**Design of Large-scale Industrial Water Networks Based on Multiple Objective Mathematical Programming**

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Abstract

Structural optimisation of water networks can be used to generate alternative solutions, providing the basis for the detailed comparison of their relative merits, and a sound framework for environmental footprint reduction. Nonetheless, when based on single-objective optimisation, network degeneracy and modelling simplifications may result in a large number of alternative solutions, ultimately burdening the decision-making process. To overcome this limitation, this work focuses on a multiple objective optimisation strategy applied to the general structural design of industrial water networks.

**Keywords**: multiple objective optimisation, water network optimisation, decision making, network degeneracy

* 1. Introduction

The synthesis of process networks through the application of structural optimisation methodologies (based on superstructure concepts) has been widely studied in many engineering design domains with realistic sized problems, including *Industrial Integrated Water/Wastewater Networks* (*IWWNs*; e.g., Patrocínio *et al.* 2022). In complex systems, this framework usually leads to the appearance of alternative degenerated solutions (Faria and Bagajewicz 2010), with distinct topologies and characteristics but with comparable performance, requiring the enumeration of multiple solutions and a detailed posterior analysis step, to identify the final configuration. In some situations, this methodology may prove to be impractical. It also employs structural integer variables, which may complexify the formulation. Problems may be intensively degenerated (or quasi-degenerated) with hundreds of possibilities, where pinpointing an attractive solution can become cumbersome. Also, the search of alternative solutions is a local procedure, heavily leaning on the original result, which may fail to thoroughly explore the feasibility domain. A distinct second group of techniques tries to address these limitations through *Multiple Objective Mathematical Programming* (*MOMP*). The latter incorporates decision-making aspects of the problem during the solution process, directly tracking multiple objectives in the optimization formulation and can produce a more manageable set of interesting solutions. Although the application of these techniques to the optimisation of water networks has been conducted in the past, it regarded smaller specific sections of water networks (e.g., Boix *et al.* 2011). This work considers the design problem of an entire and complete *IWWN* in a *MOMP* aiming for broad, yet tractable, exploration of the feasible domain, supporting the decision on the adopted network.

* 1. *IWWN* optimisation framework

An *IWWN* model is comprised by a process network superstructure (Figure 1), a set of contaminants or quality indexes, and a flow model expressing the conservation relations. The superstructure includes multiple producer nodes *i* () and consumer nodes *j* (), accounting for freshwater sources (), process () and treatment units (), and effluents (). All possible node connections are accounted by the superstructure, together with existing flow and concentration (quality) constraints (Karuppiah and Grossmann, 2006, Patrocínio *et al.* 2022).



Figure 1 - *IWWN* superstructure.

The usual general mathematical problem formulation corresponds to a mixed integer non-linear program (*MINLP*), generalised in eq. 1. A single objective function () is minimised, subject to equality and inequality network constraints . Relevant constraints in this set are nonlinear, per the bilinearities in the partial contaminant mass balances formulation (i.e., continuous flow variables multiplied by continuous concentration variables). The solution vectors x and y represent continuous variables (in the problem feasibility set X) and binary variables, respectively.

|  |  |
| --- | --- |
|  | (1) |

* 1. Multiple Objective Optimisation

Network optimisation problems can be solved considering multiple different objectives *o* (). Eq. 2 mathematically defines the new *MOMP* problem. The original constraints and variables remain unchanged, although new ones can be introduced to solve this problem. *Pareto Efficiency* is an important characteristic of an *MOMP* solution, and it is achieved if there is no other feasible point in the domain capable of improving at least one of the objectives without deteriorating the others (Ehrgott 2005).

|  |  |
| --- | --- |
|  | (2) |

To apply multiple objective optimisation to *IWWN* synthesis, this work recommends the three-stage strategy illustrated in Figure 2. The *decision maker* (*DM*) intervenes in the first stage to identify the trade-offs in scope. This methodology can be applied to as many different objectives as required. For each trade-off identified in the initial stage, a *MOMP* problem is solved in the second stage, generating alternative Pareto solutions that elucidate the possible compromises within the subset of objectives considered. For simplicity, a larger set of scenarios considering the trade-offs between only 2 objectives can be considered in stage 2, to facilitate the characterisation of the corresponding Pareto surfaces. The last step compiles the results into a *solution pool*, composed by a tractable number of network solutions, spanning the feasibility domain. This tool thus allows a meaningful *a posteriori* comparison of a larger set of solution features, without the need of considerably increasing the problem complexity at stage 2. With the *solution pool* support, the *DM* is supposed to be able to elucidate in detail the relative performance of the solutions identified relative to each individual objective considered and their combination, and therefore produce a final informed choice. If necessary, the procedure can also be extended by incrementally including additional trade-offs in stage 1, and repeating the procedure from the beginning.



Figure 2 - Suggested *MOO* framework.

* + 1. MOMP techniques

Hwang and Masud (1979) introduced a broad classification for the different *MOMP* techniques according to the *DM* intervention in the solution process: *no intervention, a priori, interactive,* and *a posteriori*. The latter, particularly relevant when adopting the preconized *IWWN* *MOO* strategy of Figure 2, can be described as techniques where the *DM* makes a choice, according to some criteria, over a finite subset of the *MOMP* solutions (Hwang and Masud 1979). They can be implemented by using an Algebraic Modelling Language (*AML*) or by resorting to metaheuristic procedures, and Pareto fronts (Figure 3) can be identified to visualise the solution trade-offs.



Figure 3 - Pareto front example.

Metaheuristic-based algorithms, inspired by natural processes (e.g. genetic algorithms, simulated annealing) are often employed to solve *MOMP* problems. They focus on the problem domain exploration, although generally lacking a precise characterization of the optimality of the candidate solutions. Only deterministic global optimisation approaches can guarantee *MOMP* efficient solutions. The framework of Mavrotas (2009), using an *AML* compatible formulation and including *a priori* and *a posteriori* techniques, is suitable to produce efficient solutions and was applied to solve the *MOMP* instances of the application example. Supported by Figure 3, for simplicity reasons is limited to the trade-off between two objectives *f1* and *f2*, the algorithm description can be enunciated as:

The two targeted objectives are ranked in decreasing order of importance (here, we consider *f1* to be more important than *f2*). Lexicographic optimisation achieves the objective’s *best* and *nadir* points (, see Figure 3).

The interval between these *f2* points is equidistantly partitioned (see Figure 3) to obtain the Pareto candidates ().

*f1* is then minimized using a single objective formulation, utilising the original model constraints as well as the Pareto candidate levels as an additional constraint . This new program must be solved times, for each candidate point. To guarantee Pareto efficiency of all Figure 3 points, global minima and binding constraint objectives must be achieved, for all optimisation instances of the Mavrotas (2009) framework. If efficient, and the optimum of the routine is regarded as .

The second efficiency condition may not always be met, as *f2* is not considered in the model objective function and alternative, better levels of this objective can occur (such that ). To address this issue, Mavrotas (2009) slacks the constraint objective () and weights the new slack variable *s* in the objective function. Alternatively, here if for any instance , a new program can be solved, minimising *f2* and utilising the global optimum of *f1* as an equality constraint. It is paramount that the new result is a global optimum and will be assumed as .

* 1. Application example

The generic framework of Figure 2, was applied to the real case scenario of a crude oil refinery *IWWN*. The problem, an extended instance of Patrocínio *et al.* (2022), comprises 6 contaminants, one freshwater source, 23 processes and 6 treatment units, and two effluents. The solution of the single objective *MINLP*, minimising the hourly network expenditure, achieved an objective level of 604.68 €/h with a freshwater intake of 684.21 t/h. This problem displayed over 100 degenerated solutions with almost identical objective levels but with distinct topologies and water footprints. The trade-offs considered were: the *IWWN* hourly expenditure () *versus* the *IWWN* water footprint (), the *IWWN* hourly expenditure () *versus* the *IWWN* network complexity () and the *IWWN* yearly expenditure, accounting for piping capital and the operational cost () *versus* the environmental impact related to the pipe manufacturing and transport (). The *MOMP* problem was formulated as an *MINLP* and solved using an *AMD Ryzen 7 4800H 16GB RAM* computer and *GAMS* *40.3.0*, with the local solver *SBB* proceeded by using the global solver *SCIP*. An optimality gap of 0.001% was imposed in the local step, while *SCIP* was allowed a maximum computing wall clock time of 3 hours.

* + 1. vs.

The *f1* best and *f2* nadir levels are represented by *p1*. These levels correspond to the results of the single objective *IWWN* *MINLP*. Considering the overall result range, the *MOMP* analysis allows a 3.16% (21.65 t/h) decrease in the raw water intake with a global trade-off of increasing 10.32% the hourly network cost (62.4 €/h), as showcased in Figure 4.

* + 1. vs.

The second trade-off scenario concerns the *IWWN* hourly expenditure *versus* the *IWWN* network complexity, expressed as the number of structural connections in the optimal network. Again, the *f1* best level (*p7*, *f3* nadir as well) is identical to the single objective *IWWN* *MINLP* result. The Pareto front of Figure 5 is composed by discrete points (*p7* to *p13*), due to the nature of the *f3* objective. Here, the network complexity can be decreased by 22% (10 connections less), increasing the hourly network cost by 6.68% (40.24 €/h).

 (t/h)

(€/h)

Figure 4 - *f1* vs *f2* Pareto front.

 (Number of connections)

(€/h)

Figure 5 - *f1* vs *f3* Pareto front.

* + 1. vs.

Pipe cost data was supplied by *INTERFLUIDOS*, and the pipe unitary environmental footprint was extracted from the *SimaPro ecoinvent v3.6* database. Due to the discontinuous nature of the piping items, these parameters were corresponded to the connection flows using the strategy of Patrocínio *et al.* (2023). However, unlike the previous work, a disaggregated *MINLP* could not be applied to account for these discontinuous parameters, due to the size and the complexity of the considered *IWWN* problem. Instead, the pipe expenditure and the pipe environmental footprint were approximated by a linear trend superimposed to the parameters-flow correspondence. The surrogate *IWWN* yearly expenditure () and thesurrogate environmental impact () trade-off is displayed in Figure 6. For a 1.53% decrease in the equipment environmental footprint, the yearly network expenditures increase 10.06%. The discontinuity in Figure 6 is due to , i.e., in the mentioned interval there is no *f4* value better than the level for *p17*. To obtain the original *f4* and *f5* trade-off, the *f4\** and *f5\** *MOMP* results were converted from surrogate to the original variable space. In the latter, for the studied candidates, *p16* and *p19* are the *f5* best and *f4* nadir and *f4* best and *f5* nadir points. The other candidates were disregarded as .

With the results of the *MOMP* procedures, 14 relevant solutions were extracted (networks *p7* and *p13* are the same, and only *p16* and *p19* result from the vs. analysis). Although obtained from distinct *MOMP* routines, these solutions span and characterise the relevant compromises reachable in the feasible domain, and can be finally compared in light of the trade-offs expressed.

(105kgCO2 eq)

(106€/y)

Figure 6 ­ *f4\** vs *f5\** Pareto front.

Conclusion

Multiple objective optimisation is a suitable and recommended strategy for the solution of *IWWN* design problems. It allows the generation of alternative relevant solutions spanning the entire feasibility domain. Furthermore, the generated networks allow for a pertinent post-processing study of other solution characteristics, whose complexity renders impossible their direct incorporation in the original mathematical models. With the *MOO* support, more thoroughly informed decisions can be made by the DMs.

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