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OptWatNet - A Software for the Optimal Design of Water-Using Networks with Multi-contaminants

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Abstract

This paper presents a new user friendly software, OptWatNet, for the design of water using networks with multiple water sources and contaminants. It can handle four alternative solution strategies that differ in the initialization method used prior to the solution of the nonlinear program (NLP). OptWatNet provides an interface for easy data input, which is then converted to the GAMS format and included in the files that comprise the general linear (LP)/NLP models. Once the problem is solved, OptWatNet is able to draw the water networks corresponding to the solutions resulting from the different strategies. Overall, it is a powerful tool that can be used to easily evaluate alternative design options and compare the several strategies with respect to quality of the best solution obtained, quality of the initialization procedure and total computational effort.

Keywords: Optimization; Algorithm; Initialization procedures.

1. Introduction

Increasing water costs, restrictions on water use and increased environmental awareness, have driven designers towards more efficient water systems through the identification of re-use and recycle opportunities. Typically, two approaches have been used to obtain good designs of these systems: pinch technology and mathematical programming, [1]. Pinch technology has proved very useful for targeting minimum freshwater consumption [2] but for a large number of operations, the piping network becomes very complicated and hard to design. Furthermore, it only provides optimal solutions for single contaminant systems.

For multicontaminants, the targeting and design step have proved very cumbersome and unreliable.
Mathematical programming approaches are more general and powerful, and the design of an industrial water-using network can be accomplished through the solution of a nonlinear program [3]. However, the NLP is non-convex and may converge to a local optimal solution unless global optimization solvers, like BARON, are used. With local optimization solvers, like CONOPT or MINOS, the quality of the solution is dependent on the initial values of the model variables. In this paper, four alternative LP-based initialization methods are compared, which are able to generate structurally different networks that may be or not part of the feasible region of the original problem. Two of the methods use multiple starting points and select the best found solution of all NLPs as the optimal one. The paper also introduces a new software, OptWatNet, that greatly facilitates the comparison process by providing the water networks resulting from the different starting points and initialization methods.

2. Problem definition

The design problem of an industrial water-using network can be defined as follows. Given are a set W of fresh water sources containing certain pollutants (set C), with known concentrations, that are available to satisfy the demands of each water-using operation o, both in terms of mass that needs to be transferred ($\Delta m_{o,c}$) and maximum inlet ($c_{o,c}^{in\ \max}$) and outlet ($c_{o,c}^{out\ \max}$) concentration levels. The operations data is often expressed as a limiting flowrate ($f_o^{\lim}$), which can be related to the mass exchange by $\Delta m_{o,c} = f_o^{\lim} \cdot (c_{o,c}^{out\ \max} - c_{o,c}^{in\ \max})$. The goal is to find the network configuration that minimizes the overall freshwater demand.

3. Brief description of the four solution methods embedded in OptWatNet

The problem can be formulated as a non-convex NLP, from a superstructure that incorporates all design alternatives [3]. One important substructure corresponds to the traditional way of solving the problem, where all operations are satisfied exclusively by freshwater, typically from a single water source. This alternative has the disadvantage of not using process integration concepts, but can be formulated as a linear program. Method M1 uses the LP to generate a feasible starting point to the general NLP, which is then able to lower freshwater input through reuse. The second method (M2) features the initialization procedure proposed by Doyle & Smith [3], in which the LP consists of an approximated version of the NLP. The bilinear terms are removed by fixing the outlet concentrations in all operations to their maximum values. Although the starting point does not generally correspond to a feasible network, it is close to the feasible space since the nonlinear solvers are always able to converge. M1 and M2 can be considered as simple methods due to the use of a sole starting point and the generation of a single network.

The two remaining methods are more complex and use multiple starting points to avoid getting trapped in a suboptimal solution and missing the global optimum. Both approximate the general superstructure by a set that includes all structurally different substructures in terms of sequence of operation units (path followed by fresh/wastewater streams). For a particular sequence, M3 tackles each operation unit one at a time, with the purpose of previously determining the concentrations of all water streams that can be used to meet the demand of the operation unit under consideration. Such concentrations can be considered as parameters and hence bilinear terms are avoided, thus leading to a succession of LP problems. This initialization procedure has the advantage of providing starting points that correspond to feasible networks where a few of them may even be global optimal solutions. Overall, M3 consists on the solution of a total of |O|!·(|O| LPs+1 NLP) mathematical problems. Further details can be found in [4]. M4 uses the initialization method of Doyle & Smith for each sequence and thus leads to the solution of a total of |O|!·(1 LP+1 NLP) problems.

4. Software description

OptWatNet provides powerful functionality with a user friendly interface, a key concern in the development of computer based, decision making technologies. It was developed in Microsoft Visual Studio 2005 for Windows. Figure 1 illustrates how it works. After data input, selection of the NLP solver and solution method, OptWatNet generates a data file in a format that enables it to be included in any of the general GAMS files associated to the four alternative methods. GAMS is then called to solve the model file (see Figure 2), and upon termination, two text files are generated, one with the optimal values of the variables and another (for methods M3 and M4) with a report showing the values of the objective function after the initialization and final solution stages.

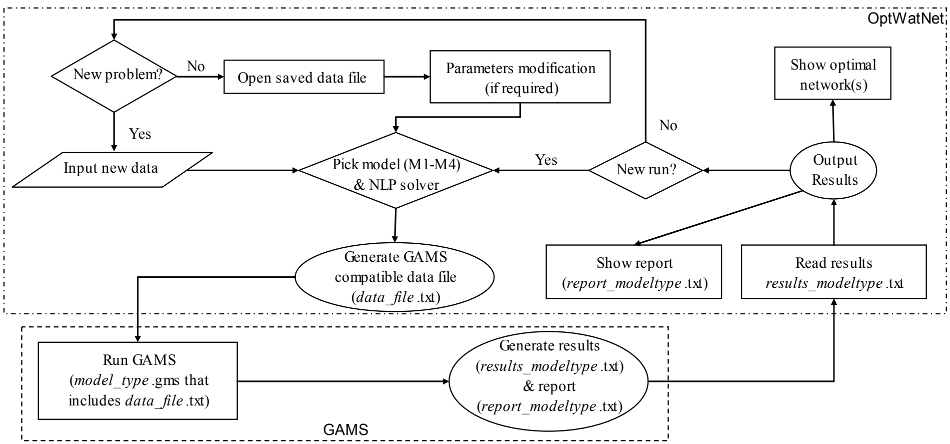

Figure 1. OptWatNet major functions including link to GAMS software

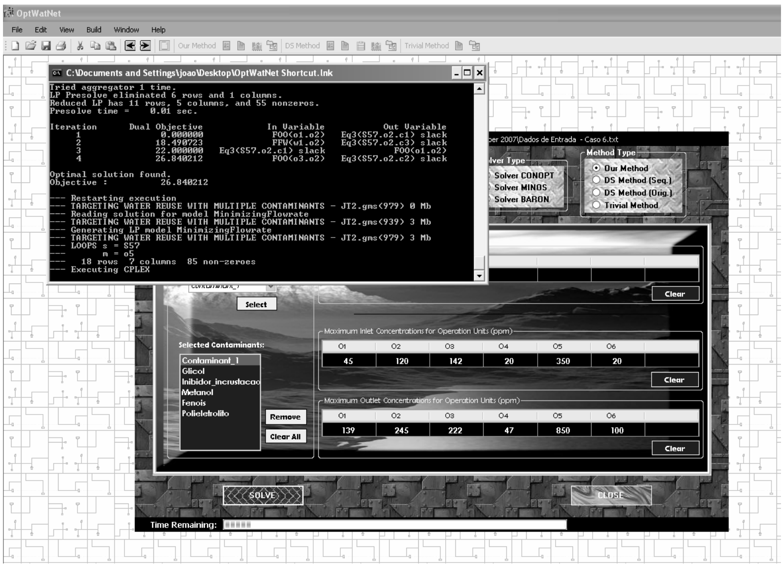

Figure 2. Screen of OptWatNet showing data input, solution method selection and GAMS run

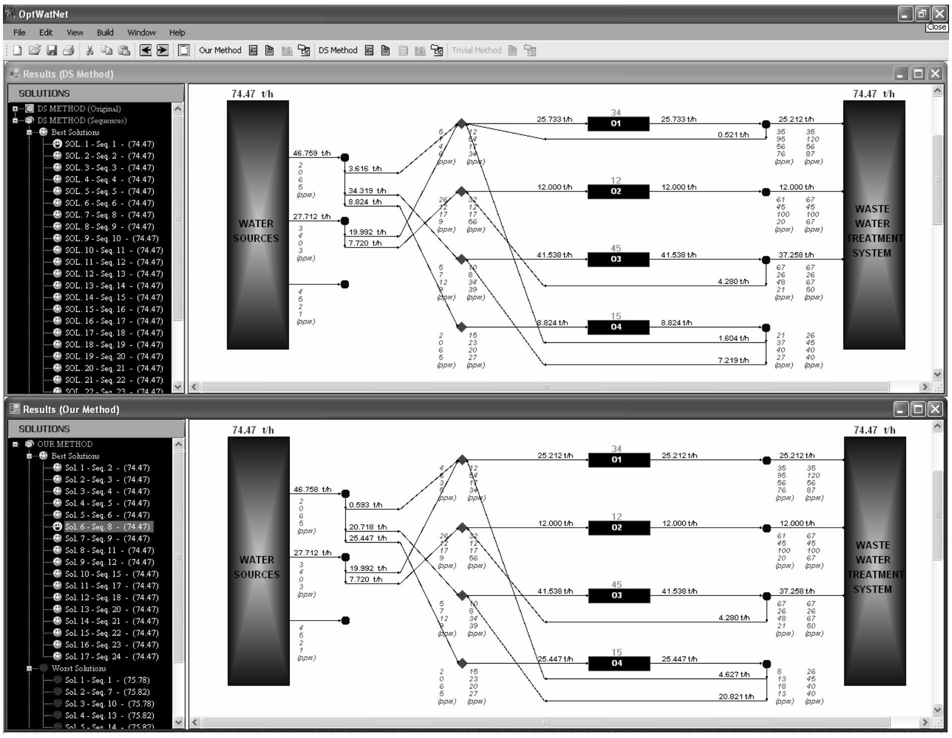

Figure 3. Comparison of degenerate solutions with different structures

The files are then read by OptWatNet, which is able to show the report file together with the several solutions in the form of a network. The results from all four methods can be accessed at any point in time, which allows for an easier comparison. It is important to emphasize that OptWatNet is designed in a way that enables an inexperienced user to use it without knowing the details of the models and solution algorithms, while a GAMS specialist can alter to some extent any model file (e.g. by adding new constraints), and still use it for viewing the results, without reprogramming. A particular problem will typically lead to a variety of solutions (with M3 or M4). OptWatNet screens them and selects those that are optimal. The best and worst solutions are accessed through different folders of the solution tree (see Figure 3). The best solutions are further analyzed in order to find structurally different networks and also identify those that feature fewer connections between operation units. Alternative designs from the same or different methods can easily be compared. In the example shown in Figure 3, two degenerate solutions are shown, where the one above features one more stream due to the recycling in unit O1.

5. Computational results

The performance of the alternative solution methods is illustrated through the solution of 7 example problems. The computational studies were performed in a Pentium-4 3.0 GHz processor running Windows XP Professional and GAMS build 22.2. In Table 1, we evaluate the quality of the solution returned (best one in bold). Due to the higher number of NLPs solved, it was expected that M3 and M4 would lead to the best solutions and this was in fact observed. M3 could always find the optimum independently of the solver, while M4 failed for Ex6 with MINOS (3.4% higher consumption). Of the simpler methods, M1 is surprisingly better than M2 and it only failed to find the optimal solution for Ex6, and Ex7 with CONOPT. The superiority of M1 over M2 and of M3 over M4 seem to suggest that it is better to use a simpler but feasible network as a starting point instead of one that is structurally more complex but that is somewhat infeasible. In terms of total computation effort (Table 2), the simpler methods are naturally faster. Between M3 and M4, the latter is solved at least twice as fast due to the solution in the initialization stage of a single LP. Thus, M4 emerges as the best method whenever a compromise must be reached between quality of the solution and total computational effort.

6. Conclusions

This paper has presented a new software, OptWatNet, for the optimal design of industrial water networks featuring multiple contaminants. It can use four alternative solution strategies to solve the problem, which are based on different initialization procedures of the general nonlinear program. Although the software does not solve the actual mathematical programming problems, this is done with GAMS, it enables easy data input and is able to read the values of the model variables and draw the corresponding water network. OptWatNet has been used for a comparative study to evaluate the performance of the methods in terms of quality of the solution and computational effort. We plan in the future to extend the software and associated models/algorithms to also deal with the distributed treatment system located downstream and also the simultaneous design problem, where some treatment units may act as regeneration units.

Table 1. Optimal freshwater consumption (t/h)

Method	M1		M2		M3[a]		M4[a]	
Solver	C=CONOPT	M=MINOS	C	M	C	M	C	M
Ex1	**193.336**							
Ex2	**74.470**							
Ex3	**143.413**							
Ex4	**142.082**		143.622	142.200	**142.082**			
Ex5	**280.771**		283.977		**280.771**			
Ex6	170.054		174.372	170.054	**164.490**		170.054	
Ex7	315.208	**312.922**	315.208		**312.922**			

[a] Value reported is the lowest of all sequences

Table 2. Total computational effort (in CPUs)

Method	M1		M2		M3		M4	
Solver	C=CONOPT	M=MINOS	C	M	C	M	C	M
Ex1	0.56	0.44	0.48	0.43	3.73	3.45	2.12	2.08
Ex2	0.31	0.55	0.56	0.33	22.9	22.4	8.69	8.02
Ex3	0.44	0.41	0.41	0.42	20.9	20.4	9.13	10.1
Ex4	0.31	0.42	0.34	0.62	128	152	41.1	63.7
Ex5	0.34	0.45	0.34	0.48	129	138	43.8	54.1
Ex6	0.33	0.34	0.44	0.34	128	121	38.3	46.9
Ex7	0.33	0.48	0.36	0.48	1148	1415	319	553

References

1. M. Bagajewicz. Comput. Chem. Eng. 24 (2000), 2093.
2. Y. Wang and R. Smith. Wastewater minimization. Chem. Eng. Sci. 49 (1994), 981.
3. J. Dyle and R. Smith. Trans IChemE, 75B (1997), 181.
4. J. Teles, P. Castro and A. Novais. In Materials of CHISA 2006. Editor: Jan Novosad, Process Engineering Publisher, Czech Republic, 1090.