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INTRODUCTION TO CHAPTER 5: MATHEMATICAL MODELLING AND SIMULATION

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The ability to predict qualitative and quantitative performances of water systems plays a key role in the management of water quality, water resources and water infrastructures. Mathematical modelling provides a framework to measure the performance based on a set of input parameters, which are typically acquired through experimentation, established databases or literature. If developed rigorously, and with due recognition to its limitations, computational simulations of such models can be used to gather critical information, which can eventually bring about changes with regards to standard regulations and policies of water systems, thus leading to a more economical and sustainable future.

This chapter contains a collection of 5 interesting research papers, which present recent advances in theoretical mathematical modelling and simulation techniques applied in the context of water systems. The selected papers used data collected from a variety of sources including experimental results, field investigation and literature. Interestingly, one of the papers used data from established databases spanning over the last 100 years.

The first two papers deal with issues related to water quality and pollution. While the first focuses on modelling heavy metal concentrations, the second uses a three step algorithm to forecast the turbidity and pH levels in water. Staying close to the subject of pollution, the third paper used modelling of field data to highlight the importance of the function of runnels in transporting fine sediments into main channels. The next paper is dedicated to quantitative modelling of the behaviour of water structures under extreme conditions such as unpredictable hydroclimatic extremes. The final paper presents modelling of fluid catalytic cracking in riser reactors using a system of partial differential equations. A brief overview of the important topics and issues addressed in each paper is provided.

The Kainji Dam, located in the North-Central region of Nigeria, is the largest dam along the River Niger and one of the country's vital sources of hydroelectric power. Since its construction in 1968, the dam improved the irrigation and strengthened agricultural and fishing industries. Recently, there have been questions on the possibility of heavy metal contamination of its reservoir, an issue which is discussed in the work of Mohammed *et al.* The authors use a Multilayer Perceptron Neural Network (MLPNN) and Radial Basis Function Neural Network (RBFNN) to model the concentration of heavy metals at various selected sites along the reservoir. Sedimentary data of the chromium (Cr^{3+}), lead (Pb^{2+})

and copper (Cu^{2+}) metals were collected from the Kainji Hydropower Station database. Both the MLPNN and RBFNN models were able to predict the actual Cu^{2+} , Pb^{2+} and Cr^{3+} levels with a reliable correlation coefficients and within tolerable limits of the Root Mean Square Error (RMSE) and Mean Relative Error (MRE). It was found that the heavy metal concentrations at the sites were within the limits of 80, 35 and 95 mg/kg, respectively, as specified by the Washington Department of Ecology Sediment Quality Guidelines.

Similar to heavy metal contaminants, the presence of impurities in aquatic environment is detrimental to the water quality. Impurities such as microorganisms, dirt, chemicals cause a cloudy appearance of water, measured as turbidity, and heavily affects the pH level. Coagulation and flocculation are fundamental processes in treatment plants to remove impurities from water and wastewater. The jar test is a common procedure to determine the optimum operating conditions of treatment plants, such as coagulant dosage. However, the task is repetitive and time consuming and, therefore, not cost-effective. In the study of Asmel *et al.*, an alternative method, also based on the RBFNN, is proposed for determining the optimum amount of alum dosage. The employed RBFNN model is basically a three step algorithm (input, hidden and output). The results showed that the RBFNN was relatively effective in its predictions, with a correlation coefficient of 0.945 and 0.812 for the observed values of the turbidity and pH, respectively. The RMSE and MSE were also within acceptable limits.

Water pollution from sedimentary fines carried by storm-water runoffs could reduce the efficacy of existing drainage facilities. This is a growing concern for the Environment Agency in England, especially in low lying coastal areas affected by climate change. Sediment transportation via these drainage networks can adversely affect the marine system into which they are released. One such area, the Portsmouth Harbour, was investigated by Mitchell and Onabule on account of its role in serving as a sheltered environment, allowing access to ships and providing an ecosystem for a number of species of flora and fauna. The authors had measured the field concentrations of suspended sediments in the drainage runnels and main channels of the harbour at different tidal conditions over the course of 2 years (2017-2018). A simple 1-D model (based on Manning's formula) was used to quantify the degree of sediment cycles. The model predicted the time period at which the water level in the main channel is sufficiently low to allow water to flow in the runnels. The results of the model and field data underlined the importance of the function of runnels in transporting fine sediments into the main channel. However, it was suggested that higher low-tide levels of water, possibly due to the effects of local engineering projects, climatic sea level rises, or atmospheric changes, may potentially reduce the efficiency of the runnels, thereby realizing the need for alternative strategies for safe disposal of drainage water and fine sediments.

Hydroclimatic extremes involving intense precipitation or drought periods is one of the challenges imposed on many countries, including Oman, as a one of the negative impact of climate change. The design of water structures such as bridges, dams, channels, drainage are predominantly reliant on the ability to predict the frequencies of such extreme events. However, most current frequency analysis models are based on the assumption

that historical extremes are stationary, which can lead to incorrect forecasts, as highlighted in the research of Xuan and Wang. Using gridded rainfall dataset, from Australia and UK, spanning over the last 100 years, the authors performed a Spatial Random Sampling for Grid-based Data Analysis (SRS-GDA) to generate the spatial patterns of annual maximum daily rainfall (AMDR). A Markov-Chain Monte-Carlo simulation was used to compute the occurrence probability of extreme events by considering both stationary and non-stationary parameters. Although this method was devised on data representing a relatively limited geographical area, the results indeed call to attention the unpredictable nature of hydroclimatic extremes. However, non-stationary modelling seemed to be more accurate in capturing the time varying distribution of rainfall extremes. Furthermore, there is evidence to suggest that rational patterns may be developed in terms of the characteristic parameters of the sampling area, such as the size and shape of the grid.

Seismic activity is another critical factor that is often neglected in the design of water structures, where seismic activity is known to occur. There is a definite need to understand the seismic behaviour of existing major water structures such as the Wadi Dayqah Dam in Oman, which is the country's largest dam. A paper by Chowdhury and Badr have addressed this matter in their examination of the sliding stability of the dam subjected to horizontal seismic loads. The paper is not included in this chapter, as it fits better within chapter 4, Water Structures. However, we thought of bringing the attention of the reader to this paper as it contains substantial computational modelling.

Reservoirs can also be formed naturally at deep subsurface levels containing deposits of petroleum, oil and gas. Fluid catalytic cracking (FCC) is one of the most critical processes used in the petroleum industries for refining crude oil into useable gasoline. As the chemical reactions involved in FCC typically occur in riser (vertical) reactors, the efficient design of the reactor is subject to the mathematical modelling of the reactions. In the past, the FCC kinetics have been defined using 3-lump and 10-lump models, both of which are unable to accurately predict the amount of coke production from the reactor. Mahfud, however, adopted a microscopic shell balance approach in conjunction with a 4-lump model to estimate the reactant conversion and yield products from the reactor. The method relies on setting up a system of partial differential equations representing infinitesimally small control volumes in the reactor and solving them simultaneously. The effect of the reactors operating temperature on the gasoline, coke yield and total conversion was analysed. It was established that a rise in the reactor temperature would lead to more liquefied petroleum gas and coke yield, but a reduction in the gasoline yield. The model also appeared to be in good agreement with available experimental data on FCC, particularly with respect to the coke yield. This is an important outcome since the coke yield is a direct indication of the degree of endothermic heat input required in the riser.

Finally, we believe that the papers selected in this chapter offer interesting and significant up-to-date contributions on the theme of mathematical modelling and simulation of water systems. They provide a valuable source of information and an interesting read for scientists, researchers, students, engineers and decision makers. In addition, they could be very helpful in steering the directions of future studies.