Dynamic Multiobjective Global Optimization of a Waste Water Treatment Plant for Nitrogen Removal

Jose A. Egea, Isabel Gracia

Department of Applied Mathematics & Statistics, Universidad Politécnica de Cartagena, Spain (e-mail: josea.egea@upct.es).

Abstract: This paper deals with the dynamic optimization of a wastewater treatment plant model for nitrogen removal. Two process variables (i.e., aeration factor in a tank and internal recycle flow rate) are selected as control variables and their time profiles are approximated using the control vector parameterization (CVP) technique. Two conflicting objectives have been considered to formulate a multiobjective optimization problem, namely the quality of the effluent and the plant economy. To solve the multiobjective problem and find the Pareto front the epsilon-constraint technique has been considered. In order to solve this complex problem and to prove its multimodality, a multistart procedure and the scatter search metaheuristic have been applied, showing that the problem is indeed multimodal. Results reveal that this approach is successful to find optimal operation policies in this type of plants.

Keywords: dynamic optimization, global optimization, multiobjective optimization, wastewater treatment plant, metaheuristics.

1. INTRODUCTION

Optimization and control are fundamental tools to meet the strict standards that wastewater treatment plant (WWTP’s) must comply with, while also trying to reduce costs. Relevant examples from the recent literature of attempts to optimize these plants are as follows: dynamic optimization design strategies using local gradient-based (Chachuat et al., 2001) or evolutionary (Balku and Berber, 2006) optimization methods, often based on simplified models; global optimization methods for simultaneously optimizing operation and design (Moles et al. 2003); an integrated approach for the optimization of control strategies, where a small selection of global and local optimization methods was used (Schütze et al., 1999); more recently, a study dealt with the PI tuning of a WWTP plant making use of global and surrogate model based optimization problems, specially designed for computationally expensive problems (Egea et al. 2007).

A common aspect in the design and optimization of WWTP’s is that their associated mathematical models present dynamic nature and non-linearity. In this context, the optimization of such models can be a very difficult task thus robust (global) optimization methods should be used to address this problem. As additional obstacles to satisfactory find the optimal operating conditions, controllers parameters, etc. of such processes we should consider (i) the high computational time needed to run a single simulation due to the large systems of differential-algebraic equations defining the mathematical models, which requires optimization methods that use a low number of simulations to locate high quality solutions, and (ii) the presence of several conflicting objectives to be optimized at the same time, like e.g. productivity and sustainability, which advises the use of sophisticated formulations to locate the Pareto front. Typical objective functions usually include operational costs and product quality measured as the amount of pollutants in the effluent.

In this work we have considered a challenging model describing a waste water treatment plant for nitrogen removal developed by European Cooperation in Science and Technology (COST) 624 work group (Jeppsson and Pons, 2004). This model was built to test different control strategies for the operation of this type of plants. The system dynamics is described by algebraic mass balance equations, ordinary differential equations for the biological processes in the bioreactors as defined by the ASM1-model (Henze et al., 1987) and the double-exponential settling velocity function (Takács et al., 1991), for a total number of around 100 differential algebraic equations.

A plant description as well as the problem formulation including selected variables and solving tools are presented in the following sections.

1.1 Plant description

To enhance the development and acceptance of new control strategies, the International Water Association (IWA) Task Group on Respirometry, together with the European COST work group, proposed a standard simulation benchmarking methodology for evaluating the performance of activated sludge plants. The COST 624 work group defines the benchmark as a protocol to obtain a measure of performance of control strategies for activated sludge plants based on numerical, realistic simulations of the controlled plant. According to this definition, the benchmark consists of a
description of the plant layout, a simulation model, and definitions of performance criteria. The layout of this benchmark plant combines nitrification with pre-denitrification by a five-compartment reactor with an anoxic zone. A secondary settler separates the microbial culture from the liquid being treated (Fig. 1).

Two manipulated variables, i.e., the aeration factor in the last anoxic reactor of the plant and an internal recirculation flow rate have been chosen to optimize two different performance indexes: the quality of the effluent (in terms of amount of pollutants) and the economy of the plant. The dynamic optimization problem has been formulated and solved using the control vector parameterization (CVP) approach (Vassiliadis et al., 1994), which divides the time horizon into a number of time intervals. The control variables are then approximated within each interval by means of basis functions, usually low order polynomials, with fixed or variable length along the time. This parameterization transforms the original (infinite dimensional) dynamic optimization problem into a non-linear programming problem where the systems dynamics (differential equality constraints) must be integrated for each evaluation of the performance index. For solving the multi-objective optimization problem (i.e., finding the solutions in the Pareto front), we have used the epsilon-constraint technique (Haimes et al., 1971), in which one of the objectives is optimized and the rest are formulated as additional constraints.

In this work, a Simulink implementation of the benchmark model by Jeppsson is used for the simulations (Copp, 2002). Each function evaluation consists of an initialization period of 100 days to achieve steady state, followed by a period of 14 days of dry weather. Calculations of the controller performance criterion are based on data from these last 14 days.

2. PROBLEM FORMULATION

The multiobjective optimization problem is formulated as follows:

\[
\text{Min } F = [f_1, f_2]
\]

With \( f_1 = EQ \), which represents the term of effluent quality in units of kg pollution units d\(^{-1}\) and it is defined by

\[
EQ = \frac{1}{T \cdot 1000} \int_{t_0}^{t_{14 \text{days}}} \left[ \beta_{\text{TSS}} \Delta \text{TSS}_e(t) + \beta_{\text{COD}} \Delta \text{COD}_e(t) + \beta_{\text{BOD}} \Delta \text{BOD}_e(t) + \beta_{\text{TKN}} \Delta \text{TKN}_e(t) + \beta_{\text{NOx}} \Delta \text{NOx}(t) \right] Q_e(t) dt
\]

Where \( T \) is the time horizon, \( \text{TSS}_e, \text{COD}_e, \text{BOD}_e, \text{TKN}_e, \) and \( \text{NOx} \) are, respectively, the total suspended solids, chemical oxygen demand, biological oxygen demand, total Kjeldahl nitrogen and nitrates/nitrates nitrogen, all of them measured in the effluent. \( Q_e \) is the effluent flow rate. The coefficients \( \beta_i \) are taken from Vanrolleghem et al. (1996).

The second objective function \( f_2 \) is a weighted combination of the operational costs which include aeration energy, pumping energy and sludge production.

\[
f_2 = AE + PE + 3 \cdot P_{\text{sludge}}
\]

The weights are chosen based on the work by Vanrolleghem and Gillot (2002). More details about how to calculate these terms as well as the system dynamics (not shown here for the sake of brevity since it consists in more than 100 differential algebraic equations) can be found in Copp, 2002. and in the web page maintained by the benchmark authors

In the formulation above, \( x \) is the set of state variables (and \( x^\prime \) is its time derivative), \( u \) is the decision vector which represents the control variables (both the control values and the length of the time intervals), \( F \) represents the systems of differential-algebraic equations which define the plant’s mathematical model, \( t \) is the time (\( t_0 \) and \( x_0 \) represent the initial time and the values of the state variables at the initial time). Finally, \( u_l \) and \( u_u \) are the lower and upper bounds for

---

1 http://www.ensic.inpl-nancy.fr/benchmarkWWTP/Bsm1/Benchmark1.htm
the control variables and for the lengths of time intervals. These limits for the control values are defined as [0, 360] day\(^{-1}\) for the aeration factor and [0, 92230] m\(^3\) day\(^{-1}\) for the internal recycle flow rate.

The problem, which is highly computationally demanding (it takes around 30 s. per simulation in a standard workstation), has been solved using a multistart procedure with a sequential quadratic programming method and an advanced implementation of the scatter search metaheuristic which has successfully been applied to the solution of dynamic optimization problems (Egea et al., 2009). The application of such optimization techniques has revealed that the problem is highly multimodal and that only the robust global optimization technique (i.e., the scatter search method) is able to locate the best solutions.

3. COMPUTATIONAL EXPERIMENTS

3.1 Single-objective optimization

In order to check the non-convexity of the problem regardless the objective considered, we applied a multistart procedure using a sequential quadratic method (fmincon from Matlab Optimization Toolbox\textsuperscript{\textregistered}) from different initial points randomly chosen within the decision variables. Due to the high computational cost associated to each simulation, just a low number of initial points were used. Later, the scatter search metaheuristic is applied to find a more refined solution.

Effluent Quality: The histogram for the distribution of the final solutions obtained from the application of the multistart procedure is shown in Figure 2.

![Fig. 2. Histogram of the local solutions obtained for \(f_{x1}\).](image)

The histogram shows that this single objective problem is indeed multimodal. The best solution provided by the multistart procedure is 6903.9 Kg poll units/day. The number of initial points used is 10 for a total number of 18197 simulations.

In a further step, the scatter search metaheuristic, which has proved to be efficient for solving multimodal dynamic optimization problems is applied. Since it is a stochastic method, it is recommended that several runs are carried out. Table 1 shows the results of the application of the metaheuristic in 5 runs.

<table>
<thead>
<tr>
<th># run</th>
<th>Simulations</th>
<th>Final solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11781</td>
<td>6589.7</td>
</tr>
<tr>
<td>2</td>
<td>4037</td>
<td>6586.3</td>
</tr>
<tr>
<td>3</td>
<td>3988</td>
<td>6600.0</td>
</tr>
<tr>
<td>4</td>
<td>6126</td>
<td>6587.1</td>
</tr>
<tr>
<td>5</td>
<td>10119</td>
<td>6591.6</td>
</tr>
</tbody>
</table>

All the runs consistently provide the same final solution in practice, which is better than the best solution obtained with the multistart. This confirms the multimodality of the problem and justifies the use of special global optimization techniques for solving it.

Even if Table 1 shows different number of simulations for each run, this value does not indicate the number of simulation in which the best solution was found, but the total number of simulations carried out. To have clear idea about the convergence of the method, Figure 3 shows the convergence curves for the 5 runs. These curves represent the best found solution against the number of simulations.

![Fig. 3. Convergence curves for the application of scatter search over \(f_{x1}\).](image)

From Figure 3 it is clear that in every case the best solution obtained with the multistart procedure is improved by scatter search before 1000 simulations, which reveals not only the consistency but also the convergence rate of the method.

The optimal control profiles associated to the best solution found by scatter search are shown in Figures 4.
The optimal aeration factor (Fig. 4(a)) shows oscillations with time, increasing at the beginning to oxidize the ammonia and decreasing later to favor the later reduction of nitrites and nitrates to gaseous nitrogen in the anoxic tanks. This sequence is repeated in the middle of the process (around the 7th day of operation). In any case, the aeration factor presents low values compared to the upper bound for that control (360 d⁻¹).

The optimal internal recycle flow rate coincides with its upper bound most of the time, which means that the maximum amount of nitrates are being recycled to the anoxic part of the plant to be reduced. This means a high pumping energy but this objective was not being optimized here.

**Economic term**: The terms which most influence the economic objective ($f_{x_2}$) are the aeration and pumping energy. From previous simulations it was clear that the values of the control variables which minimize this term coincide with their lower bounds (no aeration and no recycle flow rate). Even if it is an obvious solution, to illustrate the numerical difficulties to solve this optimization problem, the multistart procedure is applied again from different initial points. Surprisingly, the multistart SQP method is not able to locate this obvious solution, probably due to the noise in present in the objective function, (see histogram of solutions in Figure 5).

The best solution with a value of 14309 is far from the solution corresponding to the total absence of aeration and pumping energy, which is 13697 economic units. This solution is consistently found by scatter search in the 3 runs carried out with that method.

### 3.2 Multi-objective optimization

After performing the single-objective optimization and having verified that the problem is indeed multimodal, the multiobjective approach is formulated. The aim is to simultaneously optimize two competitive objectives: the effluent quality and the plant economy. The *Pareto* front provides an idea about the balance of both objectives when the solutions are optimal thus allowing to select the operation conditions which best fit our needs or requirements. Since we use the $\varepsilon$-constraint approach, we will only minimize $f_{x_1}$ and will add $f_{x_2}$ as an additional constraint to the formulation of Section 2.

$$f_2 \leq \varepsilon$$  \hspace{1cm} (5)

This problem is solved for different values of $\varepsilon$, in particular for the following values, based on the results obtained in the single-objective optimizations.

$$\varepsilon = [14500, 15300, 16100, 16900]$$

The solutions from the different optimization problems associated to each value of $\varepsilon$, together with the solutions obtained from the single-objective optimizations, are used to build the *Pareto* front. In this case we directly apply the scatter search method since we assume that the problem is
multimodal as in the case of the single objective formulations. Two runs were carried out for each value of \( \varepsilon \) performing between 10000-15000 simulations per run. Table 2 shows the results of the procedure.

**Table 2. Results for the multiobjective approach**

<table>
<thead>
<tr>
<th>( \varepsilon )</th>
<th>( f_{x1} )</th>
<th>( f_{x2} )</th>
<th>Simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>14500</td>
<td>8097.6</td>
<td>14500</td>
<td>11061</td>
</tr>
<tr>
<td>15300</td>
<td>7312.5</td>
<td>15300</td>
<td>13282</td>
</tr>
<tr>
<td>16100</td>
<td>6877.6</td>
<td>16100</td>
<td>14421</td>
</tr>
<tr>
<td>16900</td>
<td>6680.5</td>
<td>16900</td>
<td>16378</td>
</tr>
</tbody>
</table>

The Pareto front is shown in Figure 6

![Pareto front](image)

The Pareto front reveals what we suspected: both objectives are competitive and it is not possible to improve one of them without damaging the other. Besides, in this particular case we do not find any flat area in the Pareto front, which means that apparently we can not find any work conditions in which improving one of the objectives does not deteriorate the other significantly. In any case, this Pareto front allows the designer or practitioner to choose the best operating conditions to fulfill any specific requirement.

In Figure 6 we have also included the point which represents the solution provided by the default control strategy proposed by the benchmark’s authors (2 PI controllers to maintain the oxygen concentration in tank 5 and nitrates concentration in tank 2 at certain levels, see Copp 2002 for more details). We can observe that it corresponds to a suboptimal solution even if not too far from the Pareto front. We must also note that this proposed control strategy was not necessarily chosen to optimize the same objective functions we have formulated.

4. CONCLUSIONS

Dynamic optimization of wastewater treatment plants is a difficult task due to the dynamic nature of their associated mathematical models, which may involve numerical problems for their resolution (e.g., multimodality, noise). Other aspect to be considered to carry out the design and optimization of such models is the presence of more than one objective which can be competitive with each other. Last but not least, the computational effort associated to the simulation of such models is usually large due to the high number of differential-algebraic equations present.

In this work we have formulated a multiobjective dynamic optimization problem and have solved it making use of advanced metaheuristics (i.e., the scatter search method) to overcome the problems of multimodality and/or noise.

The use of efficient global optimization methods as well as the multiobjective formulation, allow the user to be able to choose among different operation conditions (all of them optimal) depending on specific needs or requirements. The Pareto front obtained reveal that indeed that proposed objective functions compete with each other thus it is not possible to optimize one single objective without damaging the other one.

Future work will be focused on the use of surrogate model-based optimization methods to reduce the number of simulations needed to locate high quality solutions, thus decreasing the computational effort required in this type of applications.

REFERENCES


