The role of mathematical models, physical models and field measurements in water pollution problems

R. Rajar

University of Ljubljana, Faculty of Civil and Geodetic Engineering, Slovenia
E-mail: rrajar@fagg.uni-lj.si

Abstract

There are three possible tools for the simulation of water quality processes: (1) physical models, (2) field measurements, and (3) mathematical models.

The present paper describes the possible application of these three tools and their efficiency. For the water quality studies the application of physical models is limited, because the phenomena must usually be simulated in large space domains and because it is difficult or impossible to simulate bio-chemical processes on physical models. Field measurements are very often applied, but the most effective methodology in water quality studies is the combination of mathematical models and field measurements.

Some special cases of the application of physical modelling are described, where physical models are used to reveal certain details of new phenomena. A short description of the role of the remote sensing technique in mathematical modelling is also presented. An example of the application of a 3D mathematical model together with field measurements is presented for the case of the simulation of the dispersion of radioactive pollutants in the Sea of Japan.

1 Introduction

Today clean water is becoming a really precious resource. In the area of water quality management, we are trying to reduce the level of water pollution at the lowest possible cost. To achieve this goal we must determine, in advance, the effect of various planned measures which could be taken to improve water quality and then determine the \textit{measure which is optimal in both an economic and environmental sense}.

How can we determine these measures? There are three main tools, or methods, that can be used:

(1) Physical models, (2) Field measurements and (3) Mathematical models.

The role of the three tools in solving water pollution problems and their efficiency is described below. We can say that the third method, i.e. mathematical models, is usually the most effective, and that the other two methods are mostly used for calibration and verification of the mathematical models. However,
sometimes physical models and field measurements have a special role, they are not always just a supplement to the mathematical models.

2 Physical Models

The main characteristic of physical models is that they are built on a reduced scale in comparison to nature, therefore they are also called scale models. Before the development of high speed computers, physical models were used successfully in several fields of water management and to a lesser extent they are still used today. However, there are two important limitations on their application:

1. Only relatively small domains can be modelled, e.g. river sections or areas around underwater outlets.
2. Generally, only hydrodynamic circulation can be simulated on scale models and therefore their applications are more in the field of hydraulics (e.g. river and coastal engineering) than in the area of water quality studies.

On the contrary, in water quality studies, we must usually simulate processes over large space domains and must usually simulate not only hydrodynamic circulation, but also biological and chemical processes. For both of these reasons, the application of physical models in water quality (WQ) studies is fairly limited.

Physical models are always more or less limited in space, therefore it is difficult or impossible to simulate, on a scale model, the physical phenomena which occur over very large regions in nature. If the modelling scale becomes too large, several phenomena cannot be properly simulated. This is especially true of the phenomenon of turbulence, which cannot be properly modelled, as we cannot achieve a similar Reynold's number for the field and model flows. Besides this, in water quality studies there are often several parameters which are very difficult to simulate on scale models, such as the distribution of temperature and salinity. On the other hand, it is also very difficult or impossible to properly simulate on a scale model most of the bio-chemical processes which play a crucial role in WQ studies. These processes are not only occurring in large space domains, but are also long-term processes on a time scale.

It should also be mentioned that in order to find out the best trade-off solution, we have to simulate many different cases, some of which require a rebuilding of the model. Therefore, physical models are also expensive.

There are three possible ways to solve these two problems, i.e. to determine how to simulate bio-chemical processes in large space domains:

1. In some cases it is possible to use the sc. pilot facilities (or pilot models). Pilot models are not really scale models, as they are not constructed on a reduced geometric scale. We could say that they are just segments of nature, or of the original reactor, usually prepared in laboratories, where we are trying to establish conditions for some bio-chemical processes which should be as close to natural conditions as possible. It is difficult to establish exactly equal conditions (light, temperature, suspended sediments...), therefore the results should be treated with caution. It is also important that the turbulent and mixing processes in the pilot
plant are not essentially different from the processes in nature. If there are several simultaneous processes involved, we may simulate just one or some of the most relevant, but we must be aware of the possible interaction effects. Such pilot models are used relatively often to simulate the different processes taking place in waste-water treatment plants.

(2) Since increasing the modelling scale deforms most bio-chemical phenomena, the scale should be reduced and we are approaching a scale of 1:1, i.e. the nature. Therefore, field measurements became very important in WQ studies.

(3) Since mathematical models can simulate (to a certain degree of accuracy!) many bio-chemical processes in very large domains, they are the most important tool in WQ studies (see Ch. 5.)

For the above-mentioned reasons, one can see that the direct application of physical models in WQ studies is limited. However, there is another area of applications of physical models, which is often very important. The goal is to reveal some not quite well understood phenomena, e.g. special details of some density currents, headland eddies, processes connected with sediment transport and resuspension, etc. (see Section 5.1), for which science does not yet have a reliable mathematical description. Hydrodynamic and dispersion phenomena are more often modelled on scale models than biological or chemical processes. Basic research on turbulence is also widely performed, but this is not a typical WQ problem, since this phenomenon is very important in different fields of science.

Today, more effort and research is being directed away from the field of hydraulic engineering towards environmental engineering, where physical modelling is more seldom applied, thus hydraulic laboratories specialised in scale modelling are losing their jobs everywhere in the world. However, many of these laboratories have maintained their existence by one of the following solutions.

(1) Re-orientation of their activity into field measurements
(2) Re-orientation of their activity into mathematical modelling
(3) Some of the hydraulic laboratories have succeeded in attaining a very high level of quality in a narrowly specialised field. They are able to simulate special, not yet well-known or well understood phenomena, usually at a world-class level. This has lead to a more profound understanding of physical, biological and chemical phenomena and has helped to describe these phenomena using mathematical relations, which will eventually be applied to the development of even better mathematical models (see Ch. 5)

3 Field Measurements

Field measurements are often indispensable, but usually it is not possible to solve a water quality problem completely by using field measurements. We can get very important information on water quality parameters (more accurately than by physical or mathematical modelling), but there are two limitations on their effectiveness: (1) only actual real time state of the water quality parameters can be measured, although with long term measurements we can also determine some future trends. Still it is difficult or impossible to predict the future development of
water quality. (2) As it is difficult (i.e. expensive) or inadmissible due to environmental damage to repeat measurements on a 1:1 scale, it is usually not possible to verify the effectiveness of different possible sanitation measures and, thus, to find out the optimal solution in this way.

For these reasons the most effective method for solving WQ problems is a combination of field measurements and mathematical modelling.

3.1 Conventional Measurements versus Remote Sensing

There are two types of field measurements: (1) classical ("in situ") measurements, carried out from ships or buoys and (2) remote sensing, using aircraft and satellites. Remote sensing (RS) has become an extremely important methodology in oceanography and WQ studies during the last 15 years. It is regarded as a complement rather than as an alternative to conventional measurements. An excellent review of the RS technique and of its application to modelling is given by Robinson. Basically, remote sensing provides regular or occasional data over very large areas with a high spatial sampling density, while conventional "in situ" measurements are carried out in one or several locations with high temporal sampling rates. As RS can register only surface parameters, conventional measurements are sometimes indispensable for their complementarity with measurements taken along the depth.

Because RS is extremely useful in many fields of environmental research, it is subject to very fast developments. It is difficult to list all the parameters which can be measured. To name just some of the parameters which are very useful for the verification and calibration of mathematical models in WQ studies:

1. **Sea-surface temperature** (SST) can be very useful in detecting some hydrodynamic features of the circulation. As different plumes, especially from rivers, differ in temperature, it is possible to trace the pattern of the plumes and eddies by the variation in temperature (by RS it can be detected to the accuracy of 0.2 degree C).

2. **Chlorophyll concentration** A lot of effort has been put into improving the RS technique for more accurate detection of chlorophyll pigment associated with phytoplankton in the upper layers of coastal seas or oceans. On the one hand chlorophyll pigment can indicate the pattern of the HD circulation, and on the other hand it is the basic indicator of nutrient contamination and of primary production.

3. **Other water quality parameters**. There are various other factors which influence the water colour, e.g. yellow substance or suspended particulates. In general, RS spectral coverage has proved unable to separate the various constituents from each other. Suspended sediments are an exception, but calibrations should be carried out using simultaneous measurements at sea. However, ocean colour imagery can still provide a lot of useful information from the various passive tracers in the upper layers of the sea, such as turbulent eddy structures. In coastal seas, the turbidity, shown by the surface layer colour, can indicate the extent of river plumes, sediment transport, beach erosion and can also provide useful information of the dispersion processes of various contaminants.
(4) **Detecting larger contaminated patches or objects.** Large oil-spill patches can be detected using satellite imagery, which, together with the on-line connection with environmental protection services, has a very important role in clean-up actions. Permanent tracking of icebergs is also carried out, which contributes to navigation safety.

3. 2 Remote Sensing and Modelling.

Remote sensing can be an extremely useful tool in environmental modelling. The RS data can be used for obtaining initial and boundary conditions (e.g. for better determination of the always problematic open boundary conditions) and especially for the calibration and verification of the models themselves. As RS data cover large regions with detailed sampling density, it matches well with the computational domain of global ocean models or mesoscale models, and often also with coastal seas models. Temporarily sparse sampling can be a problem, but, often, a single image with the instantaneous distribution of a certain parameter can also be very useful. Only surface conditions can be registered. When the parameters are well mixed along the depth, this corresponds very well with 2D depth-averaged modelling. When 3D simulations of phenomena with non-uniform distribution of parameters over the depth is carried out, the surface conditions obtained by RS can be compared with the conditions obtained by the simulation of the upper model layer. In such cases the RS data are often combined with *in situ* measurements over the depth.

Robinson presents an interesting case study where a 2D model of HD circulation and temperature distribution was driven using RS image data. The goal of the modelling exercise was “to test the effect of different parameterisations of diffusion and different advecting residual flows in order to reproduce as closely as possible the temperature patterns from the satellite data.” Robinson emphasises that such a model, tuned for reproducing the temperature field, could then be applied to modelling of other tracer distributions. He also points out that such a modelling approach is only made possible by the use of remote sensing.

Even more than physical models, RS can be used to better understand several large-scale physical phenomena. Even some new and interesting phenomena have been found by the RS. Usually when the RS imagery of the ocean reveals interesting phenomena, physical oceanographers try to simulate it by numerical models in order to understand the processes controlling the features. Sometimes the satellite observations merely inspire further study of a phenomenon, while in other cases the image data are used to define the length scale of the process and the image provides an approximate test for qualitative validation of the model.

Robinson also describes some phenomena where the RS helped reveal the basic physical phenomenon: headland eddies, tidal turbidity fringes, shelf-sea mixing fronts, mixing in the islands’ wake, coastal current eddies, equatorial waves, etc. Usually an advance in fundamental knowledge is most effectively achieved by the interaction of RS and numerical modelling.
4 Mathematical Models

As indicated in the introduction, the final goal of research in the field of water quality protection is to find out the optimal measures of improvement of the water quality. The extremely important role of mathematical models (MM) in such studies is well known.

A special kind of model is being developed in which simulations of several possible measures are integrated into the model together with the economic evaluation of their consequences. These models are directly used as a management tool. Theoretically the output of such a model simulation is the final, optimal measure for the water quality sanitation. But practically it is rarely possible to obtain the final solution to the problem without a sound engineering appraisal, especially since it is usually difficult to make a precise economical evaluation of the effect of different measures on the environment.

Most often, the solution to such environmental problems can be achieved using mathematical models, complemented by field measurements and sometimes with physical model experiments. Let us point out the crucial role and the advantages of mathematical models.

(1) As already pointed out, field measurements usually cannot predict the future consequences of different measures. In addition, it is not possible to execute different possible sanitation measures in nature due to economic and environmental protection reasons. The physical models are often unable to simulate physical processes, especially over very large space domains. Biological and chemical processes can rarely be simulated by physical models. So, many WQ processes can only be simulated by mathematical models.

(2) As a rule, MM are much more economical than either physical models or field measurements. When a mathematical model is developed, well-calibrated and verified, it can be used for the solution of other similar problems, which economises the solutions.

(3) The solution can usually be obtained in a much shorter time with MM than with physical models or field measurements. This is often a great advantage.

(4) Another advantage of MM is that we can very easily store data for possible later applications. Even the data for a very complex topography of a computational domain can be saved on a small file. Physical models must most often be destroyed to make way for new models.

(5) Another advantage of water quality MM is that we can simulate different, even not very well-known, processes and the response of a physical system to a certain kind of forcing. By comparing the results of such simulations with field measurements and observations we can better understand physical, biological and chemical processes and find more accurate mathematical descriptions of these processes.

(6) It is very important to understand that the right choice and use of mathematical models can reduce to a minimum the number of necessary - usually very expensive - field measurements. With mathematical models, the best locations for taking samples in field measurements can also be determined.
What are the limitations of mathematical models? More than in the computer facilities, the limitations are in our knowledge of the physical, chemical and biological processes and in our ability to describe them by mathematical relations.

5 Examples of Application of Physical Models and Field Measurements

With the fast development of sophisticated numerical models, more and more phenomena can be simulated, and many conventional experiments on physical models have been replaced by mathematical simulations. But the researchers can now concentrate on some specific, not yet well-understood phenomena and they can study them in detail on physical models. They first try to understand and to describe the phenomenon in detail, the influence of different parameters on it and then try to find an appropriate mathematical description of the process. The final goal is often to define mathematical relations which can then be used in advanced numerical models, which will simulate the phenomenon.

Purely hydrodynamic phenomena are nowadays relatively well understood. More often we find that basic research is taking place in the fields of density currents and sediment transport. We shall describe some examples.

**Physical modelling of vortices above flexible water plants.** An interesting type of research has been carried out (Ikeda and Kanazawa 3) in order to demonstrate in detail the flow over flexible water plants, typically a physical (hydrodynamic) phenomenon, which is not yet well-known or understood. The knowledge of such flow is important in understanding the exchange of momentum and substances, such as oxygen or sediments between the vegetation layer and the outer flow. Measurements were carried out in a laboratory channel 15 m long and 40 cm wide. Flexible water plants were modelled using 5 cm nylon filaments on the bed. The LDA measuring technique and a special visualisation technique were used to measure the velocities and register the vortices.

The authors have found several new details of the phenomenon. The velocity profile induced by the presence of water plants has an inflection near the top of the plant layer, where the flow becomes unstable, rolling up into discrete vortices. The turbulence intensity and the Reynolds stress are strongest near the top of the plant layer, where they are transported upwards by ejection and downward by sweeps. The findings of the research will undoubtedly be efficiently used to improve the accuracy and reliability of some rare 2D and 3D numerical models which have been developed to simulate this phenomenon.

**Research on sediment transport in rivers with a high concentration of fine suspended materials.** This research (Yang et al. 8) was carried out in the Yellow River, which is known for its enormous concentrations of suspended material. The methodology used was similar to laboratory experimentation, but since for such phenomena there is no accurate model similarity, the measurements were carried out in the river itself. It is known that the unit stream power formula for the
estimation of sediment transport in rivers is not accurate for rivers with a very high concentration of fine suspended materials. Thus, the goal of the research was to find out corrections to the basic Yang's formula for such cases. The results of the theoretical and experimental studies (over 1000 measurements were performed) have shown that modifications can be made on the values of particle fall velocity, flow viscosity, and relative specific weight without any change in the original formula.

In this way, new relations were found for special flow conditions with high concentrations of suspended material. However, the authors indicate that the modified formula can be used reliably for the Middle and Lower Yellow River, but that for other similar rivers the accuracy can be improved if some field data are available for calibration of parameters in the formula.

**Modelling bacterial decay coefficient during simultaneous sludge digestion and metal leaching (SSDML) processes.** An interesting example of modelling biochemical processes in waste water treatment plants was presented by Sreekrisham et al. The SSDML process can leach out heavy metals, achieve sludge solids reduction, and eliminate sludge pathogens. Because of applications in the wastewater treatment industry, a sound knowledge of the bio-chemical processes is required. Experiments were carried out both in laboratory batch reactors (20 L working volume) and in a 4000 L capacity pilot facility. Based on the results of these experiments, it was concluded that the degradation rate of volatile sludge matter is influenced by several parameters, among others by the sludge pH and the availability of oxygen. Some new mathematical relations were determined, e.g. the dependence of the degradation rate constant on the sludge pH. Finally, simulation studies were applied to actual experiments and the results were found to be satisfactory.

6 An Example of the Application of Mathematical Models and Field Measurements: Simulation of the Dispersion of Radioactive Pollutants in the Japan Sea

The Sea of Japan is a large, almost enclosed sea, between the Japanese islands, Sakhalin Island, the Siberian coast and Korea. It is about 1800 km long, 900 km wide (see Fig. 1) and has a maximum depth of about 3900 m.

A large amount of radioactive (RA) waste has been deposited in the Sea of Japan, off Vladivostok, at a depth of about 3500 meters. Research should answer the question of where the RA waste might be transported by currents and dispersion, and especially after what time they would reach the surface layers, where they might contaminate fish and other marine organisms (Cetina et al. 1). In the simulations, the possible leakage of the radionuclides was supposed to be at the location No. 9. (see Fig. 1).

This is typically a problem to be solved by means of mathematical modelling because it is neither possible to simulate such a large domain on a physical model.
nor possible to do direct experiments with contaminants or tracers in the nature. We also had to simulate a phenomenon, which may happen in the future.

Comparison with the surface currents, measured by many authors (Fig. 1) was used for the first rough calibration of the model. Calibration included testing if inclusion of the sc. topographic stress of the Neptune effect, proposed by Holloway, in model simulations, improves the results.

To determine circulation, a 3D hydrodynamic (HD) baroclinic model was used (Rajar and Cetina). A single equation turbulence model is applied to calculate the vertical turbulent viscosity, where the influence of stratification is taken into account as a function of the Richardson number. A finite volume numerical method using a hybrid scheme is applied. The 3D circulation was driven by three forcing factors: thermohaline forcing, wind, and the inflow/outflow surface (Tsushima) currents. The computations were carried out in the diagnostic mode, taking into account the data on seasonal temperature, salinity distribution and seasonal winds. A uniform wind field was accounted for (9.5 m/s in winter, 0 m/s in summer). The inflow current through the Tsushima Strait was taken to be 1.1 Sv in winter and 2.2 Sv in summer.

The observed pattern of the surface currents (Fig.1, adapted from Yoon) was compared with the simulated summer circulation minus the Neptune effect, the value of the topographic length scale parameter being L=0 (Fig. 3a). In general, the agreement is good, but south of Vladivostok the observations show a cyclonic gyre, while an anti-cyclonic circulation is obtained by the simulations. In simulated winter circulation (not shown here, see 1), this non-realistic gyre is even stronger. When trying to eliminate this disagreement, we have carried out simulations with the Neptune effect (NE, Fig 3b). The value of L=4 km was determined by calibration (Holloway et al., have found L=6 km). Two features are improved with the NE included: the anti-cyclonic gyre off Vladivostok is eliminated (in summer it is replaced by a realistic cyclonic gyre) and under both winter and summer conditions the two cyclonic gyres in the Northern part of the Sea are enhanced, which agrees better with observations. In addition, the enhancement of the NSB with NE seems to be realistic.

The only available direct measurements of bottom currents were published by Takematsu et al. The maximum velocities in the bottom layers were surprisingly high, up to 10 cm/s, which occurred mainly in the spring. It is interesting to note that the simulations have also shown maximum velocities up to 9 cm/s in spring, while in other seasons they are up to 5 cm/s.

On the basis of the computed winter and summer hydrodynamic circulation, the transport and dispersion of radioactive contaminants were simulated by the mass-transport sub-model, using the Lagrangian particle tracking method. A total amount of 1 TBq (10^12 Becquerels), bound to 7500 hypothetical particles, was released in 90 days from dumping location No. 9 (see Fig. 1). Fig. 2 shows the particles’ distribution after 5 years of simulation at a depth of 2100 to 2550 m with L=4 km. The simulations have shown, that the RA contaminants would primarily reach the surface in the northern part of the Sea of Japan. The concentrations in the surface layers (above 180 m depth) increase over time and attain the maximum
concentration after about 30 years. But the maximum concentrations would be of the order $10^{-2}$ Bq/m$^3$, which is far below the natural background values and hence would not represent any danger for the environment.

We have also calculated the residence times during which particles, released from the bottom of the Sea of Japan, pass above a depth of 180 m. The turnover time, defined as the average of the residence times of all the water particles, was 24 years. This is a surprising result, since up to now most researchers had determined the turnover time of the Sea of Japan to be of the order of 100 years. Although not enough data from measurements were available in this study, after the verification efforts, it is difficult to doubt the order of magnitude of the obtained result.

7 Conclusions

The most effective methodology to solve water quality problems is the application of mathematical models together with field measurements. The remote sensing technique is extremely useful for calibration and verification of mathematical models. Both physical models and remote sensing technique are sometimes used to reveal some new or not well-known phenomena.

References:

Fig. 1. Observed Surface Currents in the Japan Sea (Adapted from Yoon 1995)

Fig. 2. Dispersion of particles after 5 years (depth 2100-2550m). L=4 km.

Fig. 3a. Simulated velocities in surface layer, (0 to 10 m). Summer cond., L=0.

Fig. 3b. Simulated velocities in surface layer, (0 to 10 m). Summer cond., L=4 km.