18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Multi-objective design of water quality rehabilitation interventions by response surfaces

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Abstract: Mathematical models have been intensively used to support Decision Makers (DMs) in water resources planning and management. Quantitative information about the effects of a planned intervention (e.g. the installation of impellers in a lake to increase vertical mixing and thus hypolimnetic oxygenation) can be obtained via simulation (the so called what if or scenario analysis). Combining the use of simulation models and the definition of evaluation criteria enables a rigorous, quantitative comparison of different interventions, the prediction of trade-offs between different uses of water and, ultimately, the identification of the Pareto-efficient solutions. However, with the growth in the number of interventions to be considered (e.g., not only impellers, but also combinations of multiple technologies such as impellers, mixers, oxygenators, selective withdrawal) and the necessity to fix their design parameters (e.g., not only deciding whether impellers must be installed or not, but also defining their number, location, thrust and depth) an exhaustive comparison becomes impracticable. In this case, Pareto-efficient solutions must be searched for by means of an automatic selection procedure based on methods from optimization theory (e.g., gradient-based algorithms, genetic algorithms, reinforcement learning). Unfortunately, optimization methods suffer from well known computational limits and, as the complexity of the simulation model increases, they quickly become impracticable. This is the case with the distributed-parameters, process based models traditionally used to describe the hydrodynamic and bio-chemical conditions of water bodies. For instance, the model used in this study to simulate hydrodynamics and ecological processes in a 1.21 x 10^6 m^3 volume reservoir has a real-to-run time ratio associated of 30:1 and comprises 33 x 10^4 spatially distributed state variables. To overcome this difficulty in this paper we develop and apply a procedural approach based on the iterative approximation of the function (Response Surface) mapping the alternatives (defined by a vector of design parameters such as number and position of impellers) into DM's satisfaction to identify Pareto-efficient interventions. An initial, small set of alternatives is simulated through a 3D coupled hydrodynamic-ecological model (ELCOM-CAEDYM) and their effects on the DM's satisfaction are evaluated in term of physical indicators. Using an appropriate class of functions (e.g linear interpolators, neural networks), a first approximation of the response surface is generated based on the data from simulation. The identification of Pareto-efficient solutions is performed using such approximation. Through a heuristic algorithm, interesting Paretian points are chosen and the corresponding points in the space of the alternatives obtained by inverting the response surfaces. These new alternatives are then simulated using the 3D model to enlarge the sample data set over which the Response Surface is identified and the procedure repeated until a given termination test is satisfied. The approach is demonstrated through a case study in Australia, the rehabilitation of the water quality in the Googong reservoir, the main freshwater reservoir of the city of Canberra. The reservoir is affected by high concentrations of Manganese and Cyanobacteria causing severe problems to the quality of water supply and the recreational use of the water body. Destratification was thought as a suitable way to solve these problems and 2 pairs of mixers were installed in 2007. With the approach proposed new mixers configurations (position and number) have been found that significantly improve the current solution.

Keywords: Water Quality, Response Surfaces, Multi-Objective optimization

1. INTRODUCTION

Over the last decades, developments in field instrumentation and data collection techniques as well as increasing computing power have opened up new opportunities for the development of more and more sophisticated models that can accurately reproduce the hydrodynamic and bio-chemical conditions of water bodies. As these models are mainly developed for scientific purpose, i.e. enhance our knowledge about the behaviour of a system, model complexity is considered as a clear advantage, altough it strongly limits their application for management (engineering) purpose: due to their computational burden, they can be used only to perform what if analysis over a limited, a-priori defined number of alternative interventions (generally with a relatively small number of design parameters) without any guarantee on the optimality (in Pareto sense) of the best alternatives thus obtained.

Lately, this is becoming a significant limitation, particularly considering the recent advances in water quality rehabilitation technologies (e.g., the low-energy impellers recently tested on Lake Como (Morillo *et al.*, 2009) for which many design parameters have to be decided, not to mention the great potential for water quality improvement associated to multi-technology interventions (e.g., combination of impellers, oxygenators, selective withdrawals).

In this paper, a novel approach to integrate science-oriented and engineering-oriented models and improve planning of water resources is presented. It is based on the use of few, appropriately designed model simulations to iteratively identify the multi-dimensional function (Response Surface) that maps the rehabilitation interventions into the objective function we want to optimize. Based on the Response Surface (RS), a greater number of interventions can be quickly evaluated and the corresponding Pareto front approximated. Interesting points on the front are then selected using an automated procedure and the corresponding interventions in the decision space simulated using the original process based model, thus obtaining new decision/objective samples to refine the approximation of the RS and the relevant Pareto front. The procedure ends when a suitable termination test is passed.

The RS approach has been recently explored in a number of applications, particularly in traditional design parameters problems for aerospace and transport design (see Queipo *et al.* (2005) and references therein). However, to the authors' knowledge, this is the first attempt of using the RS approach in environmental management.

2. THE PROCEDURE

Consider a planning project in which we need to fix the values of n decision variables u_k with $k = 1, \ldots, n$ (e.g. number and position of mixers). A rehabilitation intervention (alternative) is univocally represented by a decision vector $\mathbf{u}$ defined over a feasibility set $U \subseteq \mathbb{R}^n$ reflecting any physical constraint on the decision values (e.g. minimum depth of the water column, distance between mixers). The set of the Pareto efficient interventions can be obtained by solving the following optimization problem

$$\min_{\mathbf{u} \in U} \mathbf{y} = \mathbf{f}(\mathbf{u}) \tag{1}$$

where the vector $\mathbf{y} \in \mathbb{R}^m$ includes m performance indicators (objectives) that measure the satisfaction of economic and water quality targets following the implementation of a rehabilitation intervention, and the map $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ represents all the physical and legal connections in the system that relates input and output. In this paper we will consider a large class of problems where the relation $\mathbf{f}(\cdot)$ can be reproduced in a highly accurate fashion via simulation of a process-based model but the computational complexity of such model makes it impossible to solve problem (1).

For such class of problem, the Response Surface (RS) methodology can be used to derive an approximate solution through the following two steps: (i) a data set of input and output is generated through a set of suitably designed experiments (in our case, this means simulating the system with the process-based model); and (ii) statistical inference techniques are applied to identify an approximate input-output relation $\hat{\mathbf{f}}(\cdot)$ (the response surface) to be used in place of the original relation $\mathbf{f}(\cdot)$ to solve problem (1). These steps can be performed in a iterative way, in fact, the results of the optimization phase can be exploited to select the regions of the decision space that it is worthwhile further exploring to derive more and more accurate approximations of the original simulation model.

Following this idea, in this paper we propose and test an iterative procedure where the phase of learning (identification of the RS) and planning (solution of the optimization problem) are developed in parallel. Each iteration, say the k-th, foresees performing the following steps: (i) to run N_k simulations of the process-based model to derive N_k output vectors $\mathbf{y}^1, \ldots, \mathbf{y}^{N_k}$ against N_k inputs $\mathbf{u}^1, \ldots, \mathbf{u}^{N_k}$; (ii) to identify the RS $\hat{\mathbf{f}}^k(\cdot)$ via interpolation of all the input/ouput data generated up to the current iteration; (iii) to solve the MO optimization problem (1) where $\mathbf{f}(\cdot)$ is replaced by the currently available RS $\hat{\mathbf{f}}^k(\cdot)$; (iv) to analyze the Pareto frontier based on the RS and select N_{k+1} Pareto-efficient solutions to be simulated at the following iteration. The procedure is sketched in Figure 1. As it can be noticed from the figure, the procedure is completed by an initialization phase, in which the first N_0 input vectors are chosen, e.g. using Design of Experiment (DOE) techniques (see Tang (1993) and references therein); and a termination test, which indicates when the procedure can be stopped, e.g. because the average distance between the output vectors simulated via the process-based model and computed by the RS

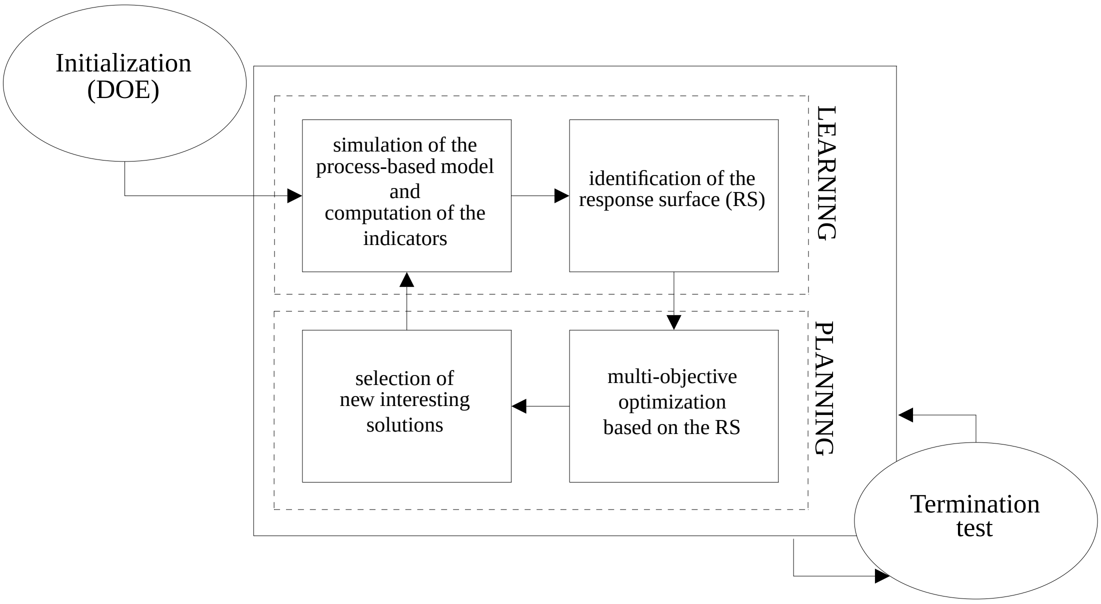

Figure 1. The learning and planning procedure implementing the Response Surface methodology.

goes below a given threshold.

3. THE GOOGONG CASE STUDY

Googong Reservoir is located in New South Wales, Australia, and is one of five sources supplying Canberra's water (Figure 2 (a) and (b)). The reservoir has a full-supply volume of 1.21 x 10^6 m^3, a surface area at full supply of approximately 3.5 km^2, an average depth of 35 m and a maximum depth of 50 m. Its waters are mainly used for potable water supply but the reservoir is also used for recreational purposes. The reservoir has a history of low to medium levels of Cyanobacteria, namely Anabaena, responsible for taste and odour problems and, at definitely higher concentration levels, for producing neurotoxins. Destratification was thought as a suitable way to solve the problem. This technique involves increasing rates of vertical mixing via mechanical means, with the objective to improve dissolved oxygen conditions at depth which in-turn reduces the likelihood of nutrient and metal release from the sediments under anoxic conditions. Two pairs of 5 m diameter WEARS (brand) surface mounted mixers have been installed for that purpose in March 2007 (point C in Figure 2). The success of this measure is still being evaluated.

3.1. The actions

The addition of new mixers and/or the reallocation of the existing ones is evaluated in this study with the purpose of improving the current solution. The search for Pareto-efficient solutions is performed according to the learning and planning procedure proposed in Section 2. The input vector $\mathbf{u}$ must univocally define the number and location of mixers. For this purpose the reservoir surface corresponding to water column depth greater than 10 m in the driest observed conditions has been divided into three macroareas (right panel of Figure 2) corresponding to an equal share of subtended water volumes. The positioning of the mixers within each macroarea reflects the functioning principle of these surface pumps and is univocally defined given the number of mixers assigned to that area in such a way that the volume of water influenced by each mixer be the same. Mixers are installed in pairs for stability reasons. The maximum allowed number of pairs of mixers compatible with the recreational use of the lake has been fixed to ten and thus this is also the maximum number of pairs of mixers that can be configured into each macroarea, i.e. there are ten possible configurations of mixer pairs for each macroarea. In conclusion, three decision variables u^i with $i = 1, 2, 3$ have been defined to form the decision vector $\mathbf{u}$, each one representing the number of pairs of mixers in the i-th macroarea subject to the constraint $\sum_{i=1}^{3} u^i \leq 10$.

3.2. The indicators

As explained above, the main water supply's concerns are about Anabaena and Manganese concentrations exceeding some reference value in the water withdrawal. As for the former, we will consider the average annual

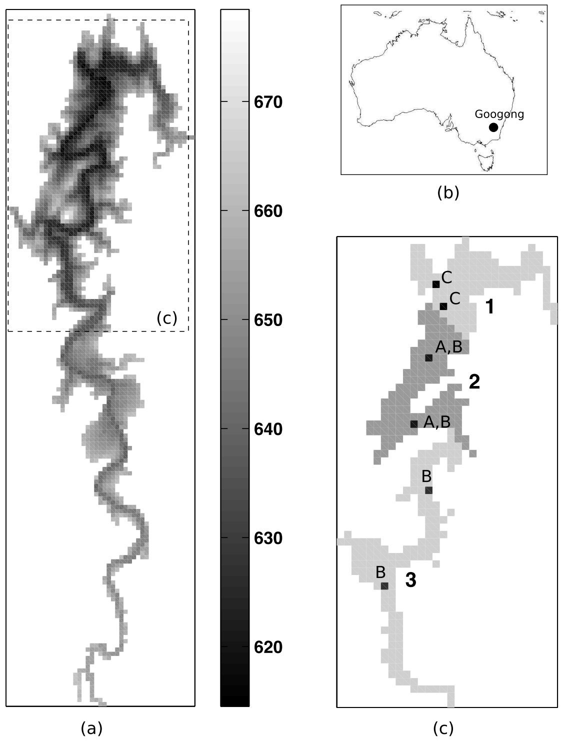

Figure 2. The Googong reservoir bathymetry (a) in New South Wales (b). The partitioning of the reservoir in three macroareas (c) with the location of the two pairs of mixers installed in 2007 (C) and the improved configurations obtained in this study (A and B, see Section 4).

number of days in which the concentration of Anabaena in the epilimnion exceeds a given threshold, i.e.

$$y_A = \frac{365.25}{h} \sum_{t=1}^{h} \chi_t, \qquad \chi_t = \begin{cases} 1 & \text{if } A_t > \bar{A} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where A_t is the average concentration of Anabaena in the epilimnion (temporal mean on day t) and $\bar{A}$ is the critical threshold (2μg chlorophyll-a/L) and h is the total number of days in the simulation horizon.
As for Manganese, any increase in its concentration in the benthic layer can be either due to poor (or null) oxygenation in the hypolimnion and/or driven by the inflow. Further, also level variations can affect the Manganese concentration as they change the ratio between the hypolimnion volume and the sediment area. Typically for low water levels (say during a drought), the oxygen will be drawn down faster and anoxic release processes will also occur more quickly, as the ratio of the region producing the problem (the surface area of the sediments) to the buffer region (the waters of the hypolimnion) increases. We will consider the average annual number of days in which the concentration of Manganese in the benthic layer exceeds a given threshold. Formally

$$y_M = \frac{365.25}{h} \sum_{t=1}^{h} \chi_t, \qquad \chi_t = \begin{cases} 1 & \text{if } Mn_t > \bar{M}n \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

where Mn_t is the average concentration of Manganese in the benthic layer (temporal mean on day t) and $\bar{M}n$ is the critical threshold (0,065 mg/L).
Finally, the cost of each rehabilitation intervention should be taken in proper consideration. Assuming such cost linearly proportional to the number of mixers installed we have the following indicator

$$y_C = \sum_{i=1}^{3} u_i \tag{4}$$

where u_i is the number of mixer pairs in the i-th macroarea.

3.3. The process-based model

The 3D coupled hydrodynamic-ecological model ELCOM-CAEDYM (Hodges and Dallimore, 2001) has been used to simulate the seasonal cycles in Googong reservoir and event driven dynamics (wind and inflow). The Estuary, Lake and Coastal Ocean Model (ELCOM) is a three-dimensional hydrodynamics model used for predicting the velocity, temperature and salinity distribution in natural water bodies subjected to external environmental forcing such as wind stress and surface fluxes. The hydrodynamic simulation method solves the unsteady, viscous Navier-Stokes equations for incompressible flow using the hydrostatic assumption for pressure. Simulated processes include baroclinic and barotropic responses, rotational effects, wind stresses, surface thermal forcing, inflows, outflows, and transport of salt, heat and passive scalars. The hydrodynamic algorithms in ELCOM are based on the Euler-Lagrange method for advection of momentum with a conjugate-gradient solution for the free-surface height. The Computational Aquatic Ecosystem Dynamics Model (CAEDYM) consists of a series of mathematical equations representing the major biogeochemical processes influencing water quality, including primary production, secondary production, nutrient and metal cycling, and oxygen dynamics and the movement of sediment. For the purpose of producing sample data for RS identification, the coupled ELCOM-CAEDYM model has been run on a 60 x 60 m grid bathymetry (left panel in Figure 2) with 1 m vertical grid resolution using a simulation step of 2 minutes. The output required by the indicators have been sampled with two different time steps, every 12 hours for the Manganese and every 3 hours for Cyanobacteria which are much more sensitive to daylight variations.

4. APPLICATION RESULTS

Given the preliminary nature of this analysis, two simplifications were unavoidable in the application of the proposed procedure and will be investigated further in subsequent research. Precisely, the DOE has been performed using a heuristic selection of the alternatives to be initially simulated with ELCOM-CAEDYM. Twenty-eight alternatives were selected in the attempt of sampling the feasibility set U in the most uniform way, including its boundary values ([0 0 0], [10 0 0], [0 10 0], [0 0 10]). Only three iterations of the procedure have been performed by significantly relaxing the termination test. In the light of these simplifications, the results reported below should be considered as a lower bound of the potential of the approach.

4.1. The identification of the RS

The identification of the RSs is a traditional model identification problem re-iterated at each iteration over an enlarged data sample. Therefore it comprises model selection and parameter estimation. Three classes of function have been evaluated including Radial Basis Function (RBF), Inverse Distance Weighted (IDW) and n-Dimension Linear (nDL) interpolator. A RBF with a 1.5 spread proved to be the best option for approximating indicator (3) while an nDL is used for indicator (2). As for the cost indicator (4), it does not need to be computed via simulation and therefore a RS approximation is not necessary.

4.2. The optimization based on RS

Once the RS has been identified, the corresponding Pareto front is calculated by solving the multi-objective optimization problem (1) where $\mathbf{f}(\cdot)$ is replaced by the currently available RS. In our application, given the relatively small number (286) of feasible alternatives, the optimization problem was solved by means of the exhaustive procedure, i.e. by computing the RS over the whole decision grid and selecting Pareto-efficient solutions via pair comparisons.

4.3. The selection of interesting solutions

Among the Pareto-efficient alternatives obtained at each iteration those which are supposed to be ‘interesting’ by the DM’s point of view are selected and the corresponding indicators’ values re-computed via simulation of ELCOM-CAEDYM, thus generating a new data sample for the RS learning process at the next iteration. As the interesting solutions are selected in the objective space, the associated decision values are obtained by inverting the RS. However, in our application, since the optimization problem was solved via the exhaustive procedure, the inversion of the RS was not required. In principle, the ‘interesting’ points on the Pareto front should be directly selected by the DM. However, the first iterations the Pareto front obtained from the procedure can be a very poor approximation of the real unknown Pareto front of problem (1). To prevent the DM’s judgment to be biased by these approximations an automated selection routine has been implemented. It is based on the idea that high curvature of the Pareto front corresponds to high trade-off solutions. Through Deulanay triangulation a continuous surface is obtained from discrete points, then the mean curvature in each point is calculated through a polynomial

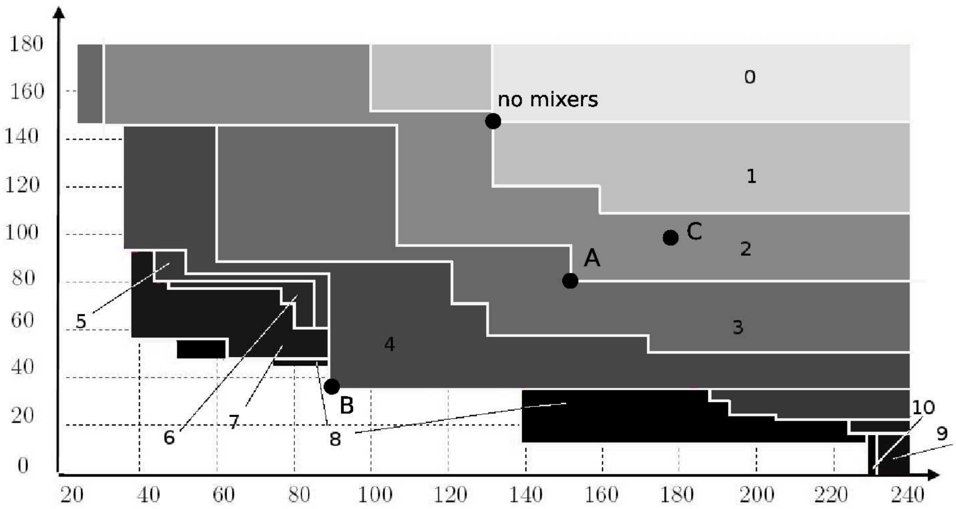

Figure 3. The approximated Pareto frontier after the third iteration of the planning and learning procedure. Horizontal axis, Anabaema indicator y_A [days/year]; vertical axis, Manganese indicator y_M [days/year]; 11 slices of the (approximate) Pareto front are reported corresponding to increasing value (from 0 to 10) of the cost indicator y_C. Point C corresponds to the current implemented mixer configuration, point A is obtained with alternative [0 2 0] and point C with alternative [0 2 2].

approximation, applying principles of differential geometry. Ideally, the DM should replace this routine in the last iterations.

4.4. Final results

The approximate Pareto front obtained at the end of the third iteration is shown in Figure 3. The current mixer configuration (C) (see also Figure 2) is dominated by point A, which is associated to alternative [0 2 0]. This means the solution so far implemented can be improved (with a reduction of 6 and 2 days respectively on indicator 2 and 3) without extra cost by simply moving the mixers in the second macroarea (point A in Figure 2). By increasing the number of mixer pairs the improvement can be even more significant. For instance, with alternative [0 2 2] (points B in in Figure 2) the current solution is improved of 91 and 52 days on indicator 2 and 3 by adding only 2 mixer pairs.

5. CONCLUSIONS

A novel procedure for multi-objective design of rehabilitation interventions of water quality in lakes and reservoir is proposed in this paper. The first results obtained on a real case study are very promising and show how the proposed approach can significantly improve traditional solutions based on what-if analysis. Further research are currently carrying on to include a formal DOE and to refine the termination test.

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