediments were advected (or transported) by the tidal currents, then the sediment concentration levels at each of the bathing water sites varied in a cyclical manner, which correlated with each tide.

Table 6.7   Predicted mean sediments concentration at the bathing water locations

ID	Beach Location (site No.)	Non-cohesive sediment mg/l	Cohesive sediment mg/l	SS mg/l
36000	Clevedon Beach, 4	286.2	2523.9	2810.1
35000	Minehead Terminus, 10	112.7	4711.3	4824.0
35200	Blue Anchor West, 7			
35100	Dunster North West, 7	90.9	4988.5	5079.4
35900	Weston-s-mare Sand Bay, 1	223.2	2526.8	2750.0
35800	Weston Main, 2			
35700	Weston-s-Mare Uphill Slipway,2	173.4	2271.7	2445.1
35500	Berrow north of Unity Form, 3			
35600	Brean, 3	95.76	1360.0	1455.8
36300	Cold Knap Barry, 18	181.4	1426.5	1607.9
36200	Whitmore Bay Barry, 14			
36100	Jacson Bay Barry, 14	213.9	1564.5	1778.4
36400	Southerndown, 17	32.3	424.7	457.0
34900	Porlock Weir, 9	25.26	508.0	533.3
34800	Lynmouth 8	17.4	315.0	332.4
36700	Rest Bay Porthcawl 15	52.0	274.4	326.4
36600	Sandy Bay Porthcawl, 16			
36500	Trecco Bay Porthcawl 16	37.43	194.3	231.7
34600	Ilfracome Hele, 6			
34700	Combe Martin 6	35.64	168.2	203.8
34450	Ilfracombe Tunnels Beach, 5			
34500	Ilfracombe Capstone 5	23.7	329.7	353.4
36900	Swansea Bay 12	1.22	2.54	3.76
37200	Langland Bay, 11			
37100	Limeslade Bay, 11			
37000	Bracelet Bay, 11	15.5	57.0	72.5
37500	Port Eynon Bay, 20	19.8	117.7	137.5
37400	Oxwich Bay, 19	21.5	70.6	92.1
36800	Abrafan, 13	0.334	0.567	0.90

The cohesive sediment predictions were based on two different averaged floc sizes, namely 0.010 and 0.063 mm. At the sites Minehead and Duster North West the average floc size was set to 0.010 mm, as the median size was found to be between 0.0085 and 0.0125 mm, see volume III of the project report (Stapleton et al., 2004). Model predicted tidal currents were also smaller at these sites. From an early investigation by Posford Duvivier and ABP Research (2000) 'mud' and 'sandy mud' were found to exist in the areas around Minehead, and 'fine sand' and 'medium sand' were found along the South Wales coast. Therefore at the remaining sites the average floc size was set to 0.063 mm. The predicted results at a number of selected sites are shown in Figure 6.30.

The suspended solids included both non-cohesive and cohesive particles and, hence, the SS concentration levels were added to the non-cohesive and cohesive sediments levels. The SS concentrations at selected sites are presented in Figure 6.31, again illustrating a similar cyclical pattern to that observed in Figures 6.29 and 6.30.
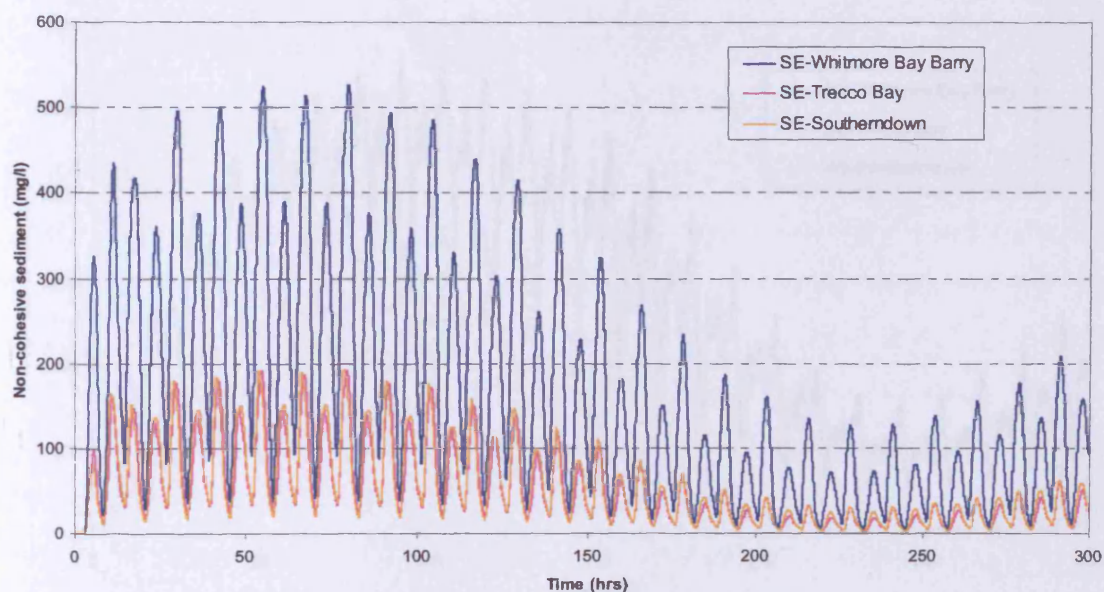

Figure 6.29   Predicted non-cohesive sediment concentration distributions at three bathing water locations
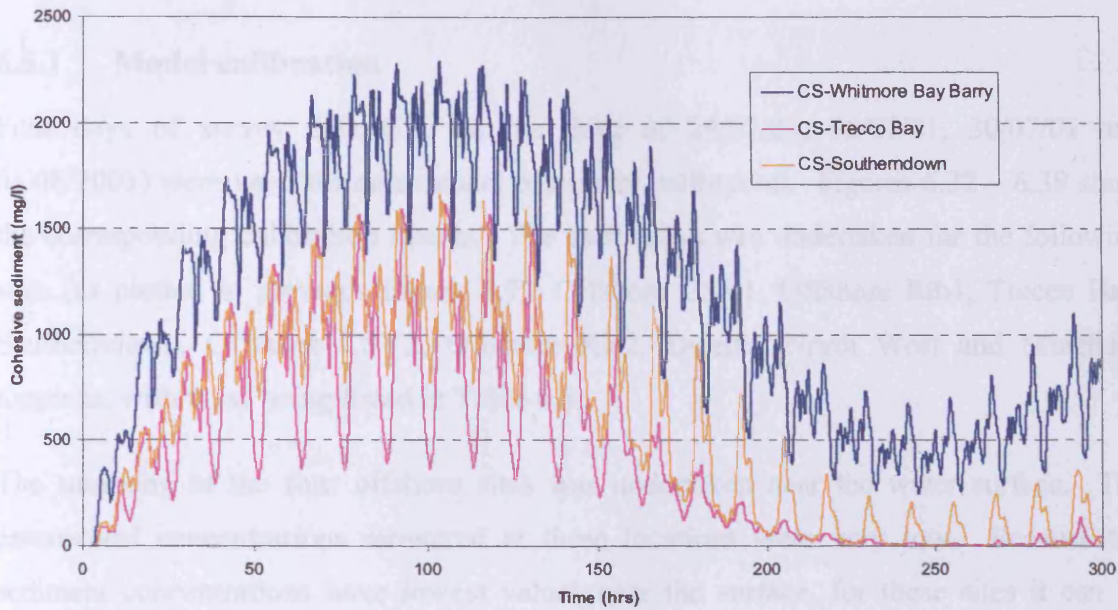
Figure 6.30   Predicted cohesive sediment concentration distributions at three bathing water locations
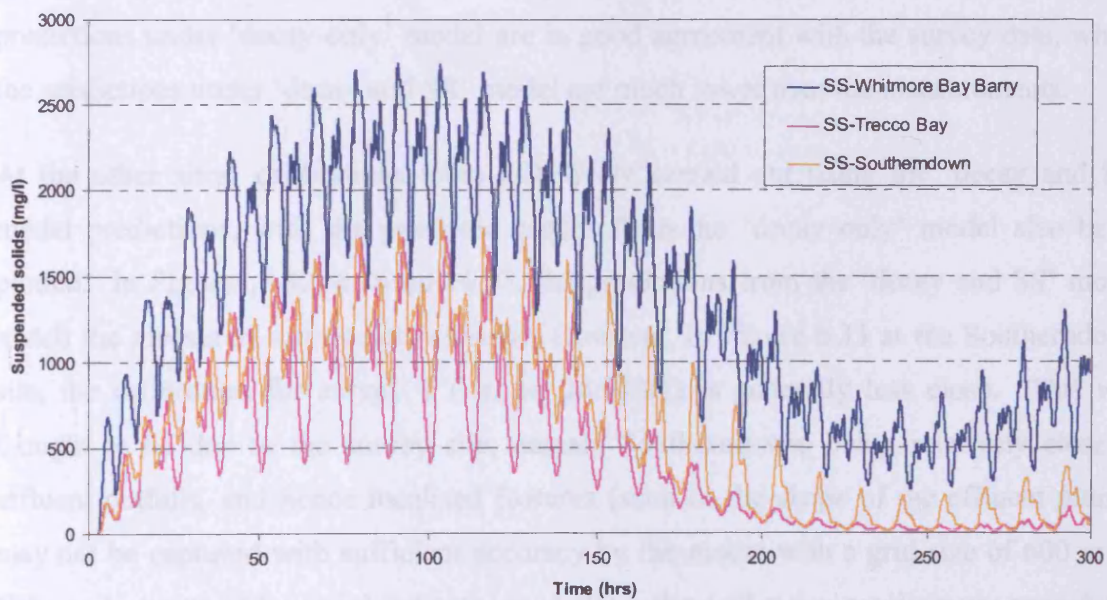

Figure 6.31   Predicted distributions of suspended solids concentration at three bathing water locations

6.5   Water Quality Simulation

6.5.1   Model calibration

Four days of survey data (i.e. on the days of 24/07/01, 26/07/01, 30/07/01 and 01/08/2001) were used for enterococci parameter calibration. Figures 6.32 – 6.39 show the corresponding calibration results. The calibration was undertaken for the following sites (as plotted in previous Figure 6.7): Offshore CSV1, Offshore Rib1, Trecco Bay, Southerndown, Offshore CSV2, Offshore Rib2, Dunster North West and Minehead terminus, with these being listed in Table 6.6.

The sampling of the four offshore sites was undertaken near the water surface. The enterococci concentrations measured at these locations were very low. Because the sediment concentrations have lowest values near the surface, for these sites it can be assumed that the increase of enterococci due to the entrainment of bed sediment is effectively zero. In addition, the re-suspension effect from sediment is particularly low in the surface zone since it was found from an early study of the Severn Estuary (ABP and Posford) that at these locations the bed sediment size is generally quite large (ABP, 1999; McLaren, 1999). As can be seen from Figures 6.34, 6.35, 6.38 and 6.39, the enterococci predictions under 'decay only' model are in good agreement with the survey data, where the predictions under 'decay and SS' model are much lower than the measurements.

At the other sites, calibrations were effectively carried out using the 'decay and SS' model predictions, with the predicted results from the 'decay only' model also being plotted. In Figures 6.32, 6.36 and 6.37, the predictions from the 'decay and SS' model match the measured survey data closely. However, in Figure 6.33 at the Southerndown site, the calibration for survey 1 (i.e. on 24/07/01) is generally less close. This was thought to be due to the survey site, namely Southerndown, being relatively close to effluent outfalls, and hence localised features (such as the shape of the effluent plume) may not be captured with sufficient accuracy by the model with a grid size of 600 m by 600 m. In terms of bacterial indicator modelling, the calibration results were considered to be satisfactory.

Figure 6.32   Model predicted and measured enterococci levels at Trecco Bay (24/07/01, 26/07/01)

Figure 6.33   Model predicted and measured enterococci levels at Southerndown (24/07/01, 26/07/01)

Figure 6.34   Model predicted and measured enterococci levels at Offshore CSV1
(24/07/01, 26/07/01)

Figure 6.35   Model predicted and measured enterococci levels at Offshore Rib1
(24/07/01, 26/07/01)

Figure 6.36   Model predicted and measured enterococci levels at Duster North West (30/07/01, 01/08/01)
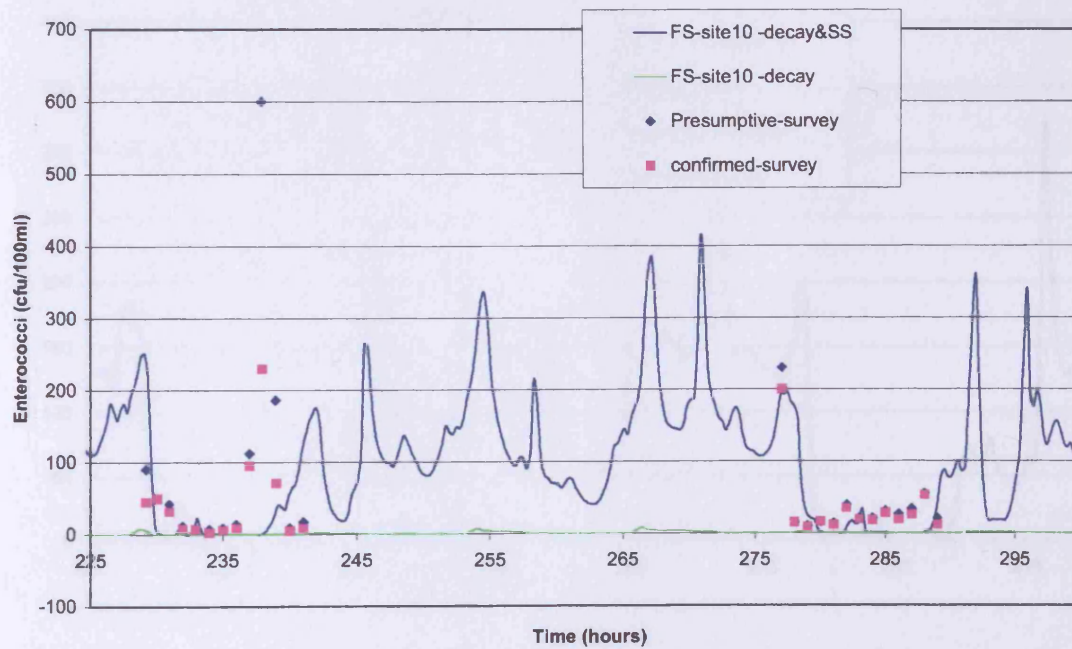
Figure 6.37   Model predicted and measured enterococci levels at Minehead Terminus (30/07/01, 01/08/01)
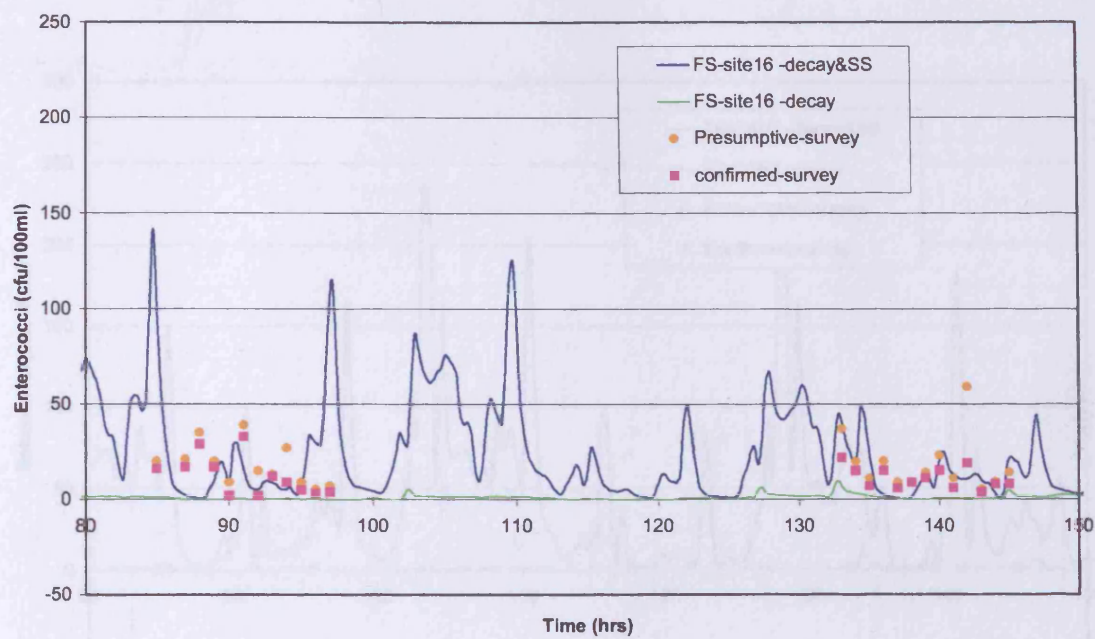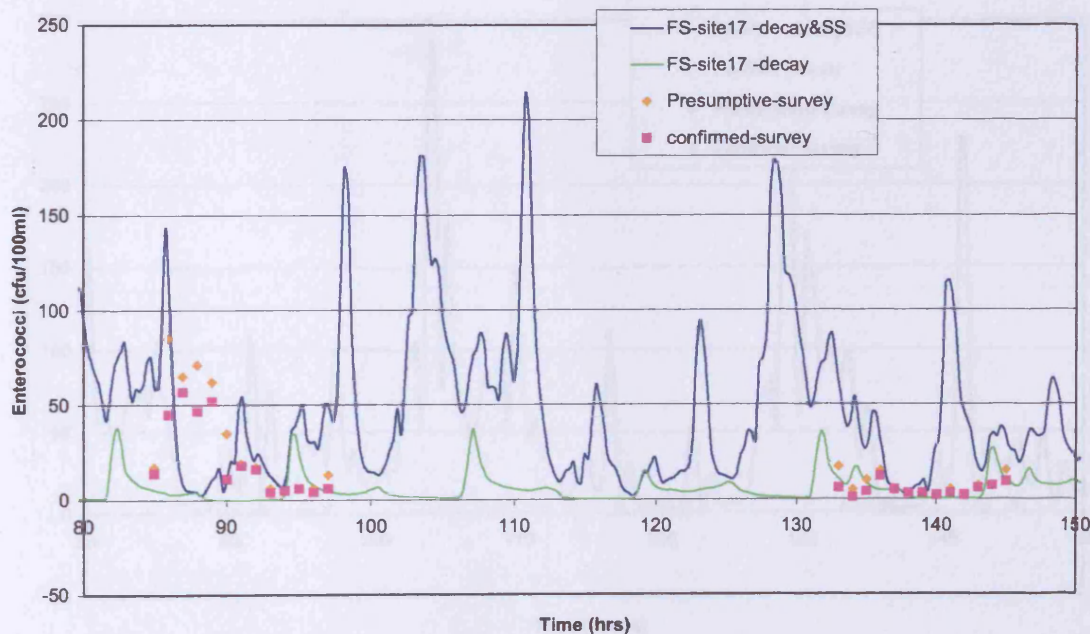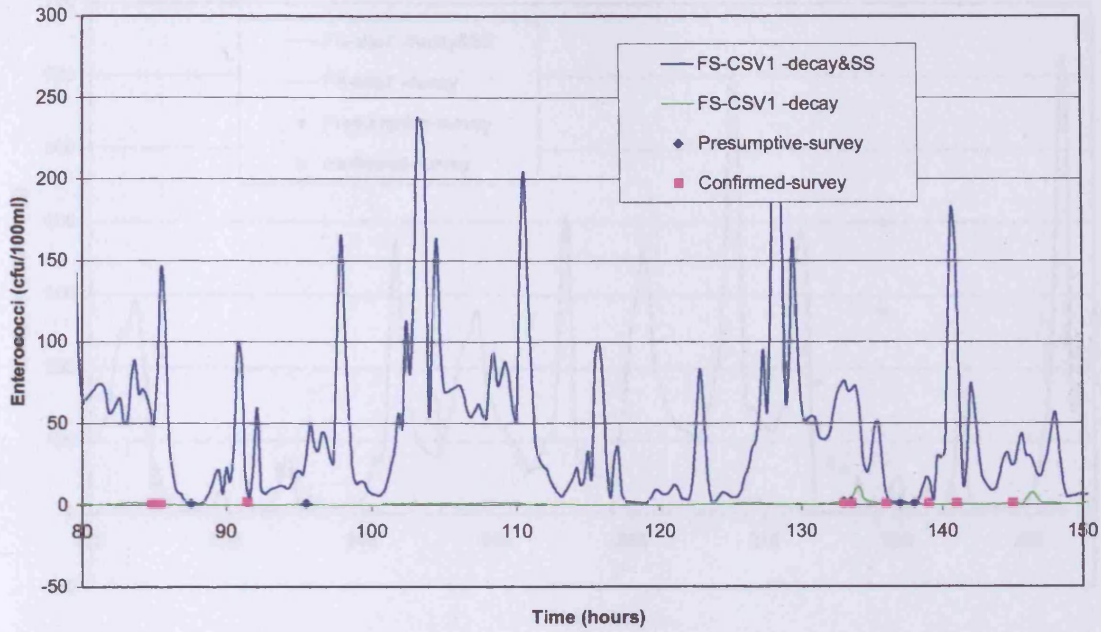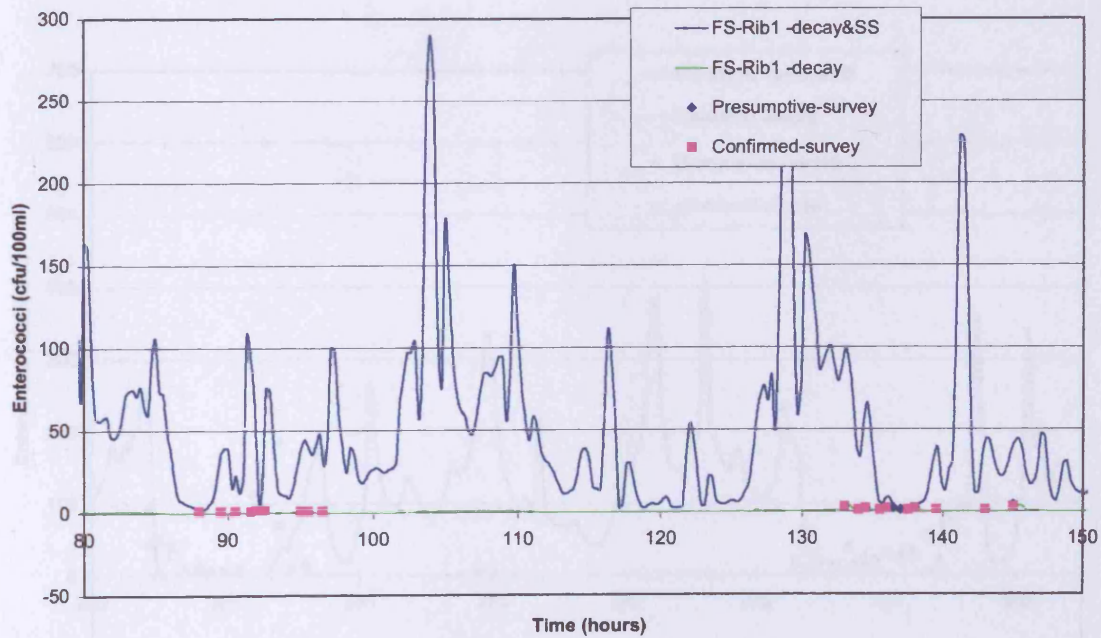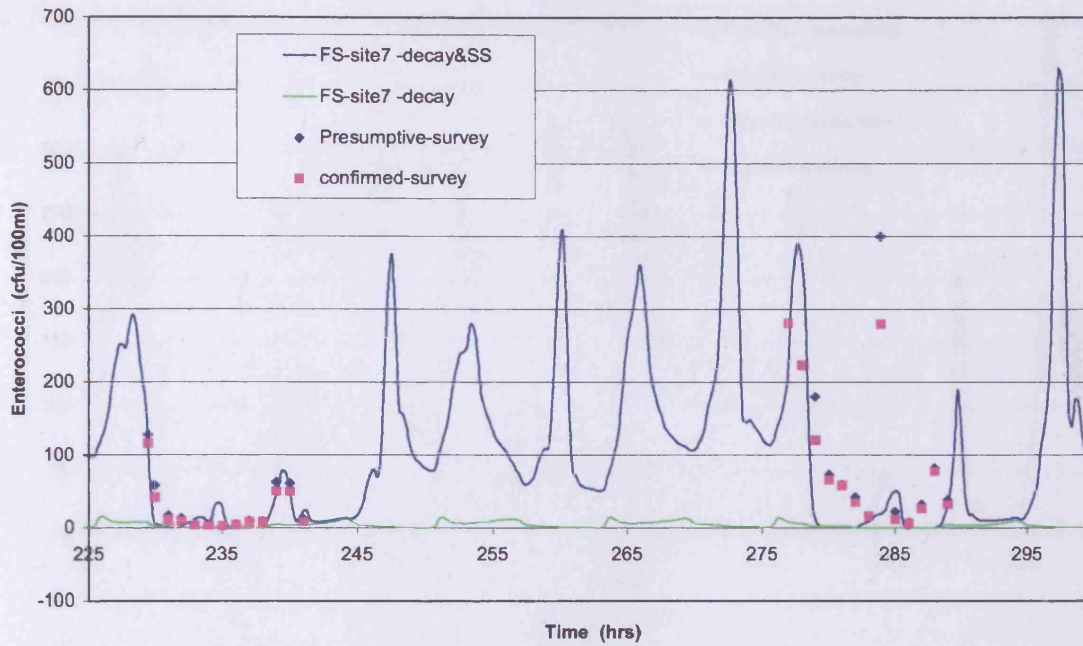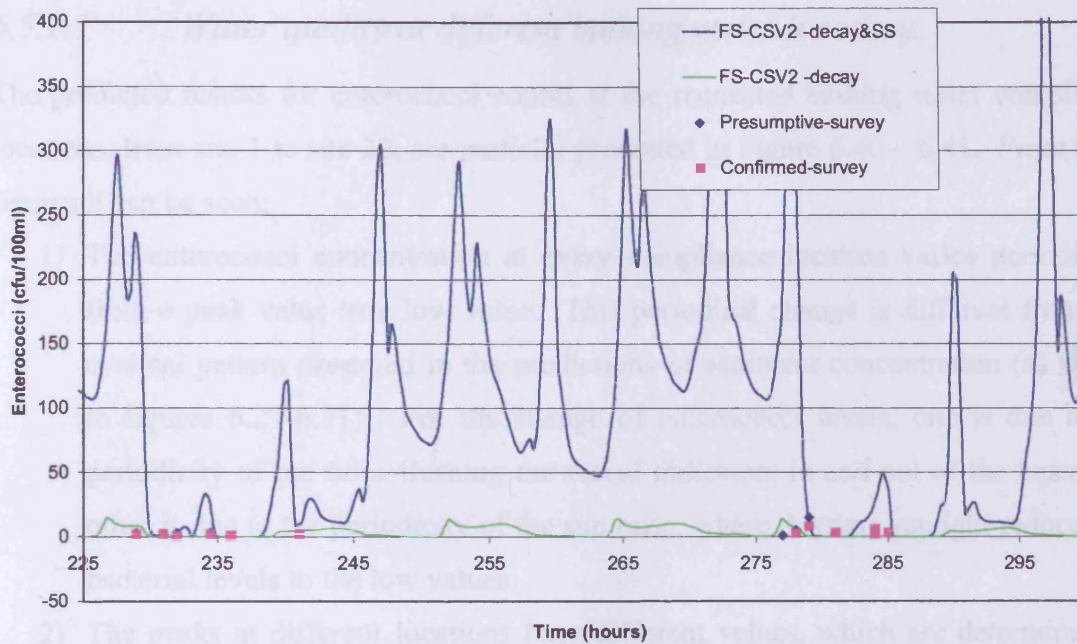
Figure 6.38 Model predicted and measured enterococci levels at Offshore CSV2 (30/07/01, 01/08/01)
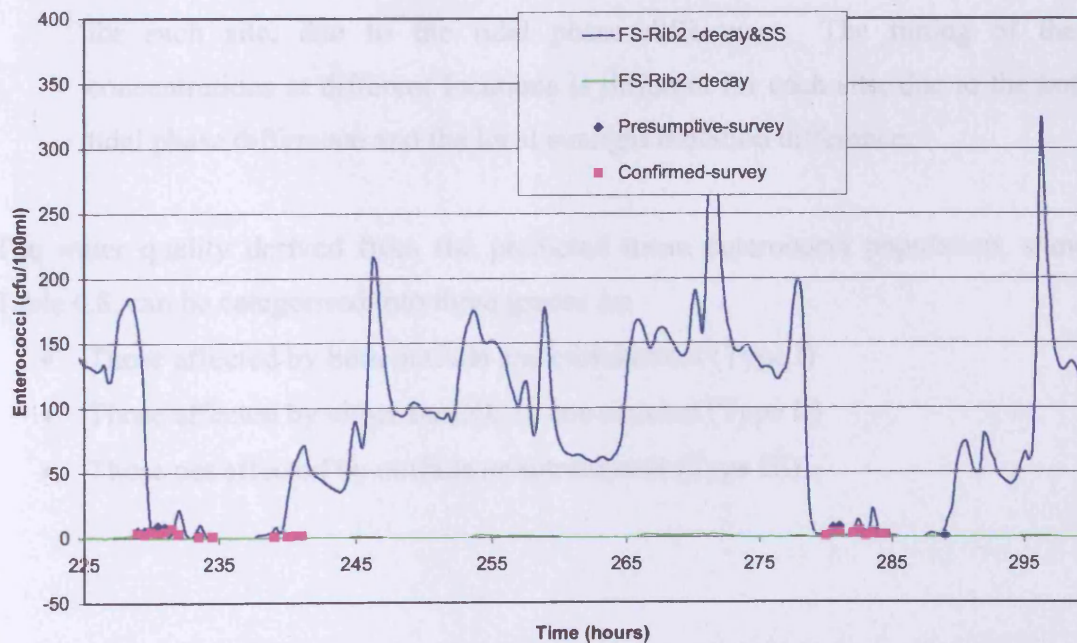
Figure 6.39 Model predicted and measured enterococci levels at Offshore Rib2 (30/07/01, 01/08/01)

6.5.2   Simulation results and discussions

6.5.2.1   Water quality at different bathing water locations

The predicted results for enterococci counts at the requested bathing water compliance locations, from site 1 to site 20, are partially presented in Figure 6.40 – 6.41. From these figures it can be seen:

1) The enterococci concentration at every compliance location varies periodically from a peak value to a low value. This periodical change is different from that cyclical pattern observed in the predictions of sediment concentration (as shown in figures 6.29-6.31). For the change of enterococci levels, one is due to the periodicity of the tides flushing the faecal indicators in and out of the basin; the other is due to the periodicity of the sun raise, where daytime sunlight reduces the bacterial levels to the low values.

2) The peaks at different locations have different values, which are determined by the exchanges between the compliance locations and the pollutant input sites and also determined by the efficiency of the sunlight radiation presented at the location which kills the bacteria. The low values at different locations are different too.

3) The timing of the peak concentrations occurred at different locations is different for each site, due to the tidal phase difference. The timing of the low concentrations at different locations is different for each site, due to the both the tidal phase difference and the local sunlight radiation difference.

The water quality derived from the predicted mean enterococci population, shown in Table 6.8, can be categorised into three grades as:

- Those affected by both outfalls and entrainment (Type I)
- Those affected by either outfalls or entrainment (Type II)
- Those not affected by outfalls or entrainment (Type III)
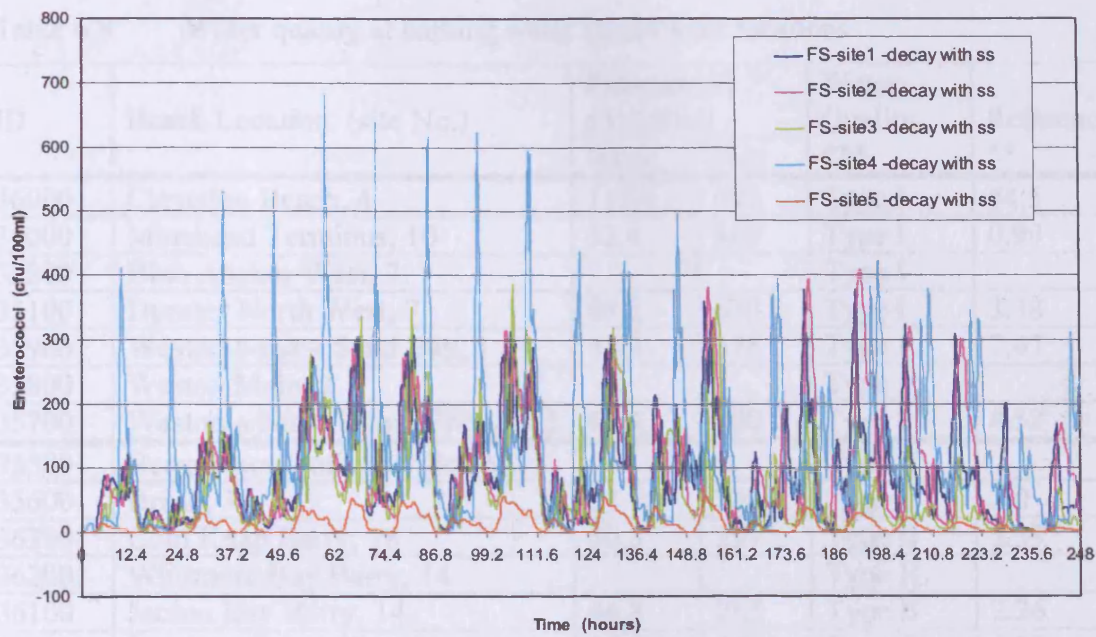
Figure 6.40   Predicted enterococci concentration levels at sites 1-5.
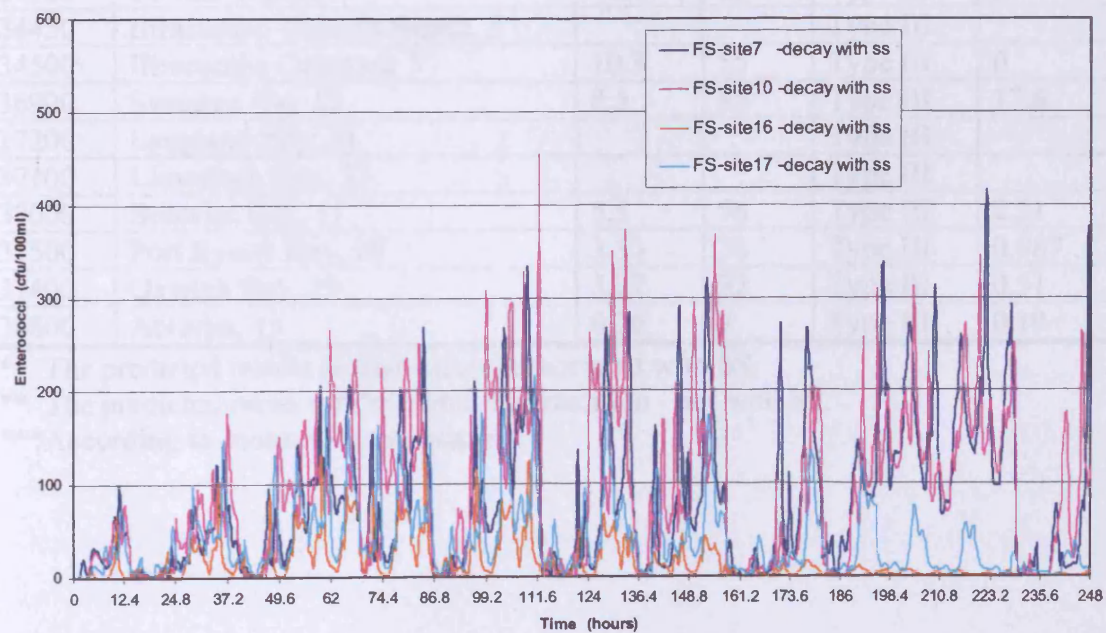
Figure 6.41   Predicted enterococci concentration levels at sites 7, 10, 16 and 17.

Table 6.8   Water quality at bathing water compliance locations

ID	Beach Location (site No.)	Enterococci * cfu/100ml		Water Quality ***	Reference **
		Mean	Max		
36000	Clevedon Beach, 4	115.0	697	Type I	44.5
35000	Minehead Terminus, 10	93.8	448	Type I	0.99
35200	Blue Anchor West, 7			Type I	
35100	Dunster North West, 7	88.2	630	Type I	3.38
35900	Weston-s-mare Sand Bay, 1	84.4	375	Type I	7.47
35800	Weston Main, 2			Type I	
35700	Weston-s-Mare Uphill Slipway,2	83.4	400	Type I	4.52
35500	Berrow north of Unity Form, 3			Type II	
35600	Brean, 3	57.1	380	Type II	2.0
36300	Cold Knap Barry, 18	50.3	297	Type II	2.33
36200	Whitmore Bay Barry, 14			Type II	
36100	Jacson Bay Barry, 14	46.8	265	Type II	2.26
36400	Southerndown, 17	32.7	210	Type II	5.92
34900	Porlock Weir, 9	34.6	253	Type II	0.086
34800	Lynmouth 8	18.5	121	Type II	0.69
36700	Rest Bay Porthcawl 15	15.4	171	Type II	1.66
36600	Sandy Bay Porthcawl, 16			Type II	
36500	Trecco Bay Porthcawl 16	13.3	141	Type II	1.03
34600	Ilfracome Hele, 6			Type III	
34700	Combe Martin 6	10.4	66	Type III	0
34450	Ilfracombe Tunnels Beach, 5			Type III	
34500	Ilfracombe Capstone 5	10.3	55	Type III	0
36900	Swansea Bay 12	8.5	85	Type III	17.6
37200	Langland Bay, 11			Type III	
37100	Limeslade Bay, 11			Type III	
37000	Bracelet Bay, 11	5.5	56	Type III	2.21
37500	Port Eynon Bay, 20	3.33	38	Type III	0.087
37400	Oxwich Bay, 19	3.27	32	Type III	0.51
36800	Abrafan, 13	0.36	7	Type III	0.19

*   The predicted results (mean values) associated with SS.
**   The predicted mean results under the condition - not with SS.
***According to enterococci population.

6.5.2.2   *Water quality – Type I*

There are five sites (seven bathing water locations) in Table 6.8 where the local water quality is affected by the WwTW outfalls (or riverine inputs) and also the strong tidal currents producing the entrainment of pollutant from the bed into the water. In other words, these locations are affected by both the close proximity of outfall discharges and the sediment re-suspension. On these sites the water quality can be regarded as 'poor'.

6.5.2.3   *Water quality – Type II*

Different from the poor-water-quality sites, these sites are affected either by the sediment resuspension or by the outfall discharges (or riverine inputs), so comparing with type I the water pollution on these sites are obviously lower. For example, at site 12 the water pollution only comes from the nearby outfalls but not the sediment re-suspension, since from figures 7.11 in chapter 7 it can been seen that the sediment fluxes at this site is dominated by sediment deposition.

6.5.2.4   *Water quality – Type III*

In Table 6.8 it is shown that the Type III sites have very low enterococci counts. The maximum concentrations on these sites are all less than 100 cfu/100ml when the predictions are carried out under the condition 'with SS' in which moderate sediment re-suspension is involved. In particular, sites 13, 19 and 20 are found to have very low enterococci concentrations, so these sites can be defined as being good water quality. These sites are located relatively far from WwTW outfalls (or riverine discharges) and exhibited very low SS concentrations.

With the same order in Table 6.8, Table 6.7 recorded the predicted mean value of sediment concentrations at the bathing water compliance locations. Comparing the predicted results in these two tables it is clearly seen that the sediment concentrations at good-water-quality sites are relatively low. Especially at site 13 the suspended solid concentration level is less than 1 mg/l, while the mean enterococci population predicted at this site is virtually below 1 cfu/100ml.

6.6   Summary

A dynamically linked 1-D and 2-D hydro-environmental tool has been developed and successfully applied as the bacterial contamination simulation model to the Bristol Channel and Severn Estuary. The model contains 29 river inputs, with different values for the microbial contaminants, and also includes 34 sewage effluent discharges from various wastewater treatment works located along the coastal zones. The study area covers receiving water area, related to an integrated catchments area of up to 15,000 km^2, including a number of bays, rivers and the main estuary.

In this study, the model developed to predict the fate of enterococci organisms in estuarine and coastal waters not only involves all WwTW outfalls and riverine discharges from a wide range of the catchments areas, but also contains the factors of significant reactions in the water column. They include: (i) a dynamic time-varying decay rate due to the variation of turbidity (the instantaneously predicted SS concentrations) and the in-situ hourly observed sunlight radiations; (ii) an additional disappearance rate due to the sediment deposition with the assumption of most bacteria being attached onto the surface of sediments; (iii) a bacterial re-appearance rate due to the entrainment of bed sediments.

To summarise, in this model the enterococci estimation has been associated with the sediment transport processes with a dynamic varying sunlight-dependent and SS-dependent decay rate, while the enterococci disapearence rate has been linked to sediment deposition and concentration increase is related to sediment re-suspension. Therefore suspended solids (SS) affect the enterococci concentration through two processes: (i) physical transport (referring to sedimentation or re-suspension); (ii) sunlight attenuation (the suspended particles prevent the light penetration so that to reduce the bactericidal effect). In this application excellent hydrodynamic calibration and satisfactory enterococci calibration were achieved.

Chapter 7

SENSITIVITY STUDY

During the model application described in Chapter 6 a sensitivity analysis of the bacteriological parameters was designed and carried out. The sensitivity analysis was aimed to reveal the knowledge of the mechanisms in various aspects of the bacteria transport and decay processes, so that to obtain an overview of the modelling results and improve the accuracy. Because of the uncertainties in predicting water quality in natural waters, a sensitivity analysis can provide information to identify the source of the uncertainties involved in the model inputs, the empirical parameters, the principle modelling formulae and the model process selections, etc. A series of tests were carried out to study the impact of the model process selections (e.g. the sensitivity of dilution effect, sediment transport effect; the model starting position effect) and the model parameter selections (e.g. the sensitivity of decay rate; bed concentration; attached bacteria ratio and the suspended solids concentration levels on the disappearance of bacterial organisms) on model results.

7.1 Dilution Effect

7.1.1 The concepts of dilution model

The Bristol Channel and Severn Estuary constitute an estuarine basin with a large flow-through volume, primarily driven by the very high tidal range of up to 14 meters. It was therefore deemed appropriate to assess the predicted dilution effects produced by these

large tidal currents and then go further to assess the sensitivity of various current related parameters. The dilution test was carried out using the same governing equations, but with a zero decay rate being assumed in the model; thus the fate of bacteria was governed purely by the physical processes of advection and dispersion, thus named 'dilution model'.

Two different runs were undertaken in order to investigate the impact of sediment transport under dilution conditions. For the first run it was assumed that the bacteria organisms were transported by the flow velocity only, which was termed as the 'dilution only' run. For the second run it was assumed that the bacteria were transported by both the flow and sediment fluxes. The second run included both flow dilution effects and the attachment to sediments in the deposition and re-suspension phases. This process of dilution with sediment transport is referred as 'dilution and SS'.

7.1.2   Results of 'dilution only' model

The predicted enterococci concentration distributions for selected bathing water sites, based on the dilution only model, were calculated to estimate the 'dilution only' effect and these results are plotted in Figures 7.1 and 7.2.
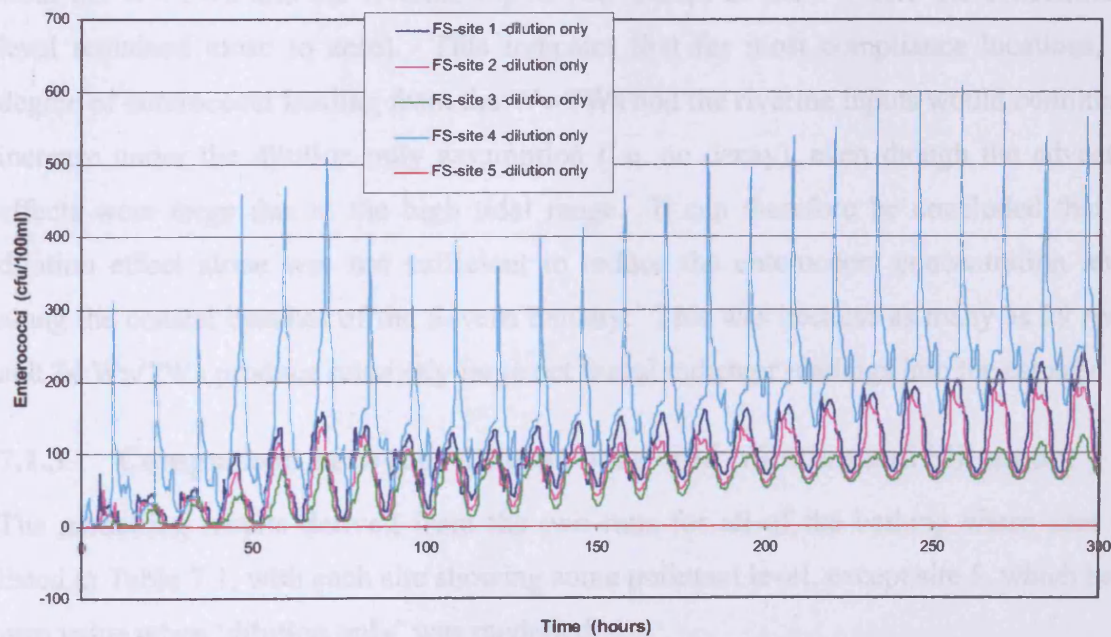
Figure 7.1 Predicted enterococci levels based on dilution only model at sites 1-5.
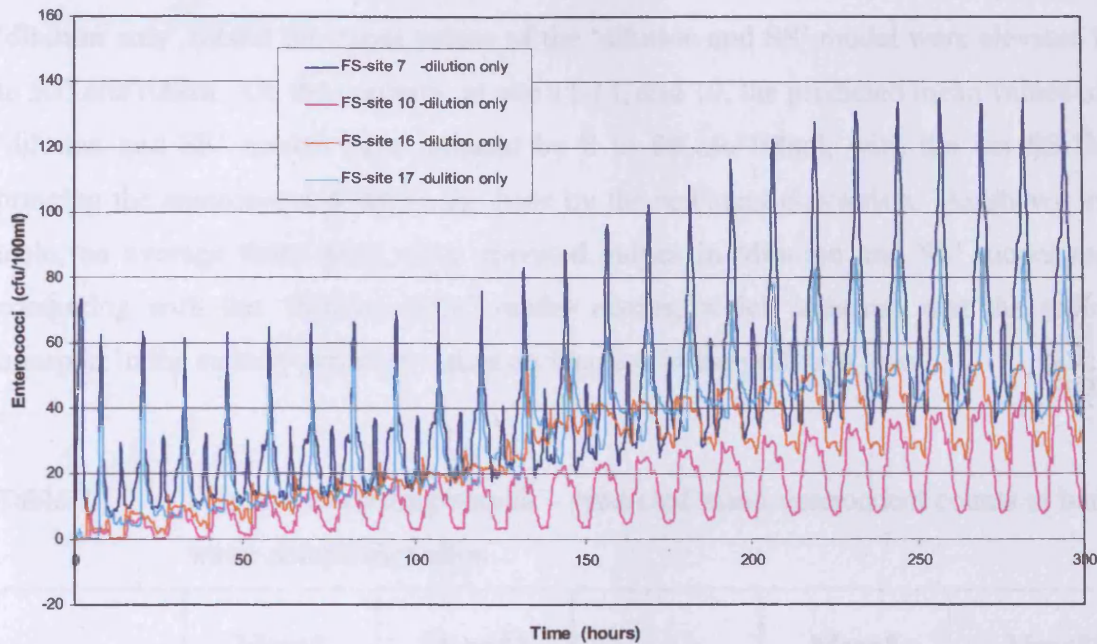
Figure 7.2 Predicted enterococci levels based on dilution only model at sites 7,10,16-17.

In Figures 7.1 and 7.2 it can be seen that, for all the sites modelled, the enterococci population level rises along the simulation time due to the accumulation of discharges from the WwTWs and the riverine inputs (i.e. except at site 5 where the concentration level remained close to zero). This indicates that for most compliance locations, the degree of enterococci loading from the WwTWs and the riverine inputs would continue to increase under the dilution only assumption (i.e. no decay), even though the advection effects were large due to the high tidal range. It can therefore be concluded that the dilution effect alone was not sufficient to reduce the enterococci concentration levels along the coastal beaches of the Severn Estuary. This was because as many as 29 rivers and 34 WwTWs produce relatively large net faecal indicator loadings into the estuary.

7.1.3   Comparison between 'dilution only' and 'dilution and SS' model

The modelling results derived from the two runs for all of the bathing water sites are listed in Table 7.1, with each site showing some pollutant level, except site 5, which had a zero value when 'dilution only' was modelled.

In the table it can be seen that at sites 1-10, 14-18, and 20, the net SS fluxes bring additional enterococci sources from beds to the water column, so comparing with 'dilution only' model the mean values of the 'dilution and SS' model were elevated by 5 to 500 cfu/100ml. On the contrary, at site 11-13, and 19, the predicted mean values of the 'dilution and SS' model were reduced by 8 to 80 cfu/100ml, with the net SS fluxes bringing the enterococci down to the beds by the sediment deposition. As shown in the table, on average there were more elevated values in 'dilution and SS' model results comparing with the 'dilution only' model results, which indicates that the sediment transport in the estuary generally cause an increase in the pollutant level.

Table 7.1   Dilution modelling results – predicted mean enterococci counts at bathing water compliance sites

Location	Mean* (cfu/100ml)	Mean** (cfu/100ml)	Location	Mean* (cfu/100ml)	Mean** (cfu/100ml)
Site 1	93.7	300.4	Site 11	37.6	11.5
Site 2	76.5	292.2	Site 12	97.9	12.6
Site 3	58.2	198.6	Site 13	25.8	0.73
Site 4	168	327.8	Site 14	68.9	176.0
Site 5	0	38.6	Site 15	26.1	44.2
Site 6	0.02	30.2	Site 16	26.3	41.3
Site 7	26.7	580.6	Site 17	34.0	91.1
Site 8	1.3	61.2	Site 18	63.5	171.8
Site 9	4.4	113.6	Site 19	16.2	8.52
Site 10	14.6	602.3	Site 20	6.5	11.9

*   Predicted from dilution only model.

** Predicted from dilution model with sediment transport.

Figures 7.3 - 7.5 show the comparison between the time-series simulations of 'dilution only' model and the 'dilution and SS' model at three selected sites, with one having the elevated enterococci counts and one having the reduced counts for the SS-linked dilution model during the whole simulation time; and the third one having an averaged rising counts but falling down in neap tides. The comparison shown in Figure 7.3 suggests that re-suspended sediments significantly added enterococci to the water column and this is the most likely case occurring in the Severn Estuary.
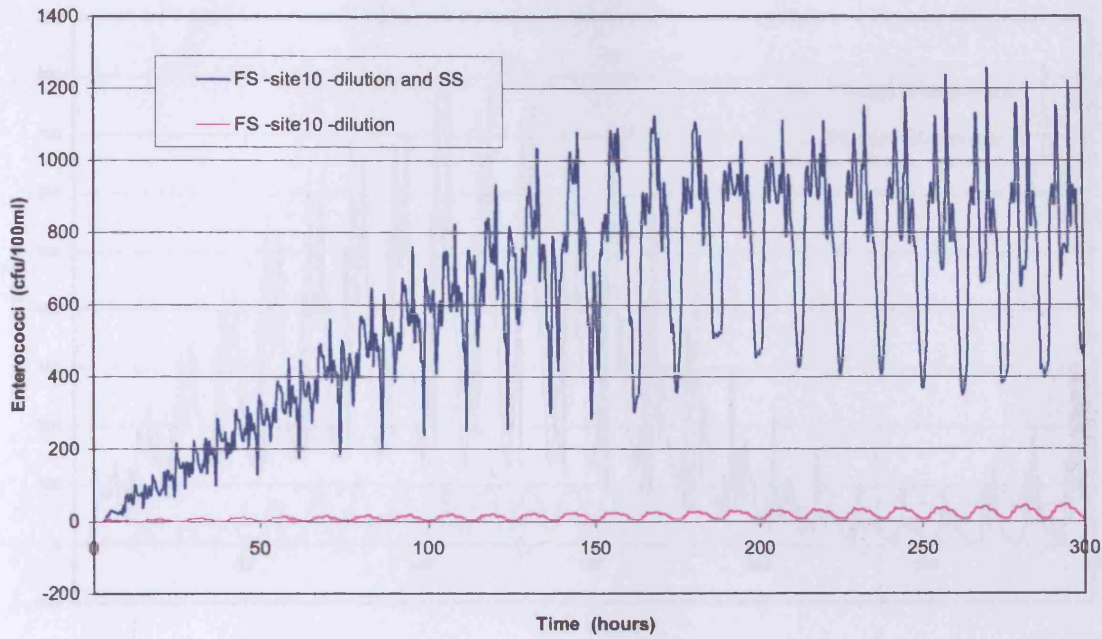
Figure 7.3 Comparison of enterococci levels for 'dilution and SS' model having elevated predictions than 'dilution only' model at site 10 - Minehead Terminus.
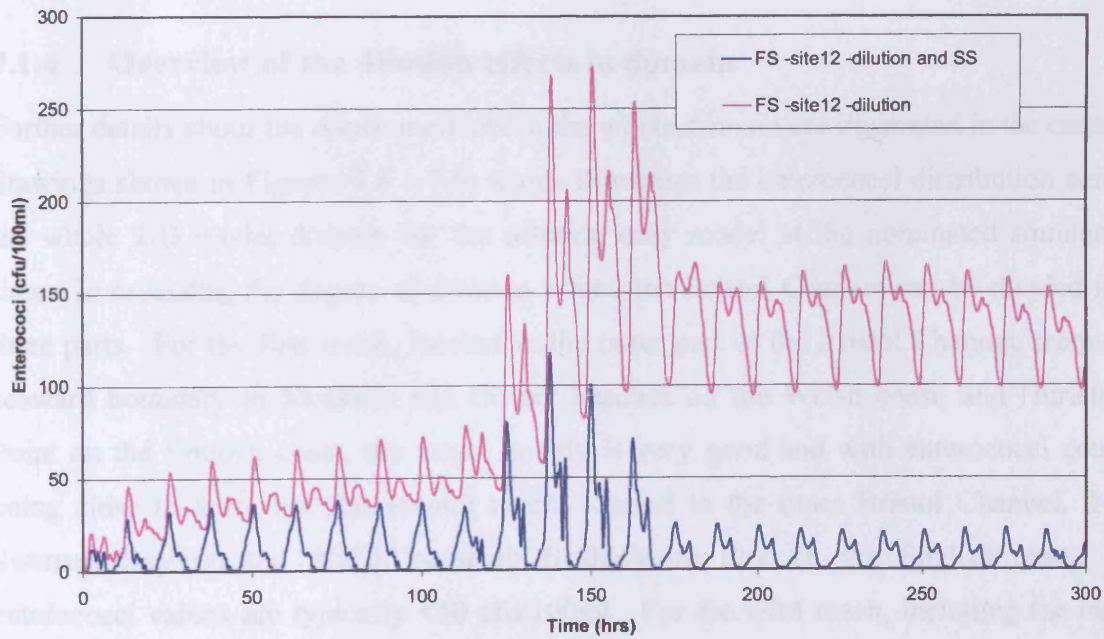
Figure 7.4 Comparison of enterococci levels for 'dilution and SS' model having fallen predictions than 'dilution only' model at site 12 – Swansea Bay.
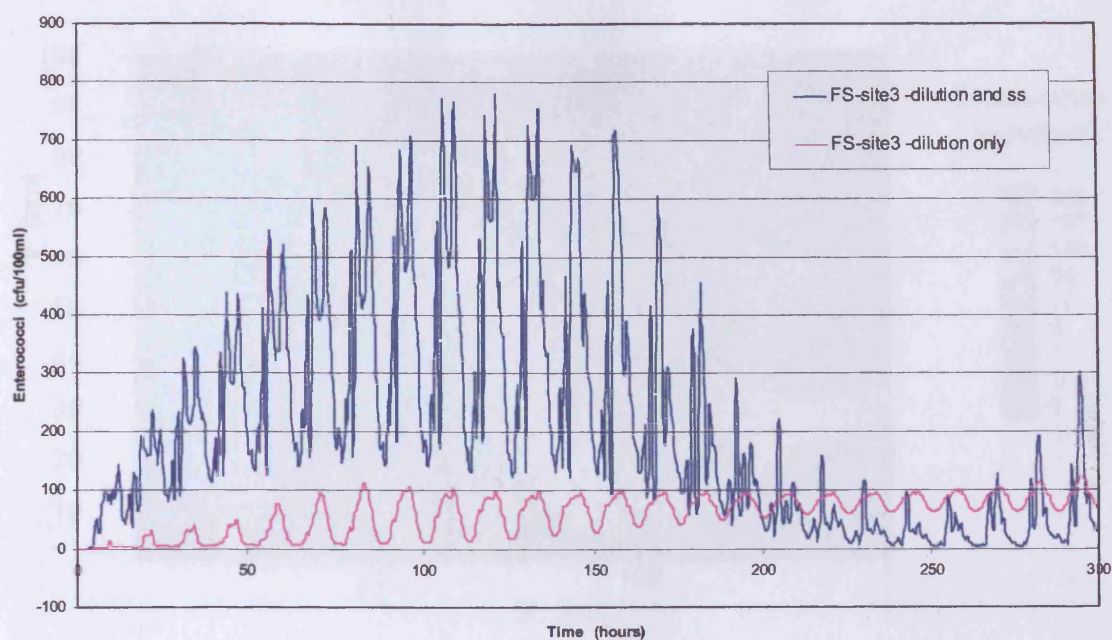
Figure 7.5 Comparison of enterococci levels for 'dilution only' and 'dilution and SS' model predictions at site 3 – Brean Beach, with rising counts at spring tides and falling counts at neap tides.

7.1.4   Overview of the dilution effects in domain

Further details about the dilution effects in the whole domain are illustrated in the contour drawings shown in Figures 7.6 – 7.9, which illustrates the enterococci distribution across the whole 2-D model domain for the dilution only model at the nominated simulation time. In assessing the degree of dilution effect, the Bristol Channel can be divided into three parts. For the first reach, located in the outer part of the Bristol Channel, from the seaward boundary to Swansea and Gower beaches on the Welsh coast, and Hurlstone Point on the English coast, the water quality is very good and with enterococci counts being close to zero. For the second reach, located in the inner Bristol Channel, from Swansea Bay on the Welsh coast to Bridgewater Bay on the English coast, the enterococci values are typically <50 cfu/100ml. For the third reach, including the inner Bristol Channel (i.e. starting from Bridgewater Bay) and the Severn Estuary the enterococci levels typically exceed 100 cfu/100ml.

Figure 7.6 Predicted enterococci distribution along bathing water sites for dilution only
model at high water during neap tide

Figure 7.7 Predicted enterococci distribution along bathing water sites for dilution only
model at mid-ebb during neap tide

Figure 7.8 Predicted enterococci distribution along bathing water sites for dilution only
model at low water during neap tide

Figure 7.9 Predicted enterococci distribution along bathing water sites for dilution only
model at mid-flood during neap tide.

7.2   Re-entrainment of Indicator Enterococci

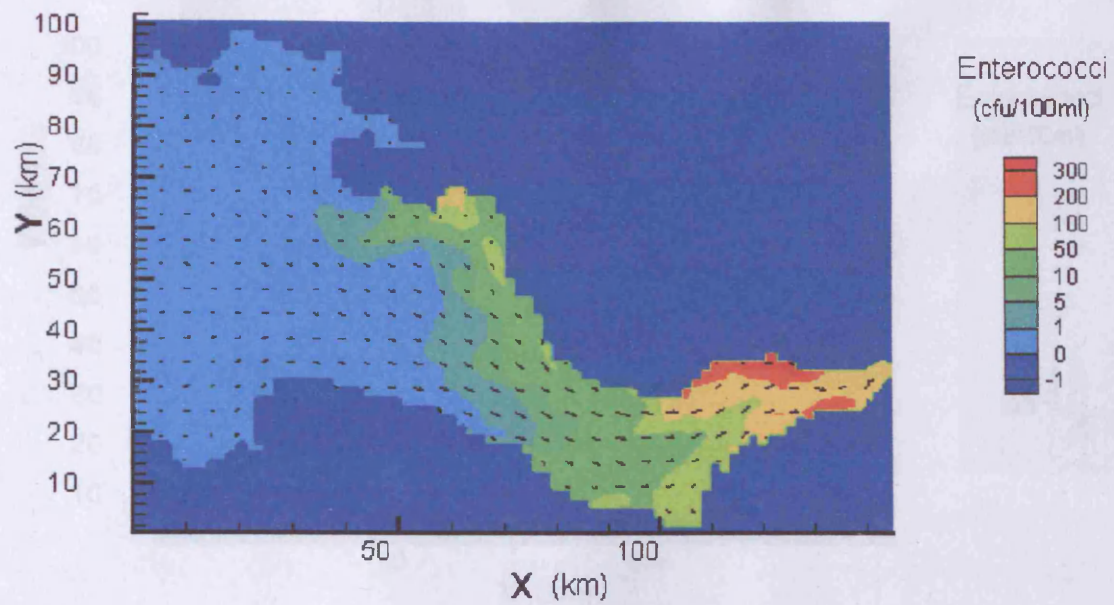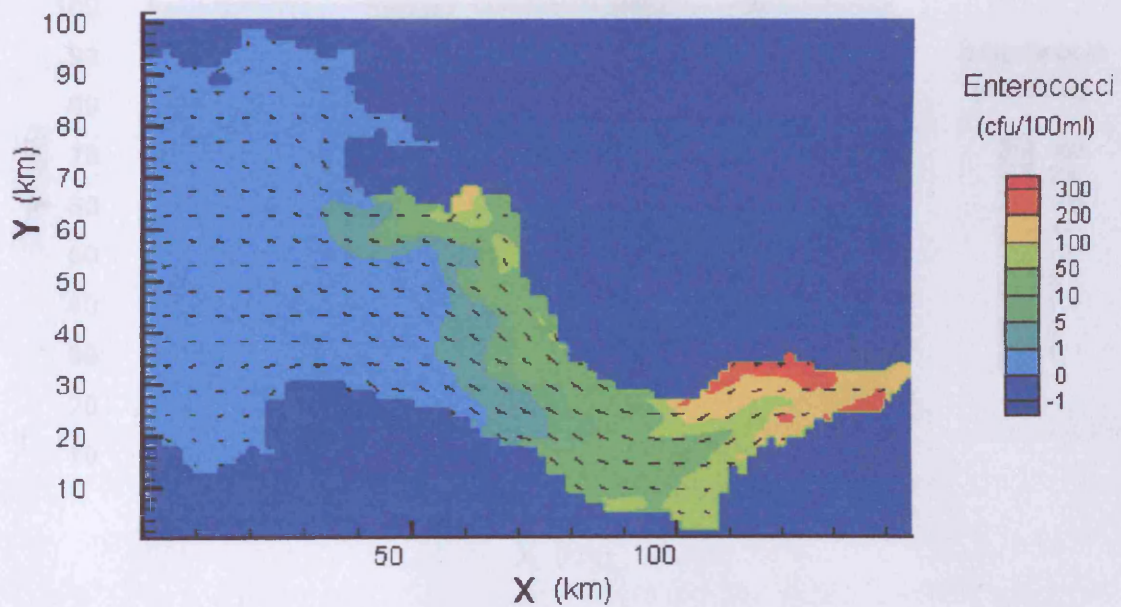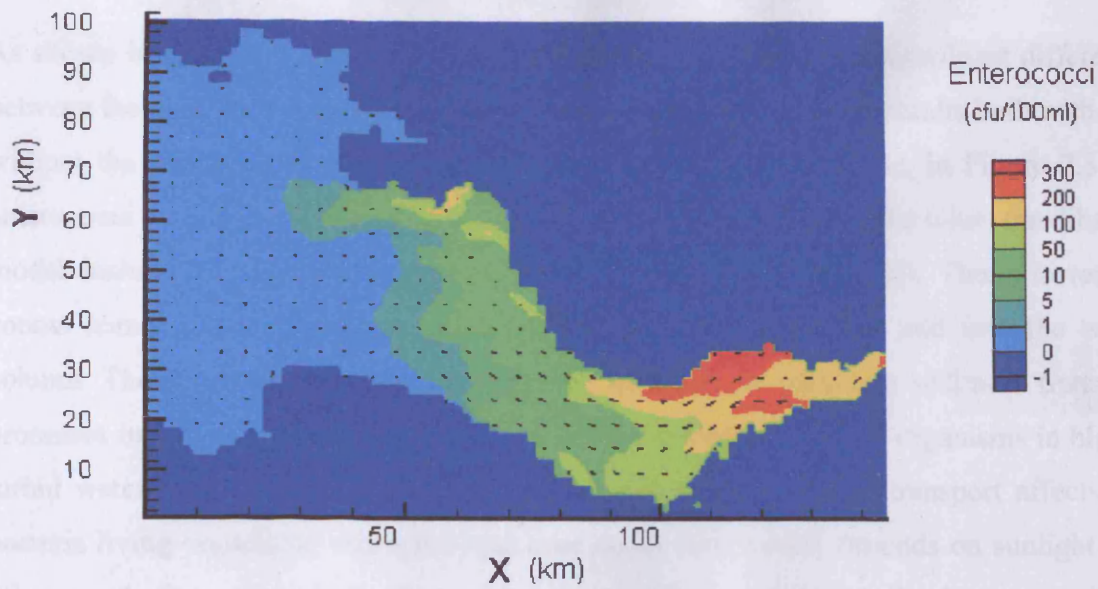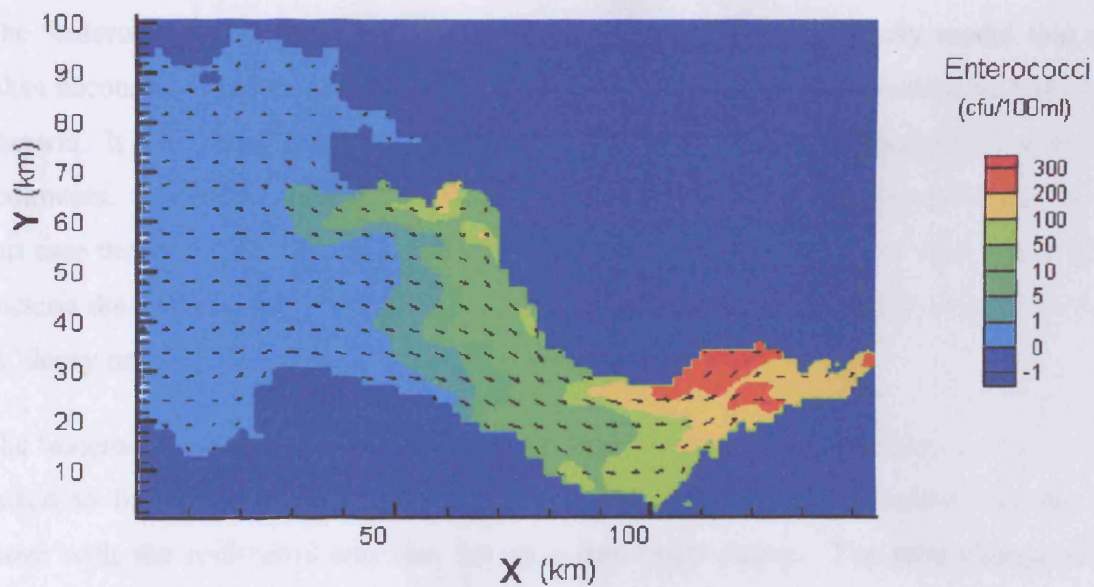As shown in Figures 7.3 and 7.5 in the previous section, there is a significant difference between the enterococci levels predicted when comparing the model results both with and without the inclusion of sediment transport processes. For example, in Figure 7.3 the enterococci counts increased significantly for all of the simulation time when the dilution model included suspended solids (i.e. the 'dilution and SS' model). These increased counts come from re-entrainment of the sediments from the bed and into the water column. These results therefore highlight the necessity of including sediment transport processes in representing the fate and transport of bacterial indicator organisms in highly turbid water basins. This section demonstrates how the sediment transport affects the bacteria living organisms when the real time decay rate, which depends on sunlight and SS concentrations, is applied. Comparisons are carried out between the decay model and the decay with SS model predictions.

7.2.1   The concepts of decay model

For comparison purposes a number of simulation scenarios are referred to and these are defined below:

The 'enterococci not with SS' scenario refers to the first order decay model that only takes account of the enterococci populations in the water column existing as free-living bacteria. It does not include the addition of bacteria arising from re-suspension of the bed sediments. It neither counts the bacteria disappearance due to sediment deposition. In this case the total disappearance of bacteria populations refers only one term, which is the bacteria die-off (or, decay). For this scenario the simulations and model outputs are cited as 'decay only'.

The 'enterococci associated with SS' scenario refers to the first order decay model being linked to the sediment transport processes. The enterococci population, thereby will move with the sediments and also act as a first order decay. The total change of the population thus includes both the bacteria die-off and the physical movements between the two phases of water column and bed sediments. For this scenario the simulations and model outputs are cited as 'decay with SS'.

A number of simulations were therefore carried out to compare the differences between the predicted enterococci population levels, both with and without the SS fluxes. When the bacteria predictions with SS were included then the enterococci concentrations associated with the sediments on beds were set at a level of 1000 cfu/gm.

7.2.2   Results of decay models

The decay model predictions for the required bathing water sites of interest are listed in Table 7.2. This table illustrates that the predicted mean enterococci counts for all of the sites, except site 12, under the 'decay with SS' model are higher than under the 'decay only' model. So the impact of suspended sediments concentrations on the indicator enterococci counts is significant. For site 12, it is likely that the velocity is generally small and deposition is the main sedimentation processes. Comparing to the 'dilution only' model results in Table 7.1, the 'decay only' predictions in Table 7.2 show on average a reduction of one order of magnitude in the mean concentration value, indicating

Table 7.2   Model results of the 'decay only' and 'decay with SS' approaches

Location	Mean* (cfu/100ml) decay with SS	Mean** (cfu/100ml) decay	Maximum (cfu/100ml) decay with SS	Minimum (cfu/100ml) decay with SS
Site 1	84.4	7.47	375	0
Site 2	83.4	4.52	400	0
Site 3	57.1	2	380	0
Site 4	115.0	44.5	697	0
Site 5	10.3	0	55	0
Site 6	10.4	0	66	0
Site 7	88.2	3.38	630	0
Site 8	18.5	0.69	121	0
Site 9	34.6	0.086	253	0
Site 10	93.8	0.99	448	0
Site 11	5.5	2.21	56	0
Site 12	8.5	17.6	85	0
Site 13	0.36	0.19	7	0
Site 14	46.6	2.26	265	0
Site 15	15.4	1.66	171	0
Site 16	13.3	1.03	141	0
Site 17	32.7	5.92	210	0
Site 18	50.3	2.33	297	0
Site 19	3.27	0.51	32	0
Site 20	3.33	0.087	38	0

*   Predictions for first order decay model with SS, i.e. 'decay with SS'
**   Predictions for first order decay model without SS, i.e. 'decay only' or 'decay'

that the bacterial first order decay processes are effectively sufficient to kill most of the released faecal bacteria from the WwTW outfalls and the riverine discharges.

7.2.3   Comparison between 'decay only' and 'decay with SS' model

Figures 7.10 to 7.12 show a comparison between the predictions made by the 'decay only' model and the 'decay with SS' model at various sites.

Figure 7.10 Comparison of enterococci levels at Site 3 for 'decay only' model and 'decay with SS' model, at Brean Beach.

In Figure 7.10, at Site 3, (Brean Beach), it can be seen that the predicted results without SS are almost zero, whereas when the SS inputs are included the predicted values are typically up to 200 cfu/100ml. This suggests that the faecal indicator concentrations at this site are primarily determined by sediment transport processes.

For this site, (see the pink line in Figure 7.10), it is shown that the decay processes are sufficient to reduce the enterococci concentration derived from the outfall discharges as the predicted enterococci levels are bellow 10 cfu/100ml when the SS fluxes are not included. This result is also supported by the data shown in Tables 7.1 and 7.2. In Table

7.1 the 'dilution only' results showed that there was a mean enterococci population level of 58.2 cfu/100ml at Site 3. Likewise, from Table 7.2 it can be seen that Site 3 had a mean enterococci level of about 2 cfu/100ml due to the effect of the kinetic first order decay ('decay only'), with the decay kinetics being sufficient to reduce the bacteria to negligible levels. In contrast, when the effect of the suspended sediments was included in the decay model, the mean enterococci level rose to 57.1 cfu/100ml (shown in Table 7.2). Thus, the model results again indicate that re-suspended bed sediments caused an increase of the predicted enterococci population levels in the water column.

Figure 7.11 shows the results for the compliance site located in Swansea Bay. In contrast to Figure 7.10, the predicted bacterial levels shown for 'decay only' simulations are generally only slightly less than those predicted for decay with SS. This prediction indicates that the pollution levels at this site are governed mainly by the outfall discharges and adjacent riverine inputs.
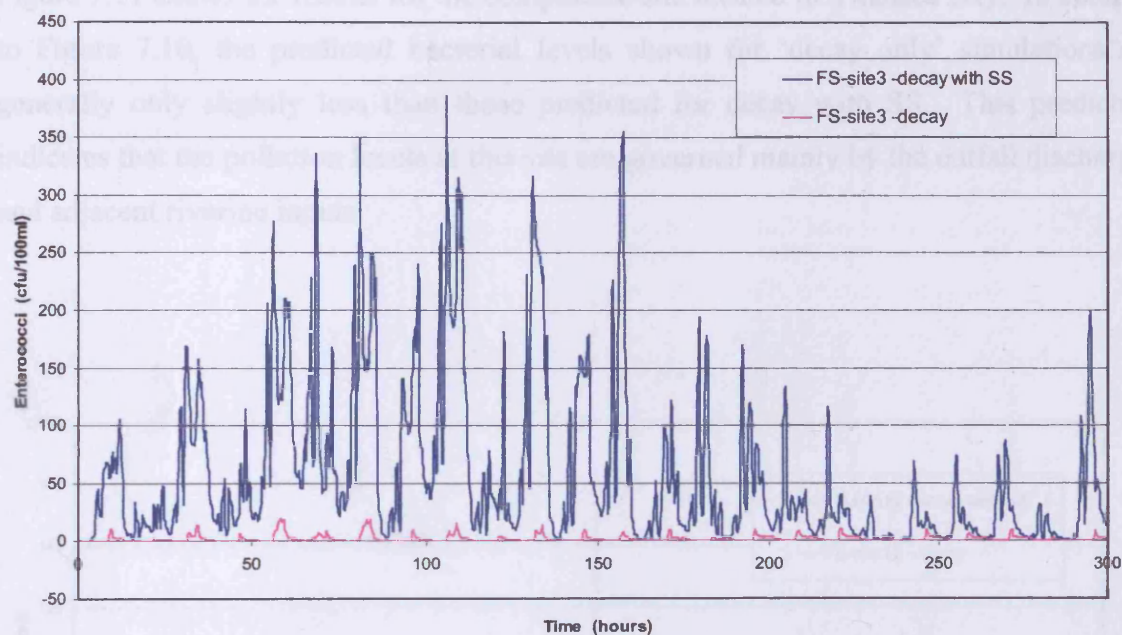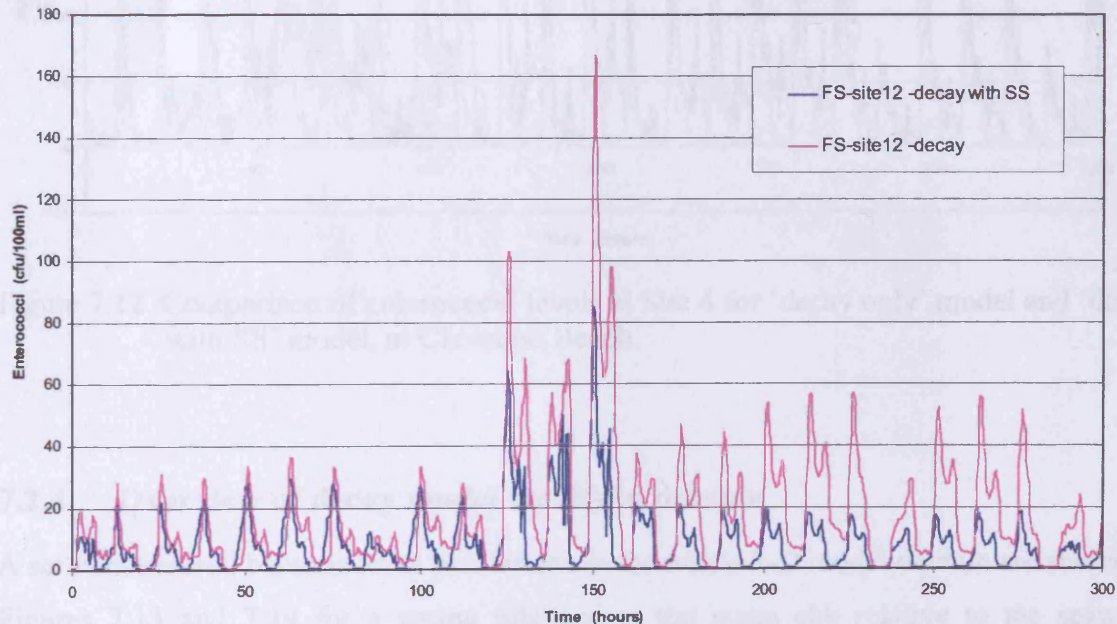

Figure 7.11 Comparison of enterococci levels at Site 12 for 'decay only' model and 'decay with SS' model, in Swansea Bay

Figure 7.12 illustrates the predicted results at Clevedon Beach, where, again, higher predicted bacteria concentrations arise due to the inclusion of SS inputs, but there are big values under the 'decay only' predictions too. This prediction indicates that the enterococci concentrations at this site arise from both inputs associated with the bed sediments and inputs from nearby effluent outfalls/or river inputs. Therefore, at this kind of site, the predicted enterococci concentrations are associated jointly with the suspended sediment and terrestrial fluxes.
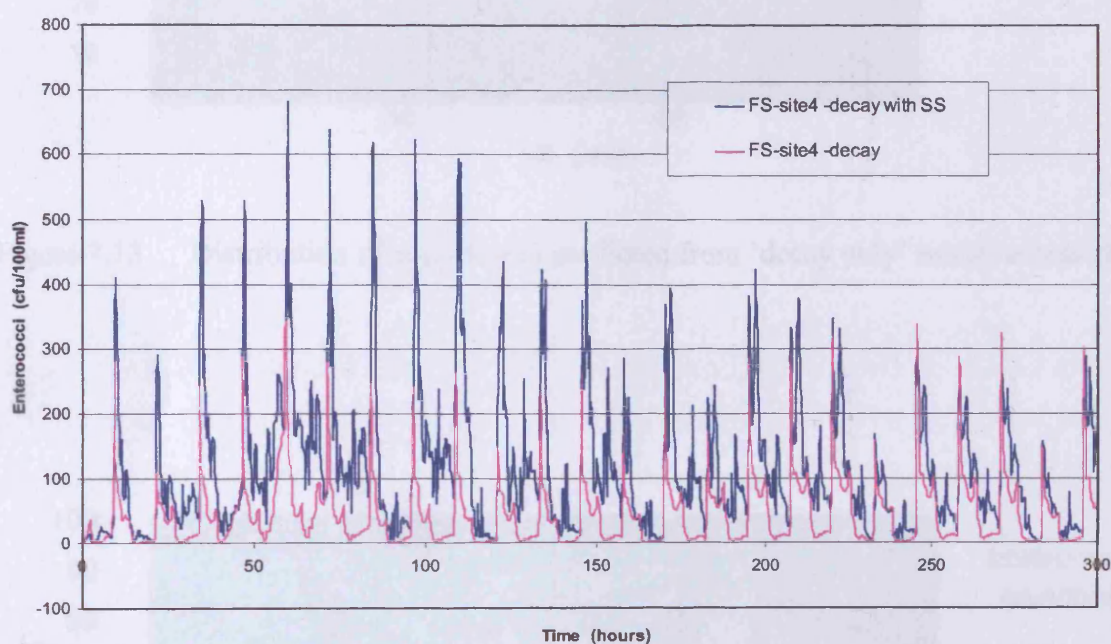
Figure 7.12 Comparison of enterococci levels at Site 4 for 'decay only' model and 'decay with SS' model, at Clevedon Beach.

7.2.4 Overview of decay model results in domain

A set of contoured bacteria level predictions in the whole 2-D model domain are shown in Figures 7.13 and 7.14 for a spring tide and at the mean ebb relative to the seaward boundary. Figure 7.13 shows the distribution of enterococci for 'decay only', whereas Figure 7.14 shows the corresponding distribution occurring for 'decay with SS'. Figures 7.13 and 7.14 suggest that the SS fluxes to the enterococci levels in the water column have a significant effect over a much larger area than terrestrially derived fluxes alone.
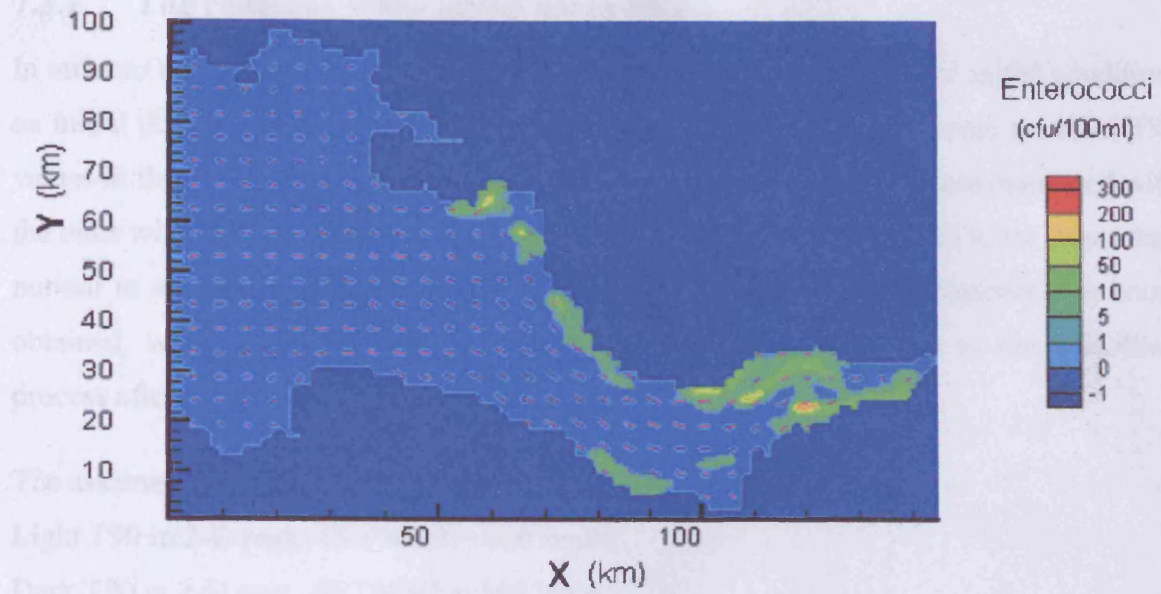
Figure 7.13   Distribution of enterococci predicted from 'decay only' model at mid-ebb.
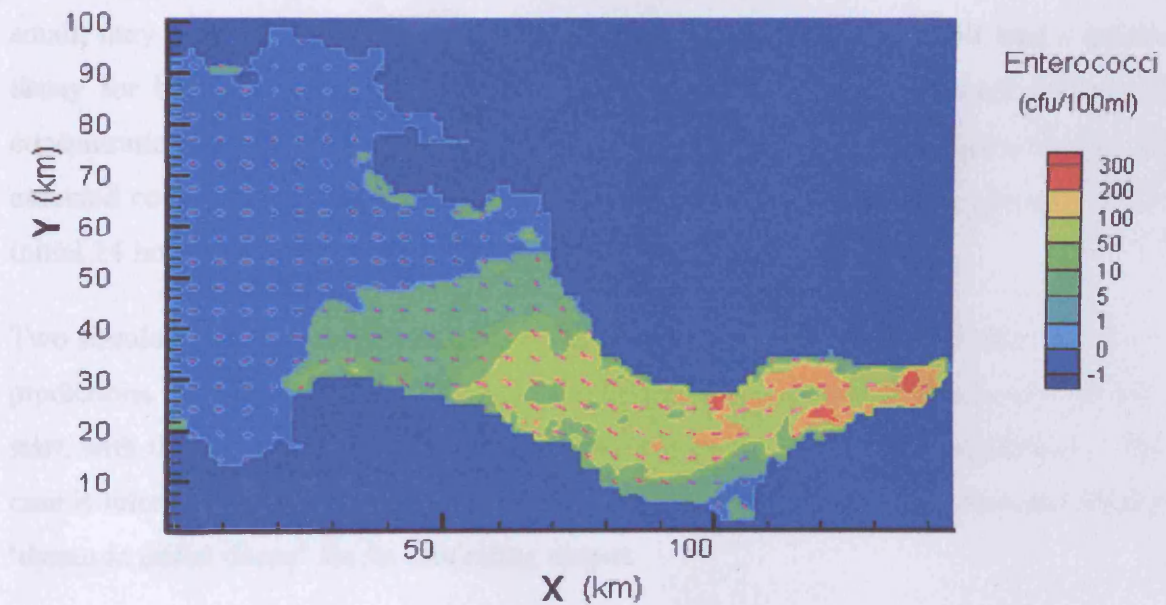
Figure 7.14   Distribution of enterococci predicted from 'decay with SS' at mid-ebb.

7.3   Sensitivity of Initial Decay Rate Representation

7.3.1   The concepts of the initial decay rate

In order to reduce the possible prediction error caused by the selection of initial condition, an initial period of 24 hours is considered for this case study. Thus, some assumed T90 values in this period during our modelling process are used and results are compared with the ones without the initial assumptions. These T90 values are assumed to be larger than normal to avoid any unexpected bacteria die-off before reliable SS concentration being obtained, which then can be used to predict its related T90 values in the modelling process afterwards.

The assumed initial T90 values are:

Light T90 in 2-D part, FST90D2 = 100 hours;

Dark T90 in 2-D part, FST90N2 = 100 hours;

Light T90 in 1-D part, FST90D1 = 120 hours;

Dark T90 in 1-D part, FST90N1 = 120 hours.

In our modelling process at t = 0, the sediment concentration was set to 2 mg/l while the actural value at some sites might be much larger. When the SS concentration such as 2 mg/l is applied in the T90-SS equations, the related-produced T90 values will be very small, may even be less than 1 hour. Thus these small T90 values will lead a quicker decay for bacteria than the actual ones. Therefore, before we get more reliable SS concentration we couldn't apply the T90-SS equations for these T90 values, instead, the assumed constant T90 values are used in these cases for both 1-D and 2-D parts for the initial 24 hours in the modelling process.

Two simulations were undertaken to establish how the initial conditions affect the model predictions. Firstly, for 'scenario 1', the decay rate was assumed to be dynamic from the start, with the deployed T90 value being time-varying from the start of simulations. This case is referred to as the model without the initial assumptions of T90 values and cited as 'dynamic initial decay' for its modelling output.

Secondly, for 'scenario 2', the T90 value was assumed to be constant for the first 24 hrs and then the same time-varying decay rate as in 'scenario 1' was applied thereafter. This

case is referred to the model with the beginning assumptions of T90 values and cited as 'constant initial decay' for the modelling output.

7.3.2 Comparison between 'dynamic initial decay' and 'constant initial decay' assumptions

Estimations are carried out under two different initial decay conditions.

The estimated results for some selected sites are plotted in Figures 7.15 to 7.18, where the blue line shows the predictions for the decay model with the assumed constant T90 value for the first 24 hours, and the red line shows the predictions obtained using the time-varying T90 values from the start of simulations. From these predictions it can be seen that, when different T90 values were used during the first 24 hours of simulation, different results occurred only for the first 40 hours of simulation. After approximately 40 hours each figure shows that the predicted bacteria levels were the same, irrespective of the initial representation of the decay rate. It was therefore concluded that when the riverine inputs and WwTW outfalls continuously discharge into the model domain, the form of the kinetic decay rate in the initial period will not affect the subsequent predictions after about 3 tides.

It can be seen from Figure 7.15 that a phase lag exists from the onset for about 3 hours, which is the time required for the water column enterococci levels to build up from the initial zero value. This can be explained by the fact that this site is not particularly close to an effluent input source and hence the initial enterococci levels of zero remain at this level for about 3 hours before the effluent from the nearest source has been transported to the site.
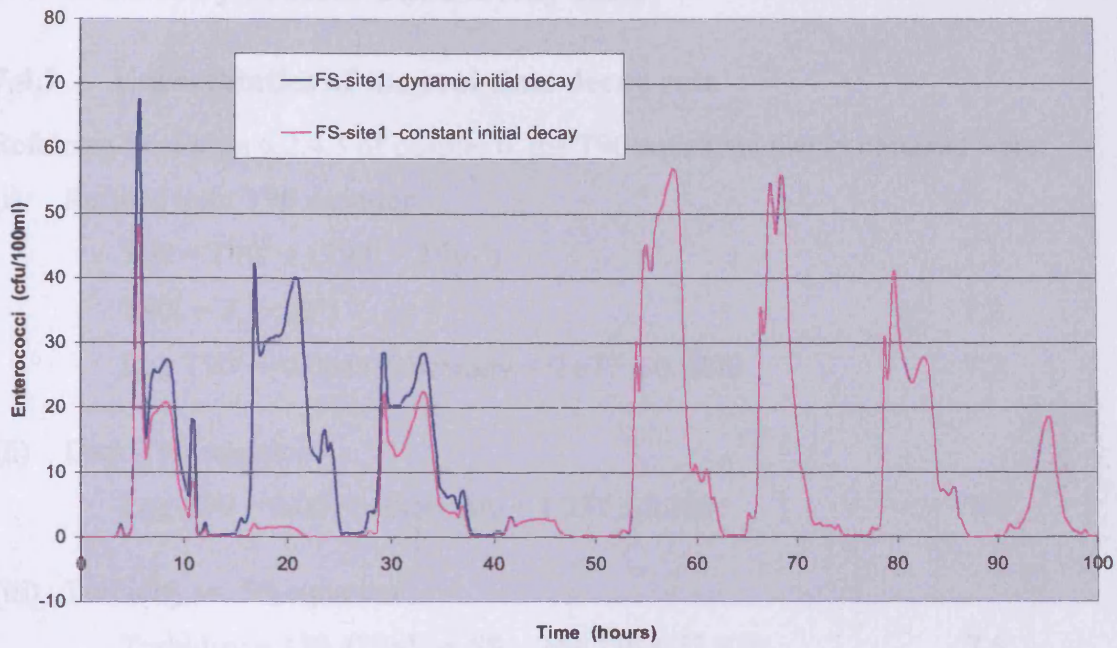
Figure 7.15 Predicted bacteria levels for different initial decay rates at Weston-s-Mare Sand Bay.
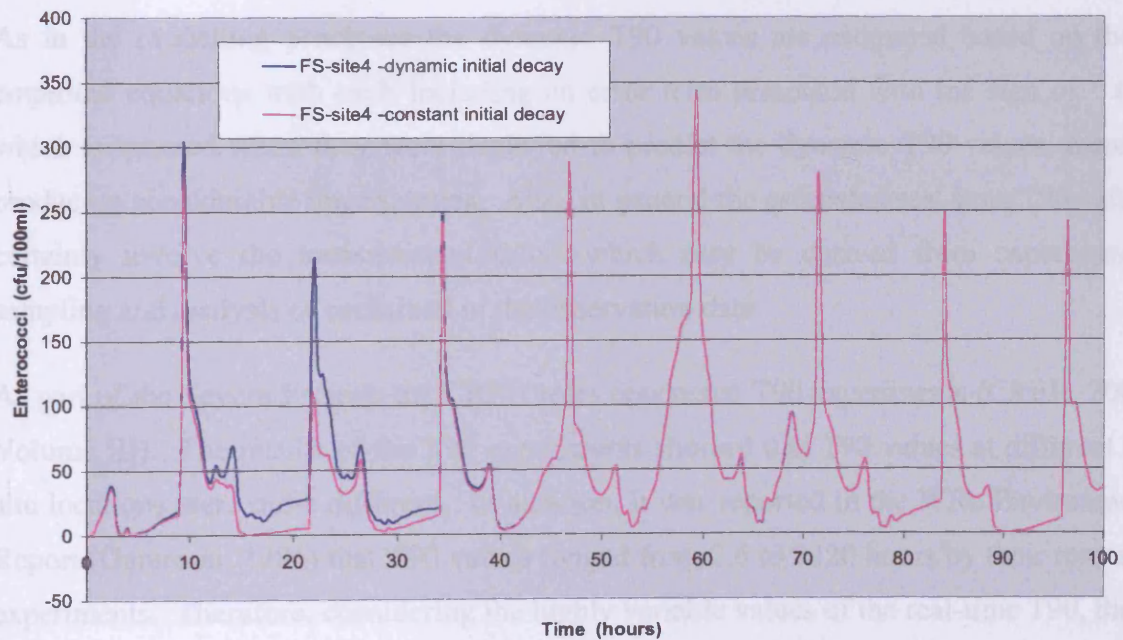

Figure 7.16 Predicted bacteria levels for different initial decay rates at Clevendon Beach.

7.4 Sensitivity of Real-Time Decay Rate

7.4.1 Uncertainties of the real-time decay rate

Referring to section 6.2.4.3 of chapter 6, the T90 equations finally obtained were:

(i) Refined light T90 equation

$$T90 = T90^2 + (T90^1 - T90_*^1) \qquad\qquad 7.1$$

$$T90^1 = 3.5 \times 10^3 \, I^{-1} \qquad\qquad 7.2$$

$$\text{Log } T90^2 = 0.0047 \times \text{Turbidity} + 0.677 \pm 0.2070 \qquad\qquad 7.3$$

(ii) Dark T90 equation

$$\text{Log } T90 = 0.0019 \times \text{Turbidity} + 1.237 \pm 0.199 \qquad\qquad 7.4$$

(iii) Turbidity vs. SS equation

$$\text{Turbidity} = 139.479 \times \text{Log SS} - 244.736 \pm 32.678 \qquad\qquad 7.5$$

where: T90 is in hours; SS concentration is in mg/l; I is the surface light intensity, W/m^2.

For daytime the real-time T90 values are represented in both sunlight-dependent and SS-dependent via equations 7.1 - 7.3 and 7.5, whilst for night time the real-time T90 values are only SS-dependent via equation 7.4 and equation 7.5.

As in the modelling processes the dynamic T90 values are estimated based on these empirical equations with each including an error term presented with the sign of ' ± ', which is ignored when they were deployed to predict the dynamic T90 values, thereby producing considerable uncertainties. Also, in general the estimated real-time T90 values certainly involve the measurement errors which may be derived from experimental sampling and analysis or contained in the observation data.

As part of the Severn Project, the CREH team conducted T90 experiments (CREH, 2004, Volume III). The results of the T90 experiments showed that T90 values at different in-situ locations were quite different. In addition, it was reported in the WRc Environment Report (Gameson, 1986) that T90 values ranged from 2.6 to 2420 hours by their research experiments. Therefore, considering the highly variable values of the real-time T90, three runs are processed to check the differences between the modelling results from various T90 values. In the processes factors of 2 and 10 for the light and dark T90 equations are applied and then the results from applying T90, 2*T90 and 10*T90 can be compared.
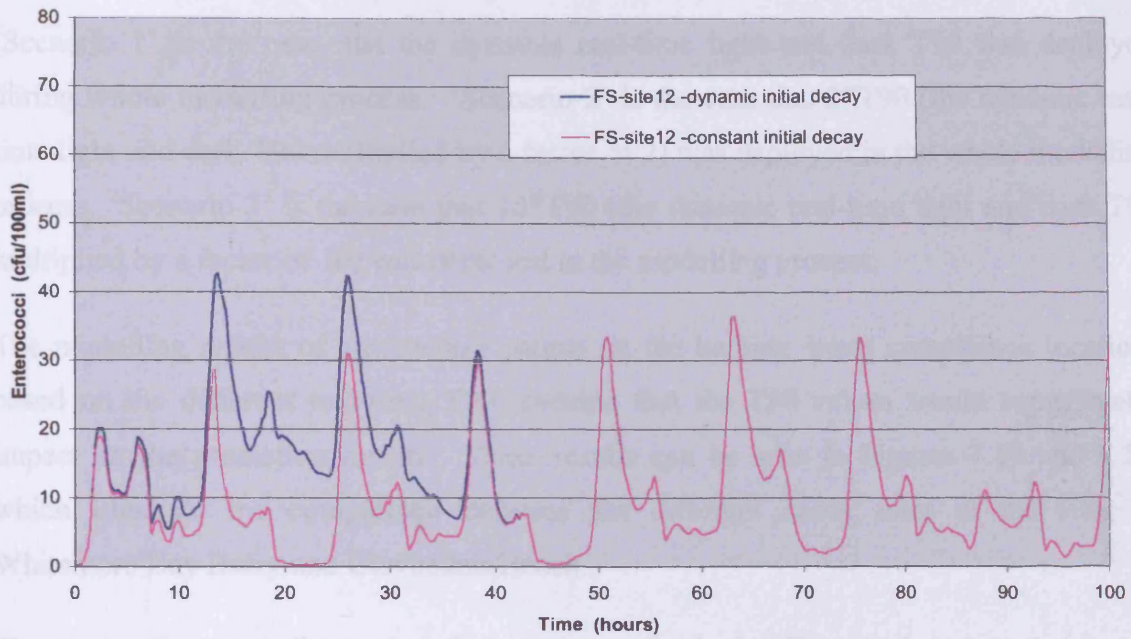
Figure 7.17 Predicted bacteria levels for different initial decay rates at Swansea Bay.
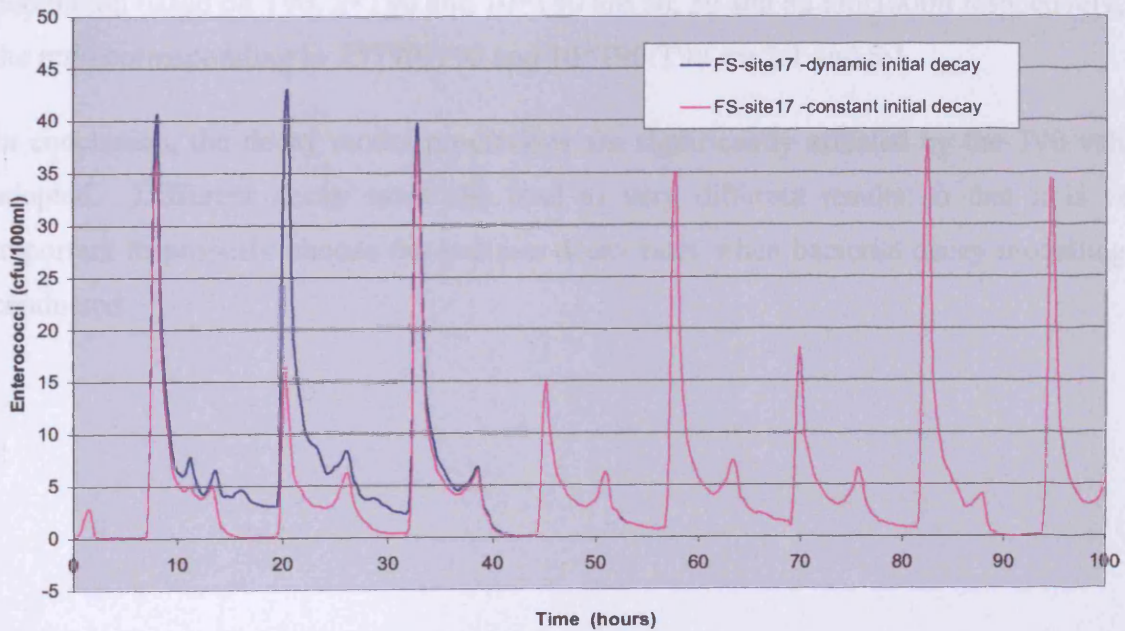
Figure 7.18 Predicted bacteria levels for different initial decay rates at Southerndown.

7.4.2   Comparison between different real-time decay rates

'Scenario 1' is the case that the dynamic real-time light and dark T90 was deployed during whole modelling process. 'Scenario 2' is the case that 2*T90 (the dynamic real-time light and dark T90 multiplied by a factor of 2) was deployed in the whole modelling process. 'Scenario 3' is the case that 10*T90 (the dynamic real-time light and dark T90 multiplied by a factor of 10) was deployed in the modelling process.

The modelling results of enterococci counts on the bathing water compliance locations based on the different real-time T90 revealed that the T90 values would significantly impact on the prediction results. These results can be seen in Figures 7.19 and 7.20, which illustrate the comparison between the different decay rates at the sites of Whitemore Bay Barry and Clevendon Beach.

These two figures indicate that there exists a marked difference between the results produced from different T90 values. For example, for the Whitemore Bay Barry site shown in Figure 7.19, the predicted peak values of enterococci population based on T90, 2*T90 and 10*T90 are 10, 19 and 75 cfu/100ml respectively, so that the ratio corresponding to 2*T90:T90 and 10*T90:T90 are 2:1 and 7.5:1. For the Weston-s-mare Uphill Slipway site shown in Figure 7.20, the predicted peak values of enterococci population based on T90, 2*T90 and 10*T90 are 16, 30 and 82 cfu/100ml respectively, so the ratio corresponding to 2*T90:T90 and 10*T90:T90 are 2:1 and 5:1.

In conclusion, the decay model predictions are significantly affected by the T90 values adopted. Different decay rates can lead to very different results so that it is very important to properly choose the bacteria decay rates when bacterial decay modelling is conducted.

Figure 7.19   Predictions under different decay rates at site 14, Whitemore Bay Barry.
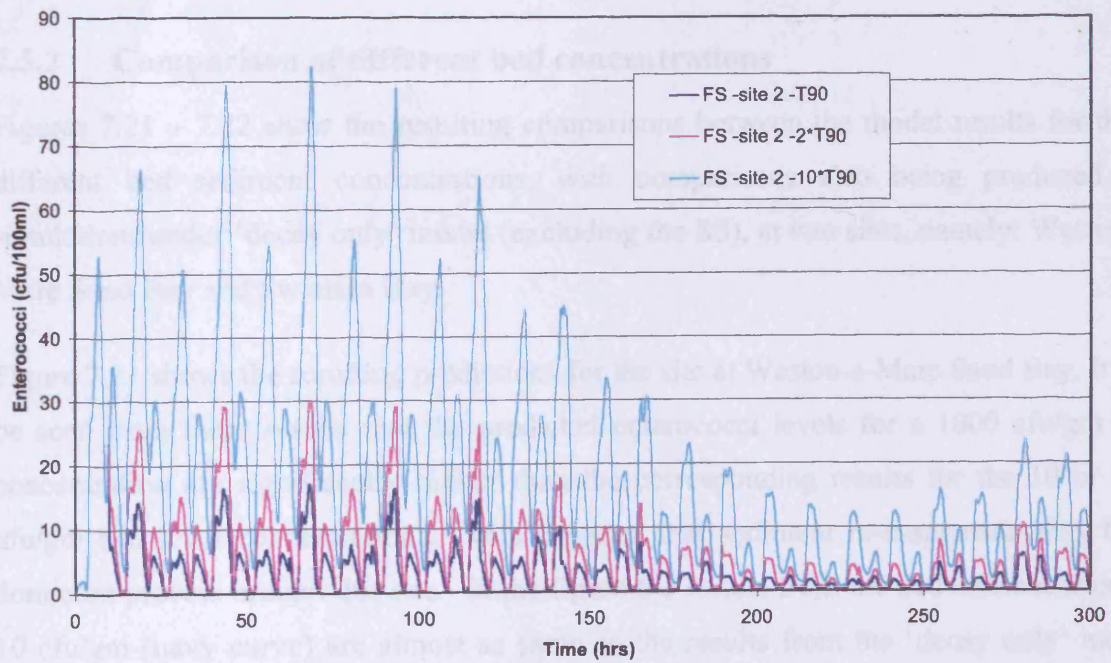
Figure 7.20   Predictions under different decay rates at site 2, Weston-s-mare Uphill Slipway.

7.5 Sensitivity of Bed Boundary Conditions

7.5.1 Introduction

A boundary concentration (C_b) representing the enterococci population levels on the bed sediments with units of 'cfu/gm' is specified in the model. This concentration can be conver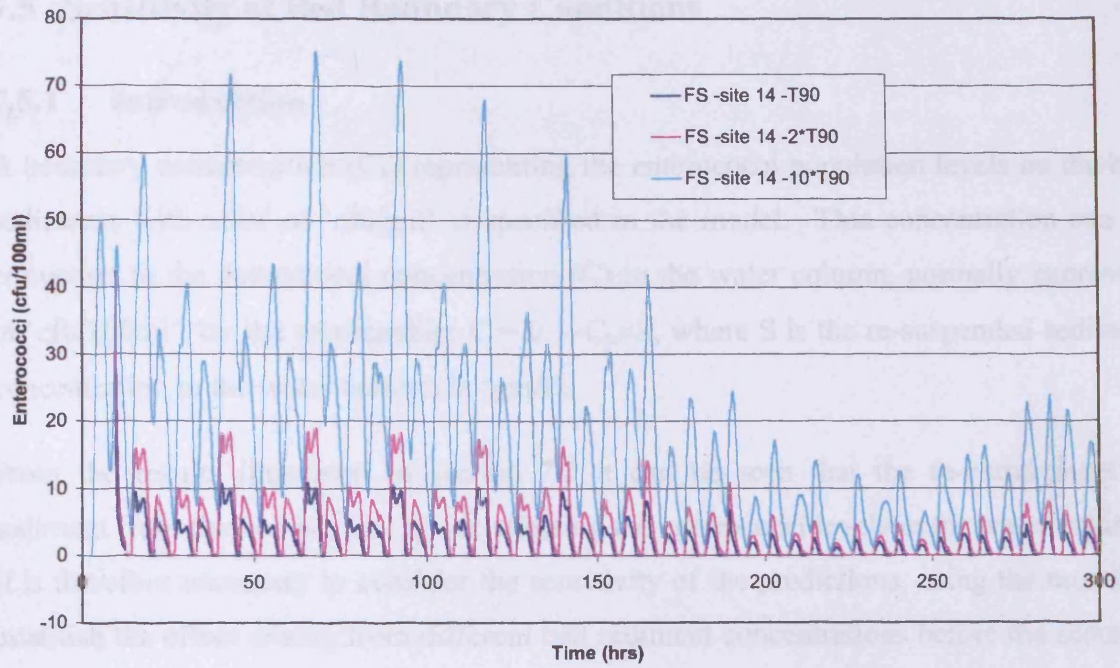ted to the enterococci concentration (C) in the water column, normally expressed in 'cfu/100ml', by the relationship: $C = 0.1 \times C_b \times S$, where S is the re-suspended sediment concentration in the water column in 'gm/l'.

From the results illustrated in section 7.2 it can be seen that the re-entrainment of sediment from the bed is a key factor affecting the enterococci levels in the water column. It is therefore necessary to consider the sensitivity of the predictions, using the model to establish the effect arising from different bed sediment concentrations before the accurate real-time bed concentrations are considered.

Three bed concentrations are considered, namely 10, 100 and 1000 cfu/gm respectively and the modelling results are cited as 10b, 100b and 1000b in the following graphs for representing each of these bed concentrations.

7.5.2 Comparison of different bed concentrations

Figures 7.21 – 7.22 show the resulting comparisons between the model results for these different bed sediment concentrations, with comparisons also being produced for simulations under 'decay only' model (excluding the SS), at two sites, namely: Weston-s-Mare Sand Bay and Swansea Bay.

Figure 7.21 shows the resulting predictions for the site at Weston-s-Mare Sand Bay. It can be seen from these results that the predicted enterococci levels for a 1000 cfu/gm bed concentration are significantly higher than the corresponding results for the 10 or 100 cfu/gm bed level concentrations. This suggests that sediment re-suspension may be a dominant process around this site. In the figure the results from the bed concentration of 10 cfu/gm (navy curve) are almost as same as the results from the 'decay only' model (blue curve), it reveals the water in this basin is deep enough for the bed entrainments to be diluted when small bed concentration is assumed, even though the pollution is dominated by the sediment transport.

In contrast to Figure 7.21, Figure 7.22 illustrates very similar concentration levels over the simulation period for the different bed concentrations; only the simulation with the exclusion of SS shows an appreciable change in the enterococci levels. This indicates that in the vicinity of this site at Swansea Bay the sediment transport processes were dominated by deposition. The blue line in Figure 7.22 highlights the results for the decay only model, which shows that higher concentration levels occur without sediment deposition.

Figure 7.21 Comparison of predicted enterococci levels for different bed sediment at Weston-s-Mare Sand Bay
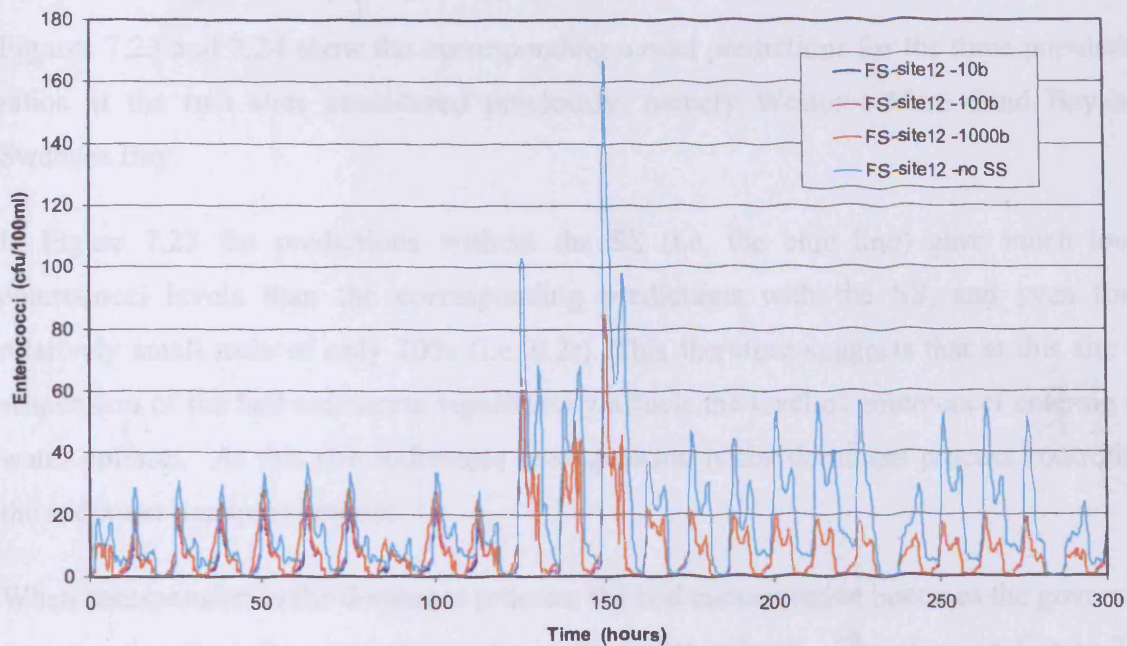
Figure 7.22 Comparison of predicted enterococci levels for different bed sediment at Swansea Bay

7.6 Sensitivity of Population Ratio

7.6.1 Introduction

The population ratio is the ratio of the attached enterococci population to the total enterococci population in the water column. In natural waters this ratio may be affected by many physical or chemical factors, such as: type of SS, concentration of SS, total enterococci population, organic matter and nutrients, water temperature, salinity, pH and etc, as cited in the literature. There was a lack of experiment data on population ratio in the Severn project, so an assumed ratio of 80% was deployed in the enterococci simulation in the application study disccused in Chapter 6.

In this chapter in order to identify the sensitivity of this parameter, three different population ratios i.e. 80%, 50% and 20% were assumed. For all of these cases the bed concentration was assumed to be 1000 cfu/gm.

7.6.2 Comparison of different population ratios

Figures 7.23 and 7.24 show the corresponding model predictions for the three population ratios at the two sites considered previously, namely Weston-s-Mare Sand Bay and Swansea Bay.

In Figure 7.23 the predictions without the SS (i.e. the blue line) gave much lower enterococci levels than the corresponding predictions with the SS, and even for a relatively small ratio of only 20% (i.e. 0.2r). This therefore suggests that at this site re-suspension of the bed sediments significantly affects the level of enterococci entering the water column. At this site sediments re-suspension is the dominant process controlling the sediment transport process.

When resuspension is the dominant process, the bed concentration becomes the governing source rather than the population ratio in the water column. Therefore, in Figure 7.23 there is only a relatively small difference between the predicted results for ratios of 0.5r and 0.8r, with the largest difference between the 0.2r (navy line) and 0.8r (orange line) ratios being 375:320, i.e. a 17% increase.
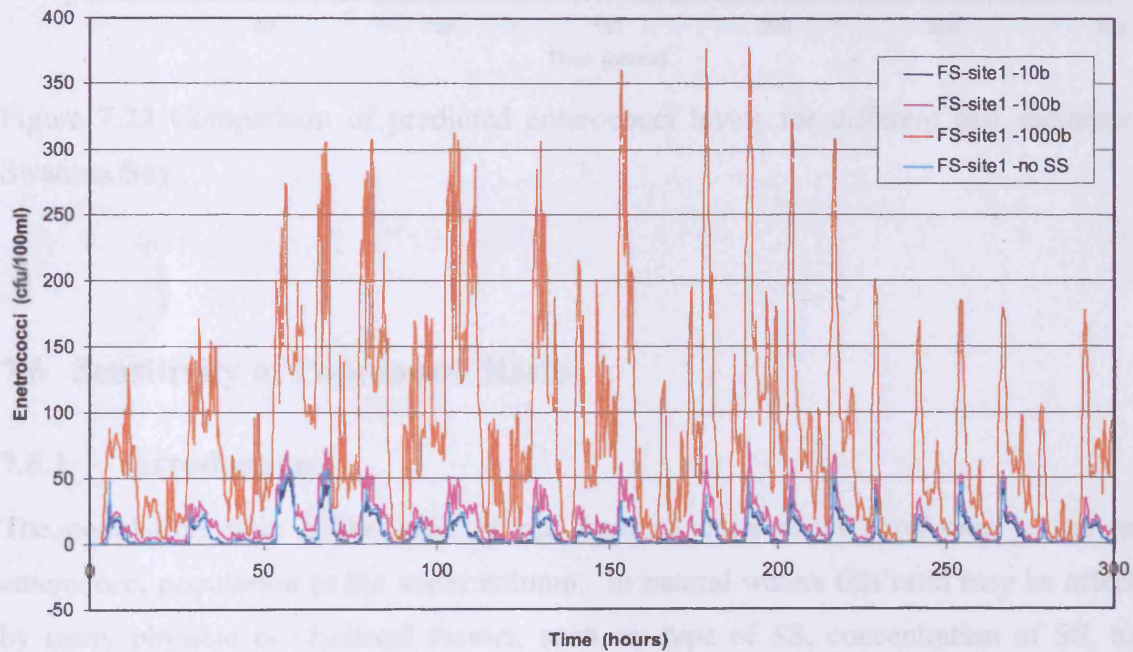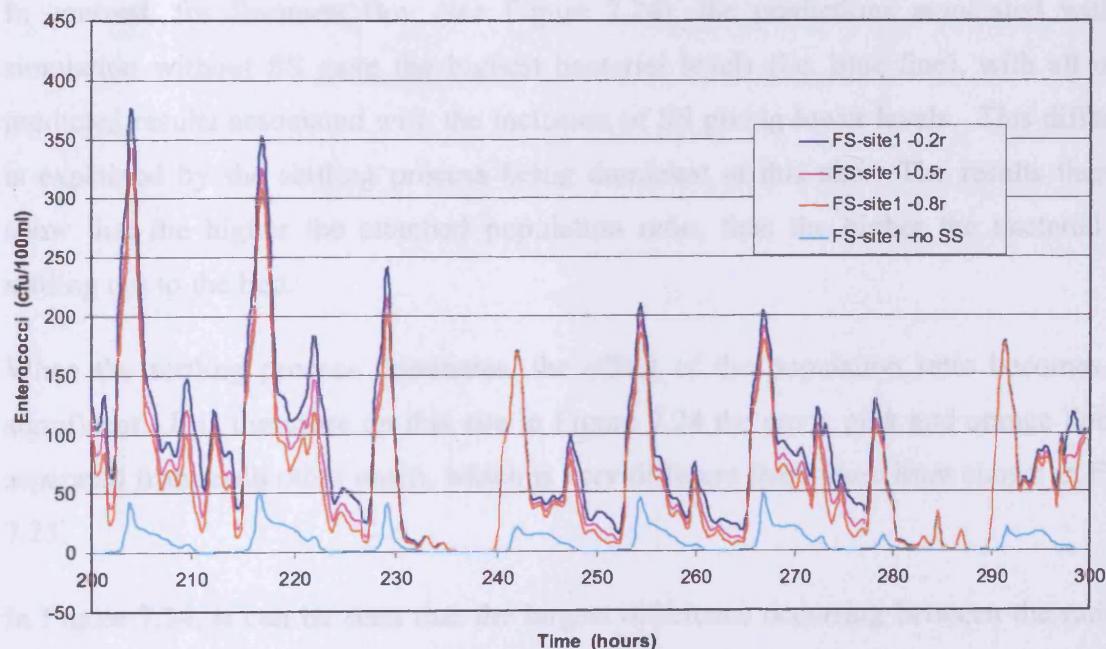

Figure 7.23 Comparison of predicted enterococci levels for different population ratios at Weston-s-Mare Sand Bay
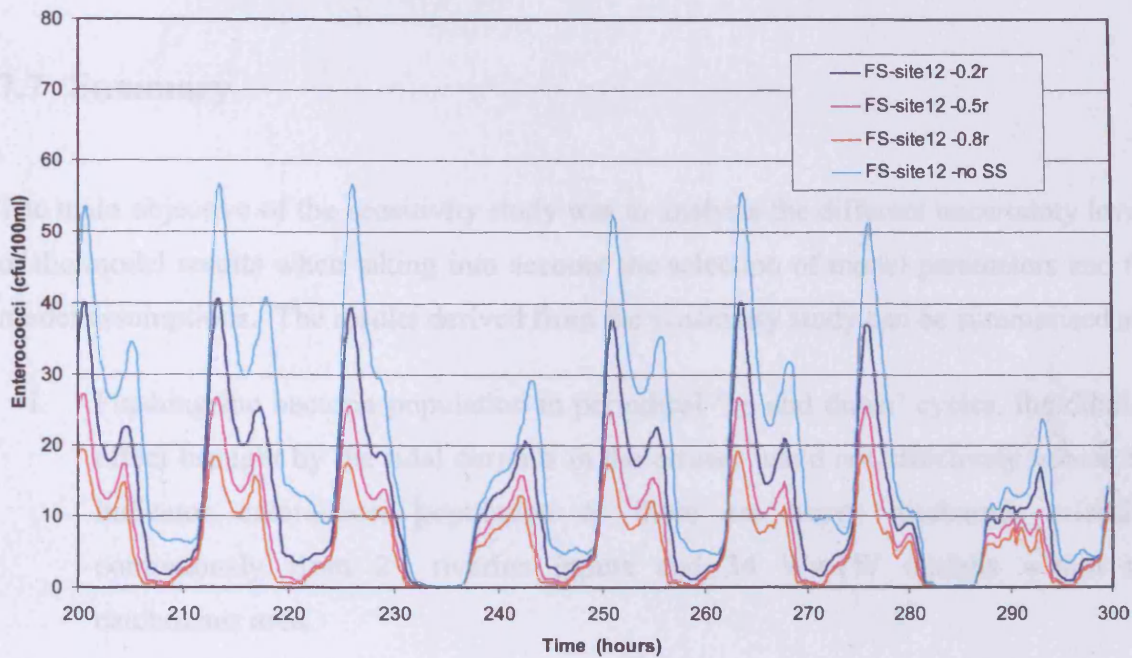
Figure 7.24 Comparison of predicted enterococci levels for different population ratios at Swansea Bay

In contrast, for Swansea Bay (see Figure 7.24), the predictions associated with the simulation without SS gave the highest bacterial levels (i.e. blue line), with all of the predicted results associated with the inclusion of SS giving lower levels. This difference is explained by the settling process being dominant at this site. The results therefore show that the higher the attached population ratio, then the higher the bacterial load settling out to the bed.

When the settling process dominates, the effect of the population ratio becomes very significant. It is therefore on this site in Figure 7.24 the navy, pink and orange lines are separated from each other much, which is very different from those lines shown in Figure 7.23.

In Figure 7.24, it can be seen that the largest difference occurring between the ratios of 0.2r (navy line) and 0.8r (orange line) is 40:19, i.e. this is over 100% , while in Figure 7.23 it was 17%.

7.7 Summary

The main objective of the sensitivity study was to analysis the different uncertainty levels of the model results when taking into account the selection of model parameters and the model assumptions. The results derived from the sensitivity study can be summarised as:

i.   Flushing the bacteria population in periodical 'up and down' cycles, the dilution effect brought by the tidal currents in the estuary could not effectively reduce the indicator enterococci population as there are heavy discharges releasing continuously from 29 riverine inputs and 34 WwTW outfalls within the catchments area.

ii. The initial condition does not affect the model results after about 3 tides from the start of the simulation.

iii. The bacterial decay rate is the most important factor with a marked effect on the decay model simulation, so attention is required in order to get better estimation of their values (e.g. the values based on T90 equations deployed in the model).

iv. The bacterial bed concentration (bed boundary condition) is an important factor in terms of the re-entrainment of sediments that brings a significant amount of bacteria into the water column from bed.

v.   Finally, the population ratio needs some attention as it contributes relatively a small percentage difference when compared with the several times differences produced by the change of bed concentration and decay rate.

Chapter 8

CONCLUSIONS AND FUTURE WORK

8.1 Summary of Research Work

This thesis presents the results of a formation and model study of enteric bacteria kinetic transformation processes in natural waters. Details are given of the development of the integrated 1-D and 2-D sediment-linked hydrodynamic and water quality model. This model has been applied to Bristol Channel and Severn Estuary to estimate the enterococci contamination along the identified bathing water compliance locations in the main estuary.

The major developments of this research work can be summarised as follows:

  i.   Insight into the principles of hydrodynamic, sediment transport and enteric bacteria modelling in 1-D and 2-D water basins.

  ii. Insight into the mechanisms of enteric bacteria surviving in estuarine and coastal waters.

  iii. Insight into the role of sediment transport processes on the adsorption and desorption of enteric bacteria and between bed load and suspended load sediments.

  iv. Upgrading an existing Fortran 77 numerical model, namely DIVAST to a Fortran 90 model with the latest advanced features.

v.   Upgrading two existing numerical models, namely FASTER (1-D model) and DIVAST (2-D model), by developing a state-of-the-art GUI system using the Visual Basic 6.0 programming language.

vi.   Development of mathematical formulations for representing the quantitative relationships between indicator bacteria and the suspended sediment concentrations.

vii.   Development of a numerical sub-model for sediment linked bacteriological transformation modelling.

viii.   Dynamically linking the FASTER and DIVAST models to encompass different flow characteristics for hydrodynamic computations in larger water basins, featuring a combined system in a modelling domain with different dimensions.

ix.   Validation and calibration of the integrated sediment-linked water quality model for the Bristol Channel and Severn Estuary projects, using data obtained from in-situ field measurements including diffuse faecal indicator sources for 29 riverine inputs; point faecal indicator sources for 34 WwTW outfalls; daily-recording of hourly observed sunlight radiation data; downstream real-time tidal water elevations; upstream Severn River flowrates; and bathymetric data across the 1-D and 2-D domains. Encouraging calibration results were obtained and the model was successfully validated to estimate the enterococci concentration levels at the bathing water compliance locations.

8.2 Conclusions

The following key conclusions have emanated from this study:

i.   From the literature review, it has been established that there is a lack of information on sediment related bacterial transport modelling. In model studies to date there has been no inclusion of the suspension from the bottom sediments and also no inclusion of separate bacterial disappearance due to a gradual-grained sediment deposition differing from bacterial decay.

ii.   New mathematical equations have been proposed for modelling the disappearance of bacteria due to sedimentation and the re-suspension from bottom sediments. In particular, in contrast to previous studies, a new bacterial disappearance equation has been developed which is independent from the first-order decay model. It has been found that the settling coefficient $K_s = V_d/H$ used in past studies, included in the overall decay rate (i.e. equation 2.18, after Canale et al., 1993 and equation 4.2, after Droste, 1997), applies only to a specific case of the bacterial carriers, for being the idealised and uniform sized particles settling in a static water column.

iii. A dynamically linked 1-D and 2-D hydrodynamic and water quality simulation model has been developed, based on the above new equations for the sediment transport associated bacteriological transformation modelling.

iv.   Object-oriented methodologies have been deployed in the integration of the sediment-linked multi-dimensional water quality model to encompass well-tested existing modules, by implementing the Fortran 90 programming language to deploy advanced numerical schemes and Visual Basic 6.0 programming language to provide a state-of-the-art GUI system.

v.   This simulation model has been successfully applied in a real case study, namely the Bristol Channel and Severn Estuary project. The project includes three main parts: hydrodynamic modelling, sediment transport modelling and sediment-linked bacteriological interaction modelling.

vi.   Accurate hydrodynamic calibration results have been achieved in the application. Based on the available survey data, calibrations of the water surface elevation, current speeds and directions were carried out for the four survey sites. The prediction of the water depths and current directions agreed well with the site survey data. The current speed predictions also agreed well with the measured data.

vii. A sensitivity study has been carried out to identify the uncertainties involved in the implementation of the new model, with the uncertainties both in the model parameters and the processes considered.

viii.   The successful application of the simulation model in the Severn Estuary project concludes that the integrated 1-D and 2-D sediment-linked model is an efficient software tool for water management and planning in real environments. It provides assistance for managers in making robust decisions to improve the water environment and for sustainable development.

From the application study, the main conclusions drawn from the enterococci contamination simulation for the Severn Estuary can be summarised as follows:

i.   Relatively high loads of faecal bacteria contaminants discharge from the riverine inputs and WwTW (sewage) outfalls into the receiving waters of the Bristol Channel and Severn Estuary, such that dilution has only limited effect on reducing the bacterial concentration or the concentration levels. The results from the dilution modelling show that the pollution load is higher along the Welsh coast and lower along the English coast.

ii.   The faecal indicator concentrations along the Severn Estuary are closely linked to both the bacterial die-off rates and the sediment transport processes.

iii.   The faecal indicator disappearance rate depends on the die-off processes in this estuarine environment, with sediment deposition having much less effect.

iv.   The faecal indicator concentration level has a close relationship with the suspended solid concentrations as it has been shown that at many locations the high concentration levels are caused by the resuspension of bottom sediments. It is deduced that in the estuary enterococci contamination is derived primarily from bacteria surviving in the bed sediments. Hence the bacteria bed concentration levels significantly affect the predicted results and the sediment resuspension significantly increases the population levels at the bathing water sites.

v.   The faecal bacteria concentrations at each bathing water location are transported in a cyclical manner in phase with the tidal oscillations. However, this cyclical manner of the bacteria concentrations is different from the cyclical pattern observed in sediment concentration predictions as bacteria are not only transported by the tidal currents but also mortality with daily sunlight intensity.

vi. The T90 value deployed in the model significantly affects the prediction results of the enterococci concentration. In this study dynamically varying T90 values were used to reflect more accurately the variation in this parameter with the diurnal hourly observations of sunlight intensity and these T90 values were predicted from empirically derived regression equations, which varied with the time-dependent and grid-dependent predicted suspended solids concentrations.

vii. Four days of site surveys were undertaken to obtain 8 sets of water quality calibration data. The calibrations showed that the measurements at the four offshore survey sites (where samples were taken near the surface) were in good agreement with the predictions using the dynamic 'decay only' model. Calibration of the model also showed that the dynamic sediment-linked 'decay and SS' model predictions gave satisfactory agreement with the measurements at the other three sites (where the samples were taken well below the water surface). Only one data set (namely the Southerndown site) did not satisfactorily match either the 'decay only' or the 'decay and SS' model predictions. These results revealed that re-entrainment from the bed sediments had a significant impact on water samples at depth and much less effect on the surface water samples in the deeper water columns at offshore sites. These findings show that the water depth affects the degree of entrainment, so that the suspended solids concentrations generally had a larger impact on the predicted enterococci levels in the shallower nearshore waters and less effect on the deeper offshore waters.

viii. In the model predictions, the ratio of the 'attached enterococci' to the 'total enterococci' concentrations did not affect the model predictions to any major extent when sediment re-suspension dominated the sediment transport processes. In contrast, this ratio noticeably affected the predicted results when deposition (or settling) was the dominant sediment transport process.

8.3 Recommendations for Further Study

Sediment transport associated bacteriological transformation modelling is a relatively new research field, which includes: hydrodynamic, sediment transport and bacterial decay

(accompanied by adsorption/desorption with sediments) modelling, dealing with the knowledge of bacterial survival (or die-off) in two phases of the water column and bed sediments. For such predictions a knowledge of the bacterial transformation between the water column and the sediments is essential. In terms of questions raised in the application to the Severn Estuary, the following recommendations have been drawn to extend the present study:

i.   Adopting smaller grid size

In the Severn Estuary the computational domain covers an area over 15,000 km^2. For such a large area, a grid size of 600m × 600m was chosen in the current study in order to model the site to a feasible running speed on PCs. For a depth-averaged model the preliminary point source concentration in the cell releasing the effluent is used via the estimated value of the released loads divided by the cell area, to give an arithmetic cell-mean concentration. This concentration is generally lower than the actual released concentration. When samples are taken near an outfall, along the main flow streamline directed to the outfall release point the measured data could be much higher than the model predictions. On the other hand, away from the main flow streamline directed to the outfall release point, the measured data could be much lower than the model predictions, since the model predictions are averaged over cell-volume. In order to trace the faecal indicator concentrations with the water column and along the flow path, smaller grid cells within a smaller model domain are recommended for any further studies. Sampling locations should be located relatively far from outfall discharge points to avoid samples being reached in the affinity of outfall flow flumes.

ii.   3-D modelling

In the enterococci calibration section, it can be clearly seen that the 'decay only' model predictions gave good agreement with the surface water samples, and the 'decay with SS' model predictions gave satisfactory agreement with the deeper water samples. This indicated that the bottom sediments had more impact on the deeper waters and less affect in the near surface waters. This was not surprising as the suspended sediments had uneven concentration distributions in the vertical water column, with high values in the lower layers, vis-à-vis the low values in the upper layers.

In any further studies a 3-D model simulation of the sediment-linked bacteriological transformation processes would give more detailed predictions of the distributions of the bacteria and suspended particles in the vertical water column. Thus a 3-D model would be expected to improve the accuracy of the model calibration and validation for the sediment-linked bacterial decay modelling. Another advantage of 3-D modelling, especially for bacterial predictions, is to represent better the surface sunlight attenuation by water depth.

iii.   T90 modelling

From the predictions for the comparisons of the different T90 values, it was noted that the dynamic real time T90 values adopted in the modelling had a significant influence on the accuracy of the predicted results. The T90 values used in this study were dynamically predicted based on the empirical regression equations, which depended upon the dynamic sunlight intensity and the suspended sediment concentrations. Obviously in turbid waters the water column depth is another significant factor affecting light penetration, which inherently reduces the effect of bacterial decay. Future T90 analyses should be conducted and then deployed in the water quality numerical model represent more accurately the real-time decay rates as a function of a number of parameters.

iv.   Investigations of bacteriological kinetics in sediments

The model developed in this study includes a number of key assumptions. Specifically, it assumes zero bacterial decay from the bed sediments and a constant initial bed enterococci concentration at all locations. The importance of this modelling component suggests that further work is needed on: (i) the spatial heterogeneity of sedimentary enterococci concentrations; and (ii) the sedimentary survival levels. Such studies would be fruitful areas of further study to enhance the model predictive capacity in estuarine environments.

Sediment re-suspension has been found to be a significant source of faecal bacteria pollution not only in this study, but also many other earlier studies (see Chapter 2). One factor is that this study has involved investigations via computer modelling based on field data, however other studies have been conducted via field or laboratory experimental study only, following on from the earliest work by Savage (1905). This research concluded that: "mud samples yield more reliable bacteriological than either water or

oyster samples." In some later documentations, the relationships of Faecal Coliform in water column and bottom sediments had been studied, with inconsistent results, such as Valiela et al. (1991) suggested that resuspension of the upper layers of sediments could account for the faecal coliform present in the water.

The mechanisms of enteric bacteria living in the bed sediments are still not clear. They may accumulate, grow or die-off in the sediment column and either the growth or die-off rate needs to be investigated further. Based on the literature on sedimental research and from the high densities of cells in the sediments, it is reasonable to expect that growth of faecal bacteria may take place in the bottom sediments, especially in areas around sewage outfall diffusers. This study suggests that if computer model is applied to bacteriological studies in natural waters in future, it would be potentially fruitful to take sediment samples at the mean while when undertaking overlying water column sample studies of the bacteria concentrations.

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