A Water Quality Modelling Tutorial using SIMULINK

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Abstract MATLAB and SIMULINK numeric computation software have been used to construct a tutorial software package to teach students how to model environmental processes. The particular application is the dynamic variation of water quality in a lake as measured by its dissolved oxygen (DO) level. All significant processes which affect DO levels are considered. SIMULINK has been found to provide a good basis for this introduction to modelling, allowing students to concentrate on model construction and operation without an undue emphasis on writing program code.

1. INTRODUCTION

Two approaches are available to introduce students to modelling of environmental systems. They can use commercially available models such as SWMM, Huber and Dickinson[1992], QUAL2E, Brown and Barnwell[1987], MIKE11, Hydrotech Research[1995], or AQUALM, WP Software[1996], or they can develop their own models using programming languages such as FORTRAN90, C, VisualBASIC, or even EXCEL, Hardisty et al.[1993]. An advantage of having students use commercially available models is that it exposes them to the packages which they will use in engineering practice. However care needs to be taken to ensure that this does not become an exercise in fitting system input and output, with little consideration of the physical, chemical and biological processes which are taking place. The second approach, having students write their own program code, forces them to consider these processes but runs the risk of concentrating too much on debugging, leaving insufficient time for the modelling process itself.

The tutorial package described in this paper was developed to utilise the advantages of both approaches, while avoiding their limitations. In this approach, students must consider the processes which affect dissolved oxygen levels in a water body and construct models to represent these processes using SIMULINK.

2. WATER QUALITY PROCESSES

2.1 General

Water quality in a water body such as a Water Pollution Control Pond, lake or estuary depends on physical, biological and chemical processes taking place at various locations throughout the water column. Some of these processes cause oxygenation of the water and therefore act as DO sources, while others cause deoxygenation and act as DO sinks.

Oxygen is a fundamental requirement for life and therefore occupies a central role in water quality as a key indicator. DO is used as the main water quality parameter in these modelling exercises.

2.2 Biochemical Oxygen Demand

Aerobic decomposition of organic material by micro-organisms, particularly bacteria, is an oxidation process which leads to the consumption of DO and hence its removal from the water. The quantity of DO needed by the bacteria is the biochemical oxygen demand (BOD). This process can be represented in terms of DO by :

$$\frac{dDO}{dt} = - K_1.L \qquad (1)$$

where K_1 is the kinetic constant for BOD decay and L is the BOD remaining to be consumed. Both K_1 and L_0, the ultimate BOD, vary with temperature.

2.3 Reaeration

Reaeration is the physical process of transfer of oxygen from the atmosphere through the air-water interface into the water. The rate at which this process takes place is proportional to the oxygen deficit, the difference between the saturation DO concentration (DO_{sat} which is close to 9 mg/L at 20C) and the actual DO in the water. This process is represented in water quality models by :

$$\frac{dDO}{dt} = K_2.(DO_{sat} - DO) \qquad (2)$$

where K_2 is the reaeration constant. K_2 depends upon the turbulence level at the interface (which for estuaries and lakes is predominantly affected by the wind speed, and for rivers by the current speed), and also on the water temperature. There are many formulations for K_2 and it is up to the modeller to select the most appropriate value for the situation being modelled.

Streeter and Phelps combined the processes of reaeration and BOD decay to yield the classical solution known as the oxygen sag curve displayed in Figure 1, Kiely[1997].

Figure 6 shows the corresponding SIMULINK block diagram.

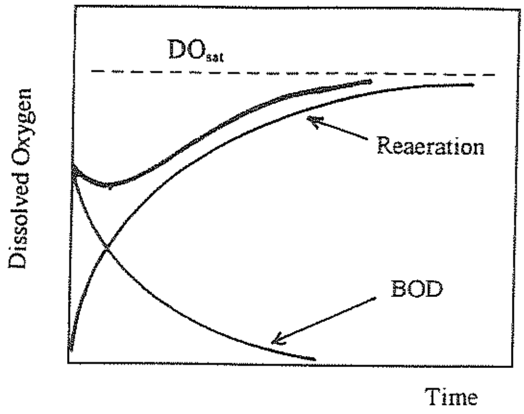

Figure 1. Streeter Phelps Oxygen Sag Curve.

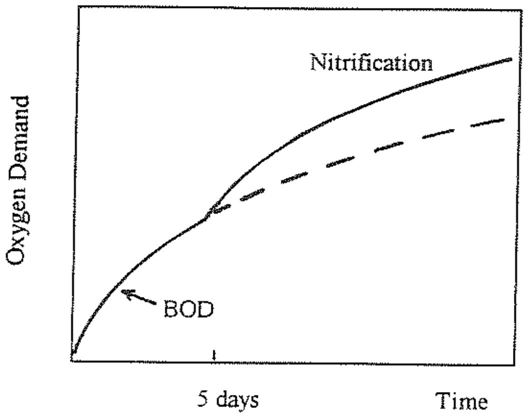

Figure 2. Oxygen Demand by BOD and Nitrification.

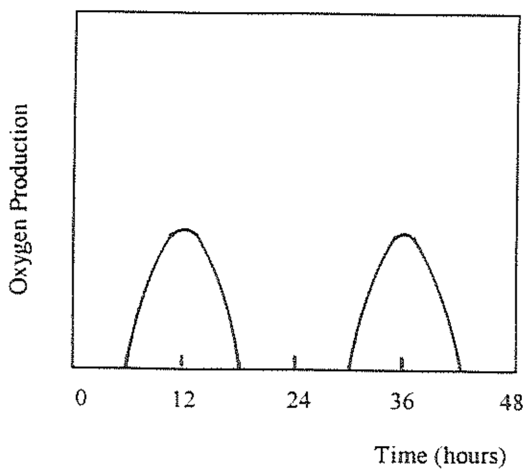

Figure 3. Oxygen Production during Photosynthesis.

2.4 Nitrification

Nitrification is a biochemical process in which aerobic nitrifying bacteria oxidise organic and ammonia nitrogen firstly to nitrite and then to nitrate. This is a two stage process involving different bacteria. The first stage is slow compared to the second and therefore governs the overall process rate.

$$2\,NH_3 + 3\,O_2 \rightarrow 2\,NO_2^- + 2\,H^+ + 2\,H_2O \qquad (3)$$

$$2\,NO_2^- + O_2 \rightarrow 2\,NO_3^- \qquad (4)$$

While there are several different representations of the nitrification process used in water quality models, it is commonly represented as an exponential demand for oxygen, dependent on the amount of nitrogen present, and adds to the BOD after about 5 days, Kiely[1997], as shown in Figure 2.

For nitrification to proceed, DO levels in excess of 1-2 mg/L are necessary. Nitrification is a significant cause of DO depletion in waterways receiving high nitrogenous loadings.

2.5 Photosynthesis and Respiration

In daylight, algae in the water utilise energy from the sun to produce carbohydrates, with oxygen as a by product. The carbohydrates are used for energy or converted to cellulose for cell wall material.

$$12\,H_2O + 6\,CO_2 \rightarrow C_6H_{12}O_6 + 6\,O_2 + 6\,H_2O \qquad (5)$$

Production of oxygen by photosynthesis varies greatly depending on sunlight intensity, temperature and the availability of a carbon source. Considering sunlight alone, the rate of oxygen production is at a peak near mid day and reduces to zero during the night. Photosynthesis is represented in models by a discontinuous sinusoidal function, Figure 3.

Respiration is the reverse process of photosynthesis and unlike photosynthesis, occurs continuously throughout the day and night. It is usually represented in models as a constant value, dependent on the biomass.

2.6 Flushing

When the water body has a stream inflow and outflow, the physical mixing process affects the concentration of pollutants by flushing. The efficiency of this flushing in purifying the water body depends on the streamflow rate relative to the pond volume, and on the degree of mixing. The particular case of BOD, with flushing and exponential decay can be represented as :

$$\frac{dL}{dt} = \frac{Q.\,L_{in}}{V} - \frac{Q.L}{V} - K.L \qquad (6)$$

where Q is the streamflow rate, V is the pond volume, Lin is the inflow BOD and L is the BOD remaining in the pond at time t.

Flushing can also be extended to the case of stream inflow (with high DO and low BOD) plus a wastewater inflow (with low DO and high BOD). In the case of a lake with stream inflow and outflow the flushing occurs continuously, but for an estuary subject to tidal flows the flushing is discontinuous and periodic.

All processes in this software package assume complete mixing, and it is therefore applicable to smaller water bodies such as Water Pollution Control Ponds, or as a first approximation to larger bodies, such as lakes.

3. THE TUTORIAL SOFTWARE PACKAGE

3.1 Modelling using MATLAB and SIMULINK

The MATLAB software provides a computing environment which combines numerical computation facilities with an array of graphical functions. SIMULINK operates as an additional module within MATLAB and is used for simulating dynamic systems, The Math Works[1994]. For this modelling tutorial, SIMULINK is used to simulate the interactions between selected water quality processes occurring in a lake.

3.2 Structure of the Tutorial Software

The tutorial consists of a set of progressively graded exercises, each of which is based on a model which is located within SIMULINK. Each exercise focuses on the governing equations for one or more water quality processes. Working from these equations, the initial exercises require the students to construct their own models using SIMULINK.

Each of these exercises is aimed at providing students with the means of simulating water quality processes, rather than teaching students about the MATLAB software itself. Thus, a Grapical User Interface for the tutorial has been developed using MATLAB's internal Handle Graphics functions. This GUI is structured to create an overall framework for the tutorial, allowing for a coherent presentation of the exercises in conjunction with the course notes provided. The tutorial GUI provides convenient access both to the model within SIMULINK for each exercise, and to the plotting and file handling functions available within MATLAB itself (Figure 4).

Given the time constraints imposed in a teaching environment, the GUI has been designed to reduce the amount of contact between the student and the standard MATLAB interface. For each exercise, the tutorial GUI provides options to perform basic file operations such as opening and saving model result files. To further create a 'user friendly' environment, an extensive range of on-line help is available from any point within the tutorial interface. In addition, the GUI has the ability to view and compare the results from each model run with either built-in analytical solutions or realistic data depending on the particular problem (Figure 5).

These features minimise the amount of time and effort needed by the student to carry out tasks in the MATLAB environment. This allows the student to focus on understanding the modelling itself, rather than devoting time to learning the variety of MATLAB commands, such as those needed to produce plots and to manage files.

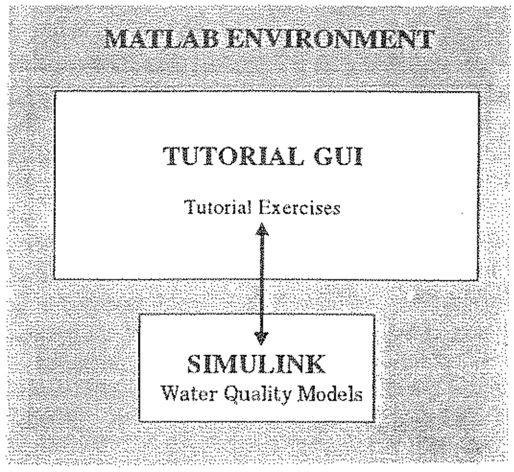

Figure 4. Structure of the Tutorial Software showing links between the GUI and SIMULINK exercises within MATLAB.

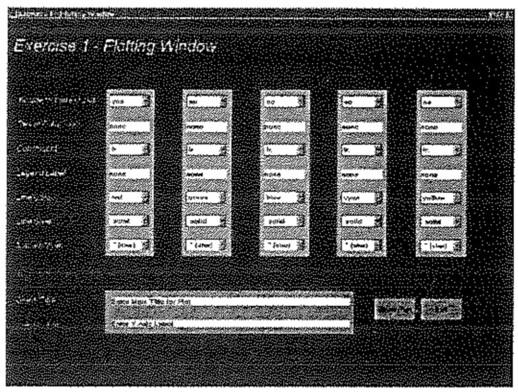

Figure 5. An example of the plotting options available for Exercise 1 of the tutorial.

4. APPLICATION OF TUTORIAL SOFTWARE TO A LAKE

The principal objective of the water quality modelling tutorial software is to introduce students to general modelling concepts. These include model building, calibration and sensitivity testing, and the assessment of model accuracy. The preliminary exercises in the tutorial package teach model building. The final exercise extends this to a realistic problem in which several interacting processes occur, and in which the data points for model calibration are not perfectly known.

Students are provided with a set of pre constructed sub-models that represent the wide variety of processes affecting DO levels in a lake. They are also provided with a range of published values of the rate constants for these processes, Corbitt[1990], Jorgensen et al.[1993], Kiely[1997], Metcalf and Eddy[1991], Tebbutt[1991], Young[1986]. They must use judgement to select appropriate values, then configure the sub-models to simulate the dynamic variation of DO concentration for the particular data set.

The volume of the lake is known and it is subjected to a stream inflow as well as a wastewater discharge from a sewage treatment plant. Both the stream flow and wastewater have known values of dissolved oxygen DO and pollutant loading in the form of BOD. Processes which may or may not be significant in controlling the DO level in the lake are : depletion by BOD, depletion by respiration of algae and zooplankton, addition by photosynthesis, addition by reaeration across the air-water interface, and depletion by nitrifying bacteria. These processes are either physical, chemical or biological, and each one has a different time scale. The DO level changes over time and the aim is to apply the water quality model to this lake.

Students are supplied with DO data points which have been measured over a 20 day period. The data contains noise which is characteristic of real data after sampling and analysis for DO. Students are required to apply the model to the lake, identifying which processes are dominant and which are not significant. Because the processes interact and also because the data contains noise, the problem is open ended with no single exact solution, and students must apply judgement in arriving at a feasible solution. In particular, some processes have only a small effect on DO, and their inclusion only adds marginally to model accuracy.

5. CONCLUSIONS

SIMULINK has been found to be an effective way of introducing students to modelling of environmental systems. The advantage of this approach is that biological, chemical and physical processes, and their interactions, can all be considered in some detail, without the distraction of writing and debugging program code.

The tutorial software uses a GUI, developed using MATLAB, to link models within SIMULINK with tutorial exercises in the GUI. The exercises are graded, requiring students to construct SIMULINK models for some processes, and providing pre constructed sub-models which are linked to represent the complex interaction of the various processes as they affect dissolved oxygen levels in the water body.

The software has been trialled on a group of final year environmental engineering students with promising results.

6. ACKNOWLEDGMENTS

This project was supported by a Teaching Development Grant from the University of Wollongong.

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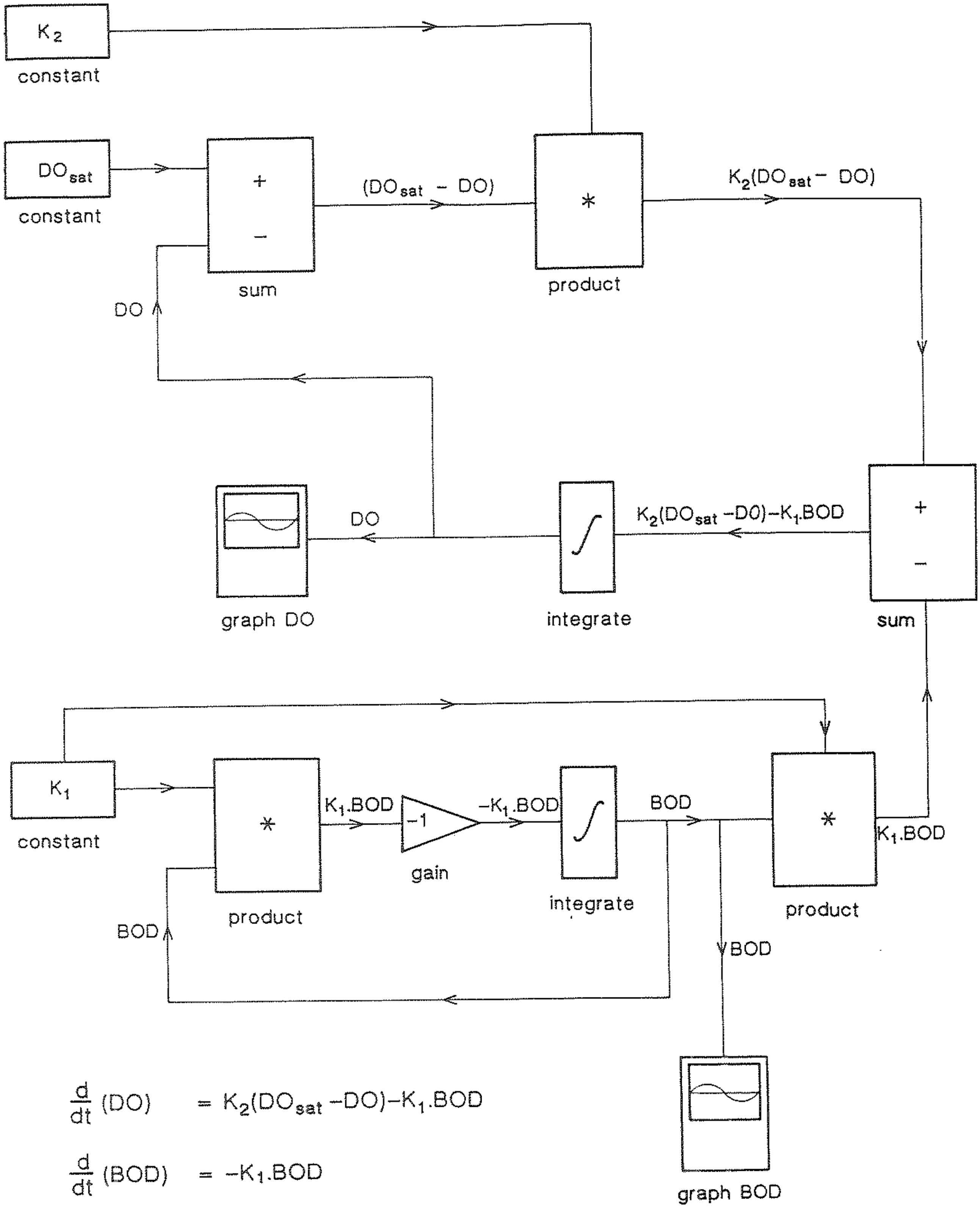

$$\frac{d}{dt}(DO) = K_2(DO_{sat} - DO) - K_1.BOD$$

$$\frac{d}{dt}(BOD) = -K_1.BOD$$

Figure 6. SIMULINK Block Diagram for Streeter Phelps Oxygen Sag Curve.