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DISSERTAÇÃO DE MESTRADO

**An improved simulation-based iterated local search metaheuristic
for gravity fed water distribution network design optimization**

Willian Carlos Souza Martinho

Programa de Pós-Graduação em Ciência da Computação

Salvador
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WILLIAN CARLOS SOUZA MARTINHO

**AN IMPROVED SIMULATION-BASED ITERATED LOCAL SEARCH
METAHEURISTIC FOR GRAVITY FED WATER DISTRIBUTION
NETWORK DESIGN OPTIMIZATION**

Esta Dissertação de Mestrado foi apresentada ao Programa de Pós-graduação em Ciência da Computação da Universidade Federal da Bahia, como requisito parcial para obtenção do grau de Mestre em Ciência da Computação.

Orientador: Prof. Dr. Rafael Augusto de Melo

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TERMO DE APROVAÇÃO

WILLIAN CARLOS SOUZA MARTINHO

AN IMPROVED SIMULATION-BASED ITERATED LOCAL SEARCH METAHEURISTIC FOR GRAVITY FED WATER DISTRIBUTION NETWORK DESIGN OPTIMIZATION

Esta Dissertação de Mestrado foi julgada adequada à obtenção do título de Mestre em Ciência da Computação e aprovada em sua forma final pelo Programa de Pós-graduação em Ciência da Computação da Universidade Federal da Bahia.

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Prof. Dr. Rafael Augusto de Melo (Orientador)
Universidade Federal da Bahia

Prof. Dr. Daniel Aloise
Polytechnique Montréal

Prof. Dr. Tiago de Oliveira Januario
Universidade Federal da Bahia

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RESUMO

O problema de otimização do projeto de redes de distribuição de água (WDND, do inglês *water distribution network design*) alimentadas por gravidade consiste em determinar os diâmetros dos tubos de uma rede de água de forma que as restrições hidráulicas sejam satisfeitas e o custo total seja minimizado. Tradicionalmente, essas decisões de design são feitas com base na experiência de especialistas. Quando as redes aumentam de tamanho, no entanto, as regras práticas raramente levam a decisões quase ideais. Nos últimos trinta anos, um grande número de técnicas foram desenvolvidas para resolver o problema de projetar de forma otimizada uma rede de distribuição de água. Este trabalho aborda o problema NP-difícil de otimização do projeto de redes de distribuição de água em um cenário multiperíodo no qual ocorrem padrões de demanda variáveis no tempo. É proposta uma nova metaheurística de busca local iterada (ILS, do inglês *iterated local search*) baseada em simulação aprimorada que explora ainda mais a estrutura do problema na tentativa de obter soluções de alta qualidade. Mais especificamente, quatro novidades são propostas: (a) uma estratégia de busca local para dimensionar de forma inteligente tubos nos caminhos mais curtos entre os reservatórios e os nós com maiores demandas; (b) uma técnica para acelerar a convergência com base em um esquema de redução agressiva do diâmetro do tubo; (c) um novo mecanismo de perturbação concentrada que permite escapar de soluções ótimas locais muito restritas; e (d) um conjunto de soluções para alcançar um bom compromisso entre intensificação e diversificação. Experimentos computacionais mostram que a abordagem é capaz de melhorar uma metaheurística estado da arte para a maioria dos testes realizados. Além disso, converge muito mais rápido para soluções de baixo custo e demonstra um desempenho mais robusto na medida em que obtém menores desvios das melhores soluções encontradas.

Palavras-chave: metaheurística, projeto de redes de distribuição de água, busca local iterada, simulação.

ABSTRACT

The gravity fed water distribution network design (WDND) optimization problem consists in determining the pipe diameters of a water network such that hydraulic constraints are satisfied and the total cost is minimized. Traditionally, such design decisions are made on the basis of expert experience. When networks increase in size, however, rules of thumb will rarely lead to near optimal decisions. Over the past thirty years, a large number of techniques have been developed to tackle the problem of optimally designing a water distribution network. This work tackles the NP-hard water distribution network design (WDND) optimization problem in a multi-period setting where time varying demand patterns occur. A new enhanced simulation-based iterated local search (ILS) metaheuristic is proposed which further explores the structure of the problem in an attempt to obtain high quality solutions. More specifically, four novelties are proposed: (a) a local search strategy to smartly dimension pipes in the shortest paths between the reservoirs and the nodes with highest demands; (b) a technique to speed up convergence based on an aggressive pipe diameter reduction scheme; (c) a novel concentrated perturbation mechanism to allow escaping from very restrained local optima solutions; and (d) a pool of solutions to achieve a good compromise between intensification and diversification. Computational experiments show that the proposed approach is able to improve over a state-of-the-art metaheuristic for most of the performed tests. Furthermore, it converges much faster to low cost solutions and demonstrates a more robust performance in that it obtains smaller deviations from the best known solutions.

Keywords: metaheuristics, water distribution network design, iterated local search, simulation.

LIST OF TABLES

2.1	Summary of used symbols.	9
2.2	Information about the instance groups.	23
2.3	Information about the available pipe types.	23
2.4	Results obtained by ILS and ILS+ for instances with less than 500 pipes.	26
2.5	Results obtained by ILS and ILS+ for instances with more than 500 pipes.	27
2.6	Additional indicators for analyzing the behavior of ILS and ILS+.	34

LIST OF ALGORITHMS

1	SOLUTION-VALIDATION($G, D, R, \mathcal{T}, h^{min}, v^{max}, S$)	12
2	INITIAL-SOLUTION($G, D, R, \mathcal{T}, h^{min}, v^{max}, T$)	13
3	LOCAL-SEARCH($G, D, R, \mathcal{T}, h^{min}, v^{max}, \alpha, f, S$)	15
4	DISPERSED-PERTURBATION($G, D, R, \mathcal{T}, h^{min}, v^{max}, S, \alpha$)	17
5	SELECTION-CRITERION(L^P, K, m)	18
6	CONCENTRATED-PERTURBATION($G, D, R, \mathcal{T}, h^{min}, v^{max}, S, \alpha$)	19
7	ACCEPTANCE-CRITERION($S^{best}, S^{cand}, S^{cur}, \Pi^v$)	20
8	SIMULATION-BASED-ILS($G, D, R, \mathcal{T}, T, h^{min}, v^{max}, time^{max}, v, \alpha, f$)	21

LIST OF ACRONYMS

- ACO: Ant colony optimization;
- BFS: Breadth-first search;
- CCEA: Cooperative co-evolutionary algorithm;
- GA: Genetic algorithm;
- GGA: Global gradient algorithm;
- ILS: Iterated local search;
- LP: Linear programming;
- LPG: Linear programming gradient;
- MINLP: Mixed integer nonlinear programming;
- NLP: Nonlinear programming;
- NLPG: Nonlinear programming gradient;
- RCL: Restricted candidate list;
- SA: Simulated annealing;
- SPT: Shortest path tree;
- WDN: Water distribution network;
- WDND: Water distribution network design.

CONTENTS

Chapter 1—Introduction	1
1.1 Motivation	1
1.2 Goals and main contribution	3
1.3 Organization	3
Chapter 2—An enhanced simulation-based iterated local search metaheuristic for gravity fed water distribution network design optimization	4
2.1 Introduction	4
2.2 The Water Distribution Network Design Optimization Problem	7
2.3 The simulation-based iterated local search metaheuristic	11
2.3.1 Solution validation using hydraulic simulation	12
2.3.2 Initial solution	13
2.3.3 Local search	14
2.3.4 Perturbations	16
2.3.4.1 Dispersed perturbation	16
2.3.4.2 Concentrated perturbation	17
2.3.5 Acceptance criterion	20
2.3.6 Simulation-based iterated local search metaheuristic	21
2.4 Computational experiments	22
2.4.1 Benchmark set	22
2.4.2 Tested approaches and settings	23
2.4.3 Computational results	24
2.4.4 Graphical summary	28
2.4.5 Analyzing the impact of each individual novelty	30
2.4.6 Analyzing additional indicators for ILS and ILS+	33
2.5 Final Remarks	35
Chapter 3—Conclusion	36
3.1 Future works	36
References	38

LIST OF FIGURES

- 2.1 Example of a water distribution network. Demand nodes are represented as dots, reservoirs as rectangles and pipes as lines. The thicker lines represent larger diameter pipes. A network which is not optimized is exemplified in (a), whereas an optimized network is illustrated in (b). 8
- 2.2 Graphical summary of the improvements achieved by ILS+ over ILS. The subfigures show the percentage of the instances for which ILS+ improved ILS, as well as the average gains of ILS+ over ILS. Subfigures (a) and (b) consider the average and best costs for all instances; Subfigures (c) and (d) examine the average and best costs for instances with less than 500 pipes; Subfigures (e) and (f) contemplate instances with more than 500 pipes. 29
- 2.3 Impact of the individual novelties on the obtained solution costs considering instances with less than 500 pipes. 31
- 2.4 Impact of the individual novelties on the obtained solution costs considering instances with more than 500 pipes 32

INTRODUCTION

1.1 MOTIVATION

A safe, adequate, and accessible supply of potable water is one of the basic necessities of any human being. According to a World Health Organization (2011) study, improving access to safe potable water not only reduces the overall risk of disease, but can also be an effective part of poverty reduction strategies. Access to safe drinkable water is important as a health and development issue at national, regional and local levels. Furthermore, it has been shown that investments in water supply and sanitation can yield a net economic benefit as the reductions in adverse health effects and health-care costs outweigh the costs of undertaking the interventions. Consequently, water distribution networks are amongst the most vital elements of a society's infrastructure, providing people with high-quality drinking water in sufficient quantities and at adequate pressures. A water distribution system is an infrastructure that consists of different elements (such as pumps, reservoirs, pipes, valves, among others) connected together to convey quantities of water from one or more sources to multiple consumers (which can be domestic, commercial, or industrial) (De Corte & Sørensen, 2013). The distribution system is designed to reliably distribute water in sufficient quantities and provide to demand patterns, pressure and velocity limitations, quality assurance, and maintenance issues. Therefore, different combinations of reservoir storage, network layout, water mains, and pumps are used, depending on the system service area, topography, and size. Very often, the reliability of these networks requires major investments and thus an efficient network design is of crucial importance.

In this direction, the design of water distribution networks (WDN) gives rise to an optimization problem called the water distribution network design (WDND) optimization problem. Given a network topology, associated demand patterns, a collection of hydraulic constraints, and a set of available pipe types, each of which with a cost per length, the purpose is to design network pipe diameters that satisfy all requirements with the minimum possible design cost. The WDND optimization problem is known to be NP-hard (Yates, Templeman, & Boffey, 1984) and can be formulated as a nonlinear constrained optimization problem due to the nonlinearity implied by the conditions of the hydraulic system. Such conditions specify that the flow going through the pipes satisfies the supply and demand nodes of the network and is compatible with

the pressure head losses (loss of "hydraulic energy"). The equations that empirically represent this relationship are nonlinear, implying that the problem constraints have a nonlinear nature. Furthermore, pipe diameters are often manufactured in a relatively small set of discrete sizes. This situation requires that the variable be discrete-valued and effectively introduce an extra layer of difficulty to the problem solution.

Many optimization techniques have been proposed to be effective and feasible alternatives for dealing with problems of that nature. Heuristic algorithms is a popular category of optimization techniques that provide feasible solutions that are not necessarily optimal and for optimization problems they usually run faster and often find high-quality solutions (Resende & Ribeiro, 2016). Further, they are capable of handling with hard problems that have an exponential sized solution space in which enumeration research became impracticable in a reasonable time, even when an implicit enumeration scheme is used to discard parts where the optimal solution cannot be found. The core of these algorithms is the use of heuristic techniques designed for tackling a specific problem. In fact, to prove that a solution is optimal or demonstrate that it does not need to be examined is generally not trivial to implement such task efficiently.

Metaheuristics (Glover, 1986) are general high-level procedures that coordinate heuristics through simple rules and are able to find high-quality solutions to computationally difficult optimization problems. These procedures are often based on different paradigms and offer mechanisms to escape from local optima solutions (Resende & Ribeiro, 2016). Metaheuristics have been proposed in the literature over the years, a few examples are tabu search (Glover & Laguna, 1998), genetic algorithms (Banzhaf, Nordin, Keller, & Francone, 1998), greedy randomized adaptive search procedure (GRASP) (Resende & Ribeiro, 2016), and iterated local search (ILS) (Lourenço, Martin, & Stützle, 2003). Metaheuristics are very useful in practice as they can explore an enormous number of solutions by effectively guiding the search with powerful mechanisms.

Combinations of optimization and simulation methods, called simulation-based optimization, is an approach of expressive presence in the research community. (Amaran, Sahinidis, Sharda, & Bury, 2016; Mota, De La Mota, & Serrano, 2015; Henderson & Nelson, 2006; Zilinskas, 2005; Fu, Glover, & April, 2005; Tekin & Sabuncuoglu, 2004). In a simulation-based optimization method, the simulation model remains embedded in the routine of an optimization algorithm with the role of evaluating solutions of the system that must be optimized by the algorithm. Note that the simulation model could be seen as a black-box structure, the proposal for optimization approaches based on simulation is to attribute efforts to the optimization algorithms and not in solving functions that describe the behavior of the system immersed in the object of study. In addition, studies that used this approach (Chong & Osorio, 2018; Luna, Ribau, Figueiredo, & Alves, 2019; Zhang, Best, Chivu, & Meltzer, 2020; Chu, You, Wassick, & Agarwal, 2015; Pourhassan & Raissi, 2017; Urayama, Fu, & Marcus, 2015) showed successful results in several study topics when compared with pure classic methods. Motivated by recently successful results of De Corte and Sörensen (2016b, 2016a), this work tackles the WDND optimization problem with a simulation-based optimization algorithm. Furthermore, this work tries to overcome the main problems of De Corte and Sörensen (2016b), such as the use of purely stochastic concepts to arrive at good solutions that faces difficulty as the size of the instances increases.

1.2 GOALS AND MAIN CONTRIBUTION

In this master's thesis, our main goal is to study simulated-based optimization approach and effectively apply them to the WDND problem. We aim to propose a new robust method for achieving solution values that improves or at least match with the current state-of-the-art. The proposal try to overcome the mainly problems of De Corte and Sörensen (2016b) incorporating a heuristic that contemplates the structure of the problem, considering from mechanisms that allow escape from the local optima to procedures that allow the compromise between intensification and diversification. The approach developed in this work follows simulation-based optimization method that combine an optimization algorithm with a simulation model responsible for evaluates the nonlinear objective function. Then, we focus on the development of robust heuristic algorithms through realistic assumptions about the system in order to optimize it.

The main contribution of this master's thesis is a robust simulation-based iterated local search metaheuristic to tackle the water distribution network design optimization problem focused on a multi-period setting with time-varying demand patterns. The approach improves over the simulation-based metaheuristic of De Corte and Sörensen (2016a) by considering relevant concepts on the structure of the problem to allow enhancements in performance. The approach presents four main novelties. Firstly, observing that low cost water distribution networks tend to have in common a structure pattern in which larger diameter pipes create paths between the nodes with highest demands and the source nodes, we attempt to smartly dimension the pipes in these paths. Secondly, it uses an aggressive pipe diameter reduction scheme based on different factors to speed up convergence. Thirdly, it introduces a concentrated perturbation mechanism to allow escaping from very restrained local optima solutions. Fourthly, it encompasses a pool of solutions to achieve a good compromise between intensification and diversification. Extensive computational experiments carried out using a set of benchmark instances show that the introduced novelties allow our new approach to outperform a state-of-the-art metaheuristic for most of the instances. Furthermore, our new approach presents much faster convergence to good quality solutions and more robustness, as the obtained solutions show much less deviation from the best ones. Additionally, we contribute new concepts that can be useful for other optimization problems.

Lastly, the contents of this master's thesis were submitted for publication in a relevant operational research journal (Martinho, Melo, & Sörensen, 2020).

1.3 ORGANIZATION

The remainder of this master's thesis is organized as follows. Chapter 2 presents the Martinho et al. (2020) work in which formalizes the WDND optimization problem in a multi-period setting with time-varying demand patterns. Furthermore, the chapter presents the description of the proposed simulation-based iterated local search metaheuristic. Finally, the chapter summarizes the computational experiments marking the improvements achieved with the newly proposed approach and discusses final comments. Chapter 3 summarizes the main contributions of this dissertation and discusses future work possibilities.

AN ENHANCED SIMULATION-BASED ITERATED LOCAL SEARCH METAHEURISTIC FOR GRAVITY FED WATER DISTRIBUTION NETWORK DESIGN OPTIMIZATION

The gravity fed water distribution network design (WDND) optimization problem consists in determining the pipe diameters of a water network such that hydraulic constraints are satisfied and the total cost is minimized. This chapter presents a new enhanced simulation-based iterated local search (ILS) metaheuristic proposed which further explores the structure of the problem in an attempt to obtain high quality solutions. The content of the chapter was submitted for publication in an operational research journal (Martinho et al., 2020).

2.1 INTRODUCTION

A safe, adequate, and accessible supply of drinking water is one of the basic necessities of human beings. The most efficient and effective way to transport drinking water is through a network of pipelines. Water distribution networks require decisions in three different phases with distinct time horizons, namely, layout, design, and planning (De Corte & Sörensen, 2016b). The *layout* phase consists of strategic decisions based on which the structure of the network is defined. In this phase, decisions taken include where the different pipes will be constructed as well as the locations to build pumps, valves, water tanks, reservoirs, and other components of the network. Traditionally, the pipe network layout is designed by the engineers and taken as fixed during the process of component sizing. The *design* phase also consists of strategical decisions which will define the type and size of each pipe, pump, valve, tank, and all other components of the network. All these decisions take into consideration the water demands, the adequacy of water facilities, and the water storage necessary to meet peak demands. Furthermore, other reliability conditions of the network should be met with provision for the estimated requirements in the future. The *planning* phase groups all tactical decisions which are taken on a daily basis and are concerned with the functioning of valves and operational pump levels to ensure that sufficient water is available in all nodes of the network.

In this master's thesis we study the water distribution network design (WDND) optimization problem in a multi-period setting in which time varying demand patterns occur. Informally, this problem can be defined as follows. Given a network topology (i.e., a set of water supply points, a set of demand points, and a set of junction points, together with a set of potential pipes connecting them), associated demand patterns, a collection of hydraulic constraints, and a set of available pipe types, each of which with a cost per length, the problem consists in assigning a particular type to each pipe in the network such that all requirements are met and the total design cost is minimized. In terms of the different phases mentioned before, the WDND can be thought of as combining the *design* phase (determining the type of pipe for each potential pipeline) with aspects of the *layout* phase (determining whether a potential pipeline should be built or not). The WDND optimization problem is challenging for several reasons. Firstly, it is known to be NP-hard (Yates et al., 1984). Secondly, the hydraulic conditions of the network are affected by every pipe and therefore changes in one of them can influence the circumstances as a whole. For these reasons, this work proposes a robust simulation-based iterated local search metaheuristic.

Originally, the proposed methods dealt with water distribution system management problems using linear/nonlinear optimization techniques. These methods were limited by the system size, the number of constraints, and the number of loading conditions. Alperovits and Shamir (1977) proposed a linear programming (LP) based approach, denoted linear programming gradient (LPG), in which the pipes were considered to be composed of segments of different sizes and the sum of these segments, each one with different diameters, was equal to the length of the pipe. The method decomposes the optimization problem in two levels. In the first level, given a set of flows, the corresponding optimal cost of the network is obtained using linear programming. At the second level, this solution is used to modify the flow of the pipes according to the gradient of the objective function with the aim of improving the cost. The authors proposed to repeat the procedure using different starting points to increase the probability of finding a global optimum. Quindry, Liebman, and Brill (1981) extended the LPG of Alperovits and Shamir (1977), but instead of the flows they considered the head (internal energy per unit weight of fluid) of the nodes as values in the formulation of the linear program. The authors also adjusted the original expression of the gradient derivation to express the interaction between paths, which enhanced the performance of the method. Fujiwara, Jenchaimahakoon, and Edirisinghe (1987) suggested an improvement of the original LPG in which the adjustments in the flows of the pipes are performed by a quasi-Newton method rather than a simple gradient search heuristic. A concise and complete study of the LPG has been adopted and restated in Kessler and Shamir (1989), where the authors successfully improved the method.

Shamir (1974) proposed a nonlinear programming (NLP) approach that uses a combination of generalized reduced gradient and penalty methods. The approach constructs a Lagrangian function by penalizing the objective function for violation of the constraints. The flow values are obtained by a Newton-Raphson method employing sparse matrix techniques. Fujiwara and Khang (1990) proposed a two-phase decomposition method called nonlinear programming gradient (NLPG), which extends the method of Alperovits and Shamir (1977) to nonlinear modeling. The method first specifies the flow distribution and pumping heads. Then, it solves the resulting convex program to get the pipes' head losses. The Lagrange multipliers of the obtained optimal solution are used to modify the flow distribution and pumping heads to achieve a reduction in the cost of the system. In the second phase the obtained pipes' head losses

are fixed, and the resulting concave program is solved for the flow distribution and pumping heads. These two phases are repeated until no further improvement can be achieved. Recently, Caballero and Ravagnani (2019) proposed a mixed integer nonlinear programming (MINLP) model considering the flow directions and the pipes diameters as optimization variables. The authors used techniques to reduce the number of nonlinear equations in the model, which was solved using a global optimization solver. The approach was used to solve to optimality network instances with up to 34 pipes.

Different metaheuristic frameworks have been applied to deal with the WDND optimization problem. Loganathan, Greene, and Ahn (1995) proposed an outer flow search-inner optimization procedure. In their approach, each pipe in the network is subject to an external search scheme based on simulated annealing (SA) and a multi-start local search that selects alternative flow configurations. Next, an inner linear program is used for the design of least-cost diameters through selected flow configurations. Cunha and Sousa (1999) also proposed an SA based metaheuristic, in which the neighborhood of a solution is any configuration having all the pipes but one with the same diameter as in the current configuration. Starting with an initial configuration of pipes with their respective diameters, at each step of the algorithm, a new configuration is randomly selected from the neighborhood of the current configuration, and then its cost is evaluated. If it is accepted, the configuration will be used as the starting point for the next step. If not, the original configuration will play that role. Each generated configuration is evaluated using the Newton-Raphson method to solve the hydraulic equilibrium equation set and determine the flows and hydraulic heads of the system.

Evolutionary algorithms represent an alternative strategy for tackling complex problems. Simpson, Dandy, and Murphy (1994) proposed an approach using a genetic algorithm (GA) that uses a binary encoding in which each tube diameter is assigned to a binary code. A Newton-Raphson method was used for hydraulic network analysis at each function evaluation to determine the flows and hydraulic heads of the system. The method assigns a penalty cost for every constraint violation, which is added to the network's total cost. The algorithm proceeds until a given total number of generations is evaluated. Results were compared with the techniques of complete enumeration and nonlinear programming.

Simulation-based heuristics are presented as an alternative for problems that have difficult solution equations. In this way, it is possible to work on improving heuristic methods for the problem, without spending too much effort on solving the equations. Savic and Walters (1997) used a genetic algorithm which adopts a Gray coding instead of the traditionally used binary coding. The hydraulic simulator EPANET (Rossman, 1993) was used to solve the equations of the system and determine the flows and hydraulic heads. Gupta, Gupta, and Khanna (1999) developed an alternative GA implementation which represents the set of solutions as the discrete pipe sizes and not in the binary alphabet as usual. Therefore, the decoding or coding required during the execution of the algorithm for each new set of solutions is avoided. The hydraulic simulator ANALIS (Bassin, Gupta, & Gupta, 1992) was used to compute the hydraulic equations. Chen et al. (2019) presented a cooperative co-evolutionary algorithm (CCEA) using the hydraulic simulator EPANET. The authors proposed an iterative trace-based decomposition method to divide a large-scale water distribution network into sub-networks. After decomposition, the sub-components are handled by an equal number of cooperative evolutionary algorithms.

Maier et al. (2003) proposed a simulation based ant colony optimization (ACO) approach in

which every decision point is associated with a pipe in the network. At each decision point, there are a number of options, corresponding to the available pipe diameters. The cost corresponding to a particular option is the product of the unit cost per meter length of each of the pipe diameters and the length of the pipe segment under consideration. The algorithm was linked with the hydraulic solver WADISO (Gessler & Walski, 1985) in order to calculate the maximum pressure deficit for each generated candidate solution. Zecchin, Simpson, Maier, and Nixon (2005) presented a similar strategy but additionally conducted an extensive study to determine the guidelines for assigning values to the various parameters in the ACO algorithm specifically for WDND optimization. Other approaches such as particle swarm optimization (PSO) (Montalvo, Izquierdo, Schwarze, & Pérez-García, 2010) and harmony search (HS) (Geem, 2006) were also applied in the context of WDND optimization.

De Corte and Sörensen (2016b) presented an approach using iterated local search (ILS) to handle the WDND optimization problem. The algorithm constructs an initial solution and then attempts to iteratively improve this solution by performing small diameter reduction moves. Therefore, neighboring solutions have configurations in which all pipes but one have the same diameter as the current solution. The decision of which pipe will be decreased in diameter depends on a greedy randomized strategy. When a local optimum is reached, a perturbation move is used to try escaping from this local optimum. The hydraulic simulator EPANET 2 (Rossman, 2000) was used to evaluate the problem constraints for each obtained candidate solution. Later, De Corte and Sörensen (2016a) extended the problem to a multi-period setting in which time-varying demand patterns occur, which is the variation we consider in our work.

A detailed critical review on gravity-fed water distribution network design optimization is given in De Corte and Sörensen (2013). D'Ambrosio, Lodi, Wiese, and Bragalli (2015) presented a survey of mathematical programming approaches widely applied to mixed integer non-linear programming models and introduced them to the context of water distribution network optimization. The authors discussed a class of challenging optimization problems related to the nonlinear network flow model and then attempted to solve them using the described techniques. More recently, Mala-Jetmarova, Sultanova, and Savic (2018) presented a systematic review and discussed limits, trends, and future research directions in the field of water distribution network design optimization.

2.2 THE WATER DISTRIBUTION NETWORK DESIGN OPTIMIZATION PROBLEM

Consider a set of nodes $N = \{1, 2, \dots, |N|\}$ representing points of water demand and supply (such as a reservoir) as well as junctions (points with both demand and supply equal to zero), and a set of water distribution pipes $P = \{1, 2, \dots, |P|\}$. Note that a water distribution network can be represented as a graph $G = (V, E)$ in which there is a vertex for each node and an edge for each pipe of the network. A water distribution network is illustrated in Figure 2.1. Define a planning horizon $\mathcal{T} = \{1, 2, \dots, |\mathcal{T}|\}$ which describes a typical network operation cycle. Let $T = \{1, 2, \dots, |T|\}$ be the set of available pipe types in which each type $t \in T$ has an associated cost $c_t \in \mathbb{R}_+$ per unit of length, roughness $r_t \in \mathbb{R}_+$ and diameter $d_t \in \mathbb{R}_+$ (in *mm*). In this work, it is assumed that the costs of the types increase as their diameters increase. It is also assumed that the elements in T are organized such that $d_1 \leq d_2 \leq \dots \leq d_{|T|}$. In addition, consider $l_p \in \mathbb{R}_+$ (in *m*) to be the length of pipe $p \in P$. Consider, for every node $n \in N$, the expected water demand

$D_{n,\tau} \in \mathbb{R}_+$ (in m^3/s) and the water supply $R_{n,\tau} \in \mathbb{R}_+$ (in m^3/s) that has to be satisfied for every period $\tau \in \mathcal{T}$. Consider $h^{min} \in \mathbb{R}_+$ (in m) to be the minimum pressure assumed for every node $n \in N$ and $v^{max} \in \mathbb{R}_+$ (in m/s) to be the maximum velocity for each pipe $p \in P$ to be satisfied for every period $\tau \in \mathcal{T}$. The water distribution network design (WDND) optimization problem consists in the selection of a type in $T = \{1, 2, \dots, |T|\}$ for each pipe in the network so that the total cost of the network is minimized without violating any hydraulic constraints. A summary of the input data and decision variables is given in Table 2.1.

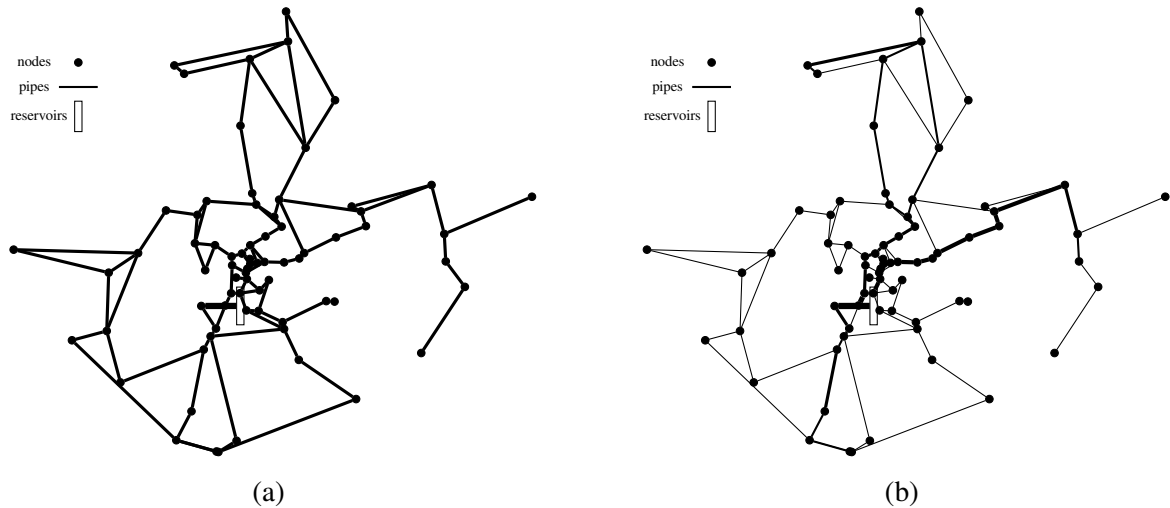


Figure 2.1: Example of a water distribution network. Demand nodes are represented as dots, reservoirs as rectangles and pipes as lines. The thicker lines represent larger diameter pipes. A network which is not optimized is exemplified in (a), whereas an optimized network is illustrated in (b).

Table 2.1: Summary of used symbols.

Symbols	Descriptions
N	Set of nodes
P	Set of pipes
\mathcal{T}	Set representing the planning horizon
T	Set of available pipe types
Ξ	Set of closed loops in the network
ξ	Set of pipes in a closed loop
c_t	Cost of pipe type $t \in T$, per unit of length
r_t	Roughness of pipe type $t \in T$
d_t	Diameter of pipe type $t \in T$ (in mm)
l_p	Length of pipe $p \in P$ (in m)
$D_{n,\tau}$	Water demand (in m^3/s) of node $n \in N$ in period $\tau \in \mathcal{T}$
$R_{n,\tau}$	Water supply (in m^3/s) of node $n \in N$ in period $\tau \in \mathcal{T}$
h^{min}	Minimum pressure (in m) allowed in node $n \in N$
v^{max}	Maximum velocity (in m/s) allowed in pipe $p \in P$
$h_{n,\tau}$	Variable indicating the pressure (in m) in node $n \in N$ in period $\tau \in \mathcal{T}$
$v_{p,\tau}$	Variable indicating the velocity (in m/s) of the water flowing through pipe $p \in P$ in period $\tau \in \mathcal{T}$
$x_{p,t}$	Binary variable indicating whether pipe $p \in P$ is of type $t \in T$
$y_{p,\tau}$	Variable representing the sign that incorporates changes in the direction of the water flow in pipe $p \in P$ in period $\tau \in \mathcal{T}$
$Q_{(i,j),\tau}$	Variable indicating the water flow from node $i \in N$ to node $j \in N$ in period $\tau \in \mathcal{T}$ (nonnegative)
$Q_{p,\tau}$	Variable indicating the water flow through pipe $p \in P$ in period $\tau \in \mathcal{T}$ (nonnegative)
$\Delta H_{p,\tau}$	Variable indicating the head loss (in m) of pipe $p \in P$, connecting nodes n_1 and n_2 , in period $\tau \in \mathcal{T}$

Let $x_{p,t}$ be a binary decision variable that determines whether pipe p is of type t ($x_{p,t} = 1$) or not ($x_{p,t} = 0$). The objective function of the WDND optimization problem can be written as

$$z = \min \sum_{p \in P} \sum_{t \in T} c_t \cdot l_p \cdot x_{p,t}. \quad (2.1)$$

A solution minimizing the objective function is conditioned to the principles of conservation of mass and energy, along with the constraints of minimum pressure head on the nodes and maximum water velocity in the pipes, for each period $\tau \in \mathcal{T}$.

Conservation of mass states that the volume of water flowing into a node in the network must be equal to the volume of water flowing out of this node. Consider variable $Q_{(i,j),\tau} \in \mathbb{R}_+$ to represent the water flowing from node i to node j in period τ . The law of conservation of mass can be represented as

$$\sum_{i \in N \setminus \{n\}} Q_{(i,n),\tau} - \sum_{j \in N \setminus \{n\}} Q_{(n,j),\tau} = D_{n,\tau} - R_{n,\tau}, \quad \text{for } n \in N, \tau \in \mathcal{T}. \quad (2.2)$$

The head loss in a piping system can be generalized as the energy used in overcoming friction caused by the walls of the pipe. Let the set $\Xi = \{\xi_1, \xi_2, \dots, \xi_{|\Xi|}\}$ represent the closed loops in the network, where each element $\xi \in \Xi$ represents a set of pipes belonging to that loop. Therefore, the energy conservation law states that the sum of head losses for every closed loop $\xi \in \Xi$ in the network must be equal to zero. Let variable $h_{n,\tau} \in \mathbb{R}_+$ (in m) be the pressure in node n at period τ and let $\Delta H_{p,\tau} = h_{n_1,\tau} - h_{n_2,\tau}$ (in m) represent the head loss of a pipe p in period τ that connects n_1 and n_2 with the direction defined by a closed loop that the nodes belong. The energy conservation law can be asserted as

$$\sum_{p \in \xi} \Delta H_{p,\tau} = 0, \quad \text{for } \xi \in \Xi, \tau \in \mathcal{T}. \quad (2.3)$$

The head losses in the pipes of a network are approximated using the Hazen-Williams equation. That equation, for a pipe p at period τ , with the parameters set as the hydraulic solver EPANET 2 (Rossman, 2000) is described as

$$\Delta H_{p,\tau} = \frac{10.6744 \cdot y_{p,\tau} \cdot Q_{p,\tau}^{1.852} \cdot l_p}{\sum_{t \in \mathcal{T}} (x_{p,t} \cdot r_t^{1.852} \cdot d_t^{4.871})}. \quad (2.4)$$

Therefore, Equation (2.3) can be rewritten as

$$\sum_{p \in \xi} \frac{10.6744 \cdot y_{p,\tau} \cdot Q_{p,\tau}^{1.852} \cdot l_p}{\sum_{t \in \mathcal{T}} (x_{p,t} \cdot r_t^{1.852} \cdot d_t^{4.871})} = 0, \quad \text{for } \xi \in \Xi, \tau \in \mathcal{T}. \quad (2.5)$$

This work considers the numerical conversion constant (which depends on the units used) as 10.6744 in Equation (2.4), as used by the simulator EPANET 2. Other values, such as 10.6750, are also possible but it is known that small variations in this parameter can lead to different results (Savic & Walters, 1997; Perelman, Krapivka, & Ostfeld, 2009). Besides, the two other constants are intrinsic to the formula and related to how it was obtained. The constant exponent 1.852 used for $Q_{p,\tau}$ and r_t is a unitless coefficient originated from the fraction $\frac{1}{0.54}$, while the constant exponent 4.871 used for d_t comes from the fraction $\frac{2.63}{0.54}$. Small variations in these last constants are possible but they are just numerical, related to the number of considered decimal places.

Remark that, $Q_{p,\tau}$ represents an alternative formulation of $Q_{(i,j),\tau}$ if the pipe p connects the nodes i and j . However, that notation requires the definition of a variable $y_{p,\tau}$, which is the sign that incorporates changes in the direction of the water flow of pipe p relative to the defined flow directions.

The minimum pressure constraint is described as

$$h_{n,\tau} \geq h^{min}, \quad \text{for } n \in N, \tau \in \mathcal{T}. \quad (2.6)$$

Assume variable $v_{p,\tau} \in \mathbb{R}_+$ (in m/s) to be the velocity of the water flowing through pipe p in time period τ , with

$$v_{p,\tau} = \frac{1.27 \cdot Q_{p,\tau}}{\sum_{t \in \mathcal{T}} (x_{p,t} \cdot d_t^2)}, \quad \text{for } p \in P, \tau \in \mathcal{T}. \quad (2.7)$$

The maximum water velocity constraint is thus represented by

$$v_{p,\tau} \leq v^{max}, \quad \text{for } p \in P, \tau \in \mathcal{T}. \quad (2.8)$$

Finally, every pipe p in the network should get exactly one type t assigned, which is ensured by

$$\sum_{t \in T} x_{p,t} = 1, \quad \text{for } p \in P. \quad (2.9)$$

The integrality requirements of the variables are defined as

$$x_{p,t} \in \{0, 1\}, \quad \text{for } p \in P, t \in T, \quad (2.10)$$

$$y_{p,\tau} \in \{-1, 1\}, \quad \text{for } p \in P, \tau \in \mathcal{T}. \quad (2.11)$$

2.3 THE SIMULATION-BASED ITERATED LOCAL SEARCH METAHEURISTIC

As mentioned in the introduction, the optimization of water distribution networks has received considerable attention from the research community. Classical exact methods often use complex formulations and can be time-consuming for solving large real-world networks, as can be observed in D'Ambrosio et al. (2015). Metaheuristic approaches have successfully produced good-quality solutions in reasonable computational time, but most of them are black-box procedures that seldom use problem-specific structure information (De Corte & Sörensen, 2013).

In this chapter, we describe a new robust simulation-based metaheuristic for the WDND optimization problem that overcomes some of the drawbacks of existing methods, both exact and heuristic. Similar to De Corte and Sörensen (2016a), the metaheuristic combines an iterated local search (ILS) approach with the hydraulic simulator EPANET 2, but improves the former in several ways by taking into consideration the structure of the problem. Firstly, we observed that low cost water distribution networks seem to have in common a structure pattern in which larger diameter pipes create paths between the nodes with highest demands and the source nodes. Hence, we attempt to dimension the pipes in some potential paths in a smart way. In this direction, we take into consideration the pipes in the shortest paths between nodes with high demands and the source nodes in the corresponding graph and postpone their reduction. This strategy can potentially lead to solutions with a reduced amount (in meters) of more expensive pipes with large diameters from which ramifications with cheaper pipes having small diameters would be originated. Secondly, we apply an aggressive reduction in the pipes' diameters, attempting to reduce the number of simulations necessary to converge to low cost solutions. Thirdly, changing a pipe diameter usually becomes harder as its neighbors reach lower diameters, leading to hard to leave local optima regions. We attempt to overcome this issue by creating a perturbation which is concentrated on the neighbors of a given pipe, allowing disturbances which can permit alternative decreases in the diameters of the involved pipes in later iterations. Last but not least, as the metaheuristic looks for fast convergence, we attempt to diversify its search using a pool of solutions. In this way, it may perform local searches in the neighborhood of different solutions, potentially allowing to encounter better solutions.

For simplicity, we assume that the water network with its sets of nodes N and pipes P is represented as a graph $G = (V, E)$, with $V = N$ and $E = P$. Note that this is a slight abuse of

notation, as we do not explicitly define the sets of vertices and edges, but rather perform a direct mapping from nodes and pipes of the network to the vertices and edges, correspondingly. We define a solution S of the problem to be an association of a type $t \in T$ to each pipe $p \in P$ of the network and $S(p)$ to be the type attributed to pipe p in solution S .

The remainder of this section is organized as follows. The procedure to perform the hydraulic simulations and evaluate every candidate solution is presented in Subsection 2.3.1. The heuristic to generate an initial solution is described in Subsection 2.3.2. The local search procedure is described in Subsection 2.3.3. Subsection 2.3.4 describes the perturbation procedures to try escaping from local optima. The criterion to accept candidates solutions is defined in Subsection 2.3.5. The complete simulation-based iterated local search metaheuristic is described in Subsection 2.3.6.

2.3.1 Solution validation using hydraulic simulation

As in De Corte and Sörensen (2016a), our algorithm uses the hydraulic simulator EPANET 2 (Rossman, 2000), which performs simulation of hydraulic and water quality behavior within pressurized pipe networks. EPANET 2's implementations are based on the global gradient algorithm (GGA) (Todini & Pilati, 1987), and the simulations consist of solving the hydraulic equations that rule the WDND optimization problem. The use of EPANET 2 allows us to concentrate our efforts on the search mechanism for good quality solutions without having to deal with the specific details of the feasibility checking of each individual solution.

The validation of a solution succeeds when all its nodes and pipes comply with the problem constraints. Therefore, this method first uses the hydraulic simulator EPANET 2 and afterwards checks the outcome, i.e., the hydraulic parameters in each node and pipe in the solution, to verify whether a constraint violation occurs.

The HYDRAULIC-SIMULATION procedure takes as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the minimum pressure h^{min} allowed at each node, the maximum velocity v^{max} permitted at each pipe, and a candidate solution S which is not necessarily feasible. The pseudocode of the procedure is described in Algorithm 1.

Algorithm 1: SOLUTION-VALIDATION($G, D, R, \mathcal{T}, h^{min}, v^{max}, S$)

```

1 for  $\tau \in \mathcal{T}$  do
2   HYDRAULIC-SIMULATION( $G, D, R, \tau, S$ );
3   for  $n \in V$  do
4      $h_{n,\tau} \leftarrow$  HYDRAULIC-PRESSURE( $n$ );
5     if  $h_{n,\tau} < h^{min}$  then
6       return FALSE;
7   for  $p \in E$  do
8      $v_{p,\tau} \leftarrow$  HYDRAULIC-VELOCITY( $p$ );
9     if  $v_{p,\tau} > v^{max}$  then
10      return FALSE;
11 return TRUE;

```

In Algorithm 1, the for loop of lines 1-10 iterates over all periods $\tau \in \mathcal{T}$. The simulation

in period τ for a network with the pipe types set as solution S occurs in line 2 with a call to `HYDRAULIC-SIMULATION(G, D, R, τ, S)`. `HYDRAULIC-SIMULATION` uses the hydraulic simulator which computes the hydraulic head of the nodes and the flow in the pipes for a fixed set of reservoir levels, tank levels, and water demands over a succession of points in time. From one time step to the next, reservoir levels and junction demands are updated according to their prescribed time patterns while tank levels are updated using the current flow solution. Determining the values for heads and flows at a particular point in time involves solving simultaneously the conservation of flow equation for each junction and the head loss relationship across each link of the network. It determines the heads and flows in period τ with pipe configuration S by solving simultaneously the conservation of flow given by constraints (2.2) for each node and the head loss relationship determined by constraints (2.3) across each pipe of the network. The for loop in lines 3-6 iterates over all nodes $n \in V$ and verifies whether constraints (2.6) are satisfied. Procedure `HYDRAULIC-PRESSURE(n)` invoked in line 4 retrieves the pressure on node n based on the latest performed simulation. Whenever (2.6) is violated, the algorithm returns `FALSE` in line 6. Next, the for loop in lines 7-10 iterates for all pipes $p \in E$ and verifies if constraints (2.8) are satisfied. Procedure `HYDRAULIC-VELOCITY(p)` invoked in line 5 retrieves the velocity on pipe p based on the latest performed simulation. Whenever (2.8) is violated, the algorithm returns `FALSE` in line 10. Algorithm 1 returns `TRUE` in line 11 if solution S is feasible.

2.3.2 Initial solution

As proposed by De Corte and Sørensen (2016b), the initial solution procedure attempts to construct a low-cost solution in which all pipes have the same diameter. The main idea of the approach is to start with all pipes having the largest diameter possible, and iteratively reduce the diameter of all pipes in the network while a feasible candidate solution can be obtained.

The procedure to build an initial feasible solution takes as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the minimum pressure h^{\min} allowed at each node, the maximum velocity v^{\max} permitted at each pipe, as well as the set of available pipe types T . The pseudocode of the `INITIAL-SOLUTION` procedure is presented in Algorithm 2.

Algorithm 2: `INITIAL-SOLUTION($G, D, R, \mathcal{T}, h^{\min}, v^{\max}, T$)`

```

1 for  $t = T, \dots, 1$  do
2    $S' \leftarrow$  solution obtained with  $S'(p) = t$  for all  $p \in E$ ;
3   if SOLUTION-VALIDATION( $G, D, R, \mathcal{T}, h^{\min}, v^{\max}, S'$ ) then
4      $S \leftarrow S'$ ;
5   else if  $t \neq |T|$  then
6     return  $S$ ;
7   else
8     terminate “No feasible solution exists using the same type for all pipes.”;
9 return  $S$ ;

```

As exposed in Equation (2.4), the head loss in a pipe is inversely proportional to the diameter of the pipe. As a consequence, the constraint of minimum pressure allowed at each node is more

likely to be satisfied by large diameter pipes. For this reason, the procedure starts with the for loop in lines 1-8 that iterates over the pipe types from the largest to the smallest diameter. A candidate solution S' , which is not necessarily feasible, is created in line 2 with all pipes set as type t . Solution S' is evaluated in line 3 and in case it is feasible, it is taken as current solution, represented by S , in line 4. A solution S from a previous iteration is returned in line 6 if at least one decrease of pipe type was performed. Line 8 deals with the case in which it is not possible to construct a feasible solution with all pipes set as the largest pipe diameter available. In case a feasible candidate solution can be obtained with all pipes set as the smallest type, i.e., the cheapest pipe with the smallest diameter, that solution is returned in line 9.

2.3.3 Local search

The local search attempts to achieve improvements by iteratively performing small changes in the obtained solutions. At each iteration of the local search, a pipe is selected using a greedy randomized (Resende & Ribeiro, 2016) mechanism to have its diameter reduced. Whenever reducing the diameter of the selected pipe leads to an infeasible candidate solution, such move is inserted into a tabu list (Glover & Laguna, 1998) to prevent the algorithm to waste computational effort trying to perform changes which were attempted without success.

Two important features differentiate our approach from that of De Corte and Sörensen (2016b). Firstly, the selection of pipes to have the diameter reduced considers a list of pipes to be avoided, which are those in shortest paths between source nodes and those with highest demands. This intends to keep these pipes with larger diameters while the other pipes are further reduced. The intuition behind this idea is to have a smaller quantity (in meters) of pipes with larger diameters from which pipes with smaller diameters would branch to serve other nodes. Therefore, our approach uses this information about shortest paths to increase the chances of achieving such type of low cost solutions.

Given an incumbent solution S , its neighborhood $\mathcal{N}(S)$ is composed of all solutions having configurations in which all pipes but one, which has its diameter reduced, have the same diameter as S . The LOCAL-SEARCH procedure takes as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the minimum pressure h^{min} allowed at each node, the maximum velocity v^{max} permitted at each pipe, the greediness factor $\alpha \in [0, 1]$, the type reduction factor f , as well as the current solution S . The pseudocode of the LOCAL-SEARCH

procedure is presented in Algorithm 3.

Algorithm 3: LOCAL-SEARCH($G, D, R, \mathcal{T}, h^{min}, v^{max}, \alpha, f, S$)

```

1  $L^{tabu} \leftarrow \emptyset$ ;
2  $L^{path} \leftarrow \text{PATH-LIST}(\text{SPT}, \mathcal{T}, D, \alpha)$ ;
3  $improve \leftarrow \text{TRUE}$ ;
4 while  $improve$  do
5    $improve \leftarrow \text{FALSE}$ ;
6    $L^P \leftarrow E \setminus L^{tabu}$ ;
7   while  $L^P \neq \emptyset$  do
8     Create  $\text{RCL}(L^P, \alpha)$  with the best elements of  $L^P$ ;
9     if  $\text{RCL}(L^P, \alpha) \setminus L^{path} \neq \emptyset$  then
10      Randomly choose  $p \in \text{RCL}(L^P, \alpha) \setminus \{L^{path}\}$ ;
11    else
12      Randomly choose  $p \in \text{RCL}(L^P, \alpha)$ ;
13    if  $S(p) > f$  then
14       $S' \leftarrow$  solution obtained with  $\begin{cases} S'(p) = S(p) - f \text{ and} \\ S'(p') = S(p') \text{ for all } p' \in E \setminus \{p\}; \end{cases}$ 
15      if  $\text{SOLUTION-VALIDATION}(G, D, R, \mathcal{T}, h^{min}, v^{max}, S')$  then
16         $S \leftarrow S'$ ;
17         $improve \leftarrow \text{TRUE}$ ;
18      else
19         $L^{tabu} \leftarrow L^{tabu} \cup \{p\}$ ;
20       $L^P \leftarrow L^P \setminus \{p\}$ ;
21 return  $S$ ;

```

In Algorithm 3, the memory set L^{tabu} that stores moves which led to infeasible candidate solutions is created as empty in line 1. Consider the base demand of node n , $d_n = \min_{\tau \in \mathcal{T}} \{D_{n,\tau}\}$ for all $n \in V$, to be its smallest demand that occurs during the planning horizon. Define $d^{max} = \max_{n \in V} \{d_n\}$ and $d^{min} = \min_{n \in V} \{d_n\}$ to be, respectively, the maximum and minimum base demands of the network G in the planning horizon. Consider a shortest path tree (SPT) obtained when finding the shortest path from the reservoirs to all other nodes in G , considering that the distance between nodes u and v is measured by the length l_e of the pipe $e = uv$ connecting them. Note that SPT can be obtained using a variation of Dijkstra's Algorithm (Dijkstra, 1959) which can be implemented to run in $O(|E| + |V| \log |V|)$. A set L^{path} is obtained in line 2 with a call to $\text{PATH-LIST}(\text{SPT}, \mathcal{T}, D, \alpha)$, which retrieves from SPT a set containing the pipes that are in the shortest path from the nodes that have a base demand d_n in the interval $[d^{max} - \alpha(d^{max} - d^{min}), d^{max}]$ to their nearest reservoirs. We remark that PATH-LIST only needs to be invoked once before the call to LOCAL-SEARCH as the information does not change throughout the algorithm, and it is shown in LOCAL-SEARCH just for easiness of explanation.

The variable $improve$, which is set as TRUE in line 3, keeps the local search procedure running

as long as improvements in the current solution S are obtained. The outer while loop of lines 4-20 iterates while the flag *improve* is set as `TRUE`, that is, the solution S was improved in the previous iteration which indicates opportunity for further improvements. For every iteration of the outer loop, the flag *improve* is set to `FALSE` in line 5. The set L^P containing all pipes of the network which are not tabu is created in line 6. The inner while loop of lines 7-20 iterates while the set L^P contains pipes that did not experience a type reduction attempt. Consider $l^{max} = \max_{p \in L^P}(l_p)$ and $l^{min} = \min_{p \in L^P}(l_p)$ to be, respectively, the maximum and minimum lengths of pipes in L^P . A restricted candidate list $\text{RCL}(L^P, \alpha)$ is created in line 8 containing pipes $p \in L^P$ with lengths l_p in the interval $[l^{max} - \alpha(l^{max} - l^{min}), l^{max}]$. Whenever $\text{RCL}(L^P, \alpha) \setminus L^{path} \neq \emptyset$ a pipe p is randomly chosen from $\text{RCL}(L^P, \alpha) \setminus L^{path}$ as shown in line 10. Otherwise, a pipe p is randomly chosen from $\text{RCL}(L^P, \alpha)$ as represented in line 12. Whenever the selected pipe p is not in the memory set L^{tabu} and its type identification is greater than the factor size f , the new candidate solution S' , which is not necessarily feasible, is created as the solution S but with the type of pipe p reduced with a factor f in line 14. Then, a hydraulic simulation is performed in line 15. Whenever the solution S' does not violate any constraints, solution S is replaced by S' as a new current solution in line 16 and the flag *improve* is set to `TRUE` in line 17. Otherwise, the attempt to reduce the type of pipe p is added to the tabu memory set L^{tabu} in line 19. Finally, pipe p is removed from the set L^P in line 20, restarting the inner loop. Algorithm 3 returns a possibly new incumbent solution S .

2.3.4 Perturbations

Perturbations are used to allow the search to escape from locally optimal solutions. Even though this can be achieved by restarting from a random solution (so-called *multistart* local search), using perturbations is a more efficient approach, since it does not completely destroy the solution built during the previous local search iteration. Two different perturbations are employed in our metaheuristic. The perturbation used in De Corte and Sörensen (2016b) randomly selects a pipe and increases its diameter by one size type until a certain percentage of pipes of the water distribution network has been disturbed. In this work, we improve this concept by attempting to increase the diameter by one size type for a certain percentage of the pipes in the water distribution network at once, which provides savings in the number of simulations required during the procedure. We call this a “dispersed” perturbation. Additionally, a new “concentrated” perturbation is added. This procedure randomly selects a pipe amongst the most expensive pipes of the network and increases a certain amount of its neighboring pipes by one type size. The intuition of the concentrated perturbation is to focus the changes in a specific region of the network that contains a high cost pipe. The aim is to allow the next local search to find some improvements in this region that could not be found without the concentrated perturbation.

2.3.4.1 Dispersed perturbation The `DISPERSED-PERTURBATION` procedure receives as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the minimum pressure h^{min} allowed at each node, the maximum velocity v^{max} permitted in each pipe, the current solution S , as well as a greediness factor $\alpha \in [0, 1]$. The pseudocode of the

DISPERSED-PERTURBATION is presented in Algorithm 4.

Algorithm 4: DISPERSED-PERTURBATION($G, D, R, \mathcal{T}, h^{\min}, v^{\max}, S, \alpha$)

```

1  $m \leftarrow \lfloor \alpha|E| \rfloor$ ;
2 while  $m > 0$  do
3    $L^P \leftarrow E$ ;
4   while  $L^P \neq \emptyset$  do
5      $P' \leftarrow$  subset with  $\min\{m, |L^P|\}$  pipes randomly chosen from  $L^P$ ;
6      $S' \leftarrow$  solution obtained from  $S$  with  $\begin{cases} S'(p) = S(p) + 1, & \text{for all } p \in P', \text{ and} \\ S'(p) = S(p), & \text{for all } p \in E \setminus \{P'\}; \end{cases}$ 
7     if SOLUTION-VALIDATION( $G, D, R, \mathcal{T}, h^{\min}, v^{\max}, S'$ ) then
8       return  $S'$ ;
9     Randomly choose  $p' \in P'$ ;
10     $L^P \leftarrow L^P \setminus \{p'\}$ ;
11     $m \leftarrow \lfloor \frac{m}{2} \rfloor$ ;
12 return  $S$ ;
```

The procedure begins initializing the maximum amount m of pipes to have their types changed in line 1 based on a percentage α of the number of pipes in the network. The outer while loop in lines 2-11 proceeds until m reaches zero or a feasible solution is obtained. The set L^P is created with all pipes of the network in line 3. The inner while loop in lines 4-10 iterates while there are still pipes remaining in L^P and a feasible solution is not found. A subset P' is populated with $\min\{m, |L^P|\}$ pipes randomly chosen from L^P as detailed in line 5. A candidate solution S' , which is not necessarily a feasible solution, is created based on the current solution S but for every pipe $p \in P'$ with its type incremented by one as presented in line 6. The candidate solution S' is evaluated in line 7. In case S' does not violate any constraints, it is returned as feasible perturbed solution. Otherwise, a pipe p' is randomly chosen from P' in line 9 and removed from L^P in line 10. Therefore, in the next iteration of the inner while loop it is guaranteed that the new set of pipes chosen for P' from L^P is different from the previous iteration. For the next iteration of the outer while loop, the value of m is rounded down with a geometric progression to the nearest integer of $\lfloor \frac{m}{2} \rfloor$. Therefore, at each iteration m tends to zero. Lastly, if a feasible perturbation could not be performed, the current solution S is returned in line 12. Algorithm 4 returns a new candidate solution S' whenever one is obtained, otherwise it returns the input solution S .

2.3.4.2 Concentrated perturbation For the concentrated perturbation, consider the breadth-first search (BFS) algorithm that traverses a graph G in layers exploring the neighboring nodes from a given source of nodes with a runtime complexity $O(|V| + |E|)$ (Cormen, Leiserson, Rivest, & Stein, 2009). Assume the sequence $K = \langle 1, 2, \dots, |K| \rangle$ as the distance levels found by BFS. Therefore, each pipe $p \in E$ can be classified with a distance level $k \in K$ from the source nodes based on the number of pipes in the path. Let $w : L^P \rightarrow K$ be a function which assigns each pipe $p \in L^P$ to a distance level $k \in K$. Consider an auxiliary procedure, denoted SELECTION-CRITERION,

whose purpose is to choose a fixed number of elements from a given set of pipes, while giving priority to pipes that are at low distance levels.

The pseudocode of SELECTION-CRITERION is detailed in Algorithm 5. It takes as input a set of pipes L^P , a sequence of distance levels K and a variable m that gives the maximum number of pipes to be selected.

Algorithm 5: SELECTION-CRITERION(L^P, K, m)

```

1  $r_1 \leftarrow \min\{m, |L^P|\};$ 
2  $P' \leftarrow \emptyset;$ 
3 foreach  $k \in K$  do
4    $C_k \leftarrow \{p \in L^P \mid w(p) = k\};$ 
5    $r_2 \leftarrow |C_k|;$ 
6   foreach  $p \in C_k$  do
7     if  $r_1 > 0$  then
8       if  $\text{random}(0, 1) < r_1/r_2$  then
9          $P' \leftarrow P' \cup \{p\};$ 
10         $r_1 \leftarrow r_1 - 1;$ 
11       $r_2 \leftarrow r_2 - 1;$ 
12     else
13       return  $P';$ 

```

SELECTION-CRITERION begins setting variable r_1 , representing the amount of elements yet to be selected by the procedure, to $\min\{m, |L^P|\}$ in line 1. Also, a set P' containing the pipes to be returned is initialized as empty in line 2. Next, for each element k of the sequence K , a set C_k is created with the pipes $p \in L^P$ such that $w(p) = k$, as shown in line 4. Let the variable r_2 , which is set in line 5, be the number of pipes in C_k that have not been evaluated by the procedure. Afterwards, for each element $p \in C_k$, whenever there are still elements to be selected, i.e. $r_1 > 0$, a pipe p is selected with a probability $\Pr(\text{random}(0, 1) < r_1/r_2)$. Remark that, $\text{random}(0, 1)$ is a real-valued random variable defined on the sample space of the uniform distribution in the interval $[0, 1]$. Whenever pipe p is selected with a probability $\Pr(\text{rnd} < r_1/r_2)$, it is inserted into P' as shown in line 9 and r_1 is decremented by one in line 10. After each evaluation, r_2 is decremented by one in line 11. Otherwise, with r_1 pipes selected, the set P' is returned in line 13. Observe that a call to SELECTION-CRITERION always returns a nonempty set P' in line 13 assuming that the input L^P is not empty.

The CONCENTRATED-PERTURBATION procedure receives as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the minimum pressure h^{\min} allowed at each node, the maximum velocity v^{\max} permitted in each pipe, the current solution S , as well as a greediness factor $\alpha \in [0, 1]$. The pseudocode of the CONCENTRATED-PERTURBATION is detailed

in Algorithm 6.

Algorithm 6: CONCENTRATED-PERTURBATION($G, D, R, \mathcal{T}, h^{min}, v^{max}, S, \alpha$)

```

1 Create  $RCL(E, S, \alpha)$  with the best elements of  $S$ ;
2 Randomly choose  $p \in RCL(E, S, \alpha)$ ;
3  $K \leftarrow BFS(G, \{u, v \mid p = uv\})$ ;
4  $m \leftarrow \lfloor \alpha |E| \rfloor$ ;
5 while  $m > 0$  do
6    $L^P \leftarrow E \setminus \{p\}$ ;
7   while  $L^P \neq \emptyset$  do
8      $P' \leftarrow \text{SELECTION-CRITERION}(L^P, K, m)$ ;
9      $S' \leftarrow$  solution obtained from  $S$  with  $\begin{cases} S'(p) = S(p) + 1 \text{ for all } p \in P', \text{ and} \\ S'(p) = S(p) \text{ for all } p \in E \setminus \{P'\}; \end{cases}$ 
10    if  $\text{SOLUTION-VALIDATION}(G, D, R, \mathcal{T}, h^{min}, v^{max}, S')$  then
11      return  $S'$ ;
12    Randomly choose  $p' \in P'$ ;
13     $L^P \leftarrow L^P \setminus \{p'\}$ ;
14     $m \leftarrow \lfloor \frac{m}{2} \rfloor$ ;
15 return  $S$ ;

```

Given a solution S , consider $\psi_S(p)$ to be the cost of a pipe p obtained as the cost of its type per unit of length $c_{S(p)}$ multiplied by its length l_p , $\psi_S(p) = c_{S(p)} \cdot l_p$. Remark that, the type t of a pipe p is determined by solution S , i.e., $t = S(p)$. Also, let $\psi_S^{max} = \max_{p \in E} \{\psi_S(p)\}$ and $\psi_S^{min} = \min_{p \in E} \{\psi_S(p)\}$ be, respectively, the costs of the most expensive and of the cheapest pipes of the network in a solution S . A restricted candidate list $RCL(E, S, \alpha)$ containing every pipe $p \in E$ whose cost lies in the interval $[\psi_S^{max} - \alpha(\psi_S^{max} - \psi_S^{min}), \psi_S^{max}]$ is defined in line 1. In order to avoid an excessively restricted list, we always ensure that at least the five best elements are included. The pipe p is randomly chosen from the list $RCL(E, S, \alpha)$ as shown in line 2. Consider as source nodes those which are incident to p . Procedure $BFS(G, \{u, v \mid p = uv\})$ invoked in line 3 traverses a graph G starting from nodes u, v and returns the distance levels as a sequence $K = \langle 1, 2, \dots, |K| \rangle$. The maximum amount m of pipes to have their types changed is defined as a percentage α of the number of pipes in the network in line 4. The outer while loop in lines 5-14 proceeds until m reaches zero or a feasible solution is obtained. The set L^P is created with all pipes of the network except p in line 6. The inner while loop in lines 7-13 iterates while there are still pipes in the set L^P and a feasible solution is not found. The $\text{SELECTION-CRITERION}(K, L^P, m)$ procedure invoked in line 12 returns $\min\{m, |L^P|\}$ pipes from the set L^P . The candidate solution S' , which is not necessarily feasible, is created based on the current solution S but for every pipe $p \in P'$ with its type incremented by one as presented in line 9. The candidate solution S' is evaluated in line 10. In case S' does not violate any constraints, it is returned as current solution in line 11. Otherwise, a pipe p' is randomly chosen from P' in line 12 and removed from L^P in line 13. Therefore, in the next iteration of the inner while loop it is guaranteed that the new set of pipes chosen for P' is different from the previous iteration. For the next iteration

of the outer while loop, the value of m is rounded down with a geometric progression to the nearest integer of $\left\lfloor \frac{m}{2} \right\rfloor$ as shown in line 14. Therefore, at each iteration m tends to zero. Lastly, if a feasible perturbation could not be performed, the current solution S is returned in line 15.

2.3.5 Acceptance criterion

As the local search algorithm converges, it may reach a local optimum caused by the intensification in certain neighborhoods. The acceptance criterion determines whether a newly proposed candidate solution should replace the current one and can be used to control the balance between intensification and diversification during the search and potentially lead to better solutions (Lourenço et al., 2003).

Differently from De Corte and Sörensen (2016b), where the authors use a first improvement paradigm which accepts a new solution whenever the current one is improved, we propose an acceptance criterion approach which uses a *pool* of solutions. The aim is to achieve a compromise between diversification and intensification. The diversification is achieved by using solutions with possibly different characteristics, i.e., with the potential to allow the search to move into unexplored regions of the search space. On the other hand, intensification is produced by the prioritization of solutions that are more likely to improve the best known. These two concepts are achieved by allowing to select solutions which are either in the pool or are the best encountered ones.

Define $z(S)$ to be the cost of a solution S defined according to the objective function in Equation (2.1). The algorithm works with two solutions indicating its current state, namely, S^{cur} represents an incumbent solution from which the algorithm iteratively generates a new candidate solution from its neighborhood $\mathcal{N}(S^{\text{cur}})$, denoted by S^{cand} . Let S^{best} be the solution with the lowest cost found so far. Consider Π^ν to be a memory structure which stores ν solutions and $S_{\Pi^\nu}^{\text{worst}}$ to be the highest cost solution in Π^ν . This memory structure is maintained through decisions that determine when a solution is replaced and guarantee its diversity.

Procedure ACCEPTANCE-CRITERION takes as inputs the best solution found so far S^{best} , the candidate solution S^{cand} , the incumbent solution S^{cur} , and the memory structure Π^ν . The pseudocode of the ACCEPTANCE-CRITERION procedure is presented in Algorithm 7.

Algorithm 7: ACCEPTANCE-CRITERION(S^{best} , S^{cand} , S^{cur} , Π^ν)

```

1 if  $z(S^{\text{cand}}) < z(S^{\text{cur}})$  then
2   if  $z(S^{\text{cand}}) < z(S^{\text{best}})$  then
3      $S^{\text{best}} \leftarrow S^{\text{cand}};$ 
4   else
5      $S_{\Pi^\nu}^{\text{worst}} \leftarrow S^{\text{cand}};$ 
6   return  $S^{\text{cand}};$ 
7 else
8   return Randomly choose an element from  $\Pi^\nu \cup \{S^{\text{best}}\};$ 

```

Algorithm 7 starts testing whether the candidate solution S^{cand} improves the incumbent one S^{cur} . Whenever this happens, in case it also improves the best solution S^{best} , S^{best} is replaced

by S^{cand} as shown in line 3. Otherwise, S^{cand} replaces the worst solution in the memory $S_{\Pi^v}^{\text{worst}}$ as shown in line 5. Later, the procedure returns the candidate solution S^{cand} in line 6. In case the candidate solution S^{cand} does not improve the incumbent one S^{cur} , the procedure returns a solution randomly chosen from $\Pi^v \cup S^{\text{best}}$ as shown in line 8. Observe that Algorithm 7 returns either the candidate solution received as input or a solution selected from the pool of solutions or the best solution found so far.

2.3.6 Simulation-based iterated local search metaheuristic

The proposed simulation-based iterated local search (ILS) metaheuristic embeds all the components presented previously in this section. The main idea consists of, starting from an initial solution, performing a sequence of local searches and perturbations until a time limit is reached. The simulation-based ILS receives as input the water distribution network G , the demands D , the supplies R , the planning horizon \mathcal{T} , the available pipe types T , the minimum pressure h^{min} at each node, the maximum velocity v^{max} permitted in each pipes, the time limit time^{max} , the size of the memory of solutions ν , the greediness factor $\alpha \in [0, 1]$, and the type reduction factor f . The pseudocode of the simulation-based ILS metaheuristic is described in Algorithm 8.

Algorithm 8: SIMULATION-BASED-ILS($G, D, R, \mathcal{T}, T, h^{\text{min}}, v^{\text{max}}, \text{time}^{\text{max}}, \nu, \alpha, f$)

```

1  $\Pi^v \leftarrow$  Populate with  $\nu$  copies of INITIAL-SOLUTION( $G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, T$ );
2  $S^{\text{cur}}, S^{\text{best}} \leftarrow S_{\Pi^v}^{\text{worst}}$ ;
3 while  $\text{time}^{\text{max}}$  not reached do
4    $S^{\text{cand}} \leftarrow$  LOCAL-SEARCH( $G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, \alpha, f, S^{\text{cur}}$ );
5   if  $f > 1$  then
6      $f \leftarrow \lfloor f/2 \rfloor$ ;
7    $S^{\text{cand}} \leftarrow$  ACCEPTANCE-CRITERION( $S^{\text{best}}, S^{\text{cand}}, S^{\text{cur}}, \Pi^v$ );
8   if  $\text{random}(0, 1) \leq (1 - \alpha)$  then
9      $S^{\text{cand}} \leftarrow$  DISPERSED-PERTURBATION( $G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, S^{\text{cand}}, \alpha$ );
10  else
11     $S^{\text{cand}} \leftarrow$  CONCENTRATED-PERTURBATION( $G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, S^{\text{cand}}, \alpha$ );
12 return  $S^{\text{best}}$ ;
```

SIMULATION-BASED-ILS starts with the creation of the memory structure Π^v (see Section 2.3.5) containing ν copies of the initial solution returned by the call to INITIAL-SOLUTION($G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, T$), as shown in line 1. The current and best solutions, S^{cur} and S^{best} , are defined according to $S_{\Pi^v}^{\text{worst}}$ in line 2, i.e., they all correspond to the initial solution. Note that such solution is both the worst and the best one in Π^v at this moment. The approach attempts to improve the current solution S^{cur} by a call to LOCAL-SEARCH($G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, \alpha, f, S^{\text{cur}}$) in line 4, and the resulting solution is stored into S^{cand} . The main while loop in lines 3-11 repeats while the time limit is not reached. Right after the LOCAL-SEARCH, whenever the factor f is greater than one, it is divided by two as shown in line 6. Thus, we are more likely to decrease the chance of getting infeasible solutions in the next attempts to perform type reductions in the local search. In line 7 the approach determines if the recently generated S^{cand} will be accepted

for further iterations via a call to `ACCEPTANCE-CRITERION($S^{\text{best}}, S^{\text{cand}}, S^{\text{cur}}, \Pi^v$)`. In line 8, the approach determines which perturbation will be executed. For each iteration the probabilities to perform a dispersed perturbation and a concentrated perturbation are, respectively, α and $1 - \alpha$. The procedure `DISPERSED-PERTURBATION($G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, \alpha, S^{\text{cur}}$)` is invoked in line 9 and `CONCENTRATED-PERTURBATION($G, D, R, \mathcal{T}, h^{\text{min}}, v^{\text{max}}, \alpha, S^{\text{cur}}$)` is performed in line 11. Both methods return a perturbed solution S^{cand} starting from the current solution S^{cur} . Lastly, Algorithm 8 returns the best feasible solution found so far S^{best} .

2.4 COMPUTATIONAL EXPERIMENTS

This chapter summarizes the performed computational experiments. All the tests were carried out on a machine running under Ubuntu x86-64 GNU/Linux, with an Intel Core i7-8700 Hexa-Core 3.20GHz processor and 16Gb of RAM. The simulation based iterated local search metaheuristic was implemented in C++, and its interaction with the hydraulic simulator EPANET was established via the Extended EPANET Toolkit 1.5 (López-Ibáñez, 2009b, 2009a). Subsection 2.4.1 describes the benchmark set of instances. Section 2.4.2 lists the tested approaches and reports the parameter settings. Section 2.4.3 reports the results comparing our newly proposed approach with a state-of-the-art metaheuristic presented in De Corte and Sörensen (2016a). Section 2.4.4 presents a graphical summary of the results. Subsection 2.4.5 analyzes the impacts of each individual novelty to the solution's quality using a subset of the instances. Subsection 2.4.6 compares some additional indicators achieved by the approach of De Corte and Sörensen (2016a) and by our new improved simulation based iterated local search metaheuristic.

2.4.1 Benchmark set

The developed algorithm was tested using a set of challenging benchmark instances generated using HydroGen (De Corte & Sörensen, 2014a), which is a tool that generates virtual water distribution networks. The input files of these networks are available via De Corte and Sörensen (2014b). The benchmark instances are divided into 30 instance groups. Each instance group contains five instances with similar size, expressed by the number of pipes, and characteristics, reflected by the meshedness coefficient. The meshedness coefficient, $M = \frac{|\Xi|}{2|N| - 5}$, is a concept in graph theory which evaluates the number of loops against the maximum number of loops in a planar graph (Buhl et al., 2006). Remark that $|\Xi|$ and $|N|$ represent, respectively, the numbers of independent loops and of nodes in the network. Note that, independent loops are loops that contain at least one element that is not part of another independent loop. The sizes and characteristics of each instance group are given in Table 2.2.

Table 2.2: Information about the instance groups.

Network	Meshedness Coefficient	Pipes	Demand Nodes	Water Reservoirs	Network	Meshedness Coefficient	Pipes	Demand Nodes	Water Reservoirs
HG-MP-1	0.20	100	73	1	HG-MP-16	0.20	606	431	4
HG-MP-2	0.15	100	78	1	HG-MP-17	0.15	607	465	4
HG-MP-3	0.10	99	83	1	HG-MP-18	0.10	608	503	5
HG-MP-4	0.20	198	143	1	HG-MP-19	0.20	708	503	5
HG-MP-5	0.15	200	155	1	HG-MP-20	0.15	703	538	5
HG-MP-6	0.10	198	166	1	HG-MP-21	0.10	707	586	5
HG-MP-7	0.20	299	215	2	HG-MP-22	0.20	805	572	6
HG-MP-8	0.15	300	232	2	HG-MP-23	0.15	804	615	6
HG-MP-9	0.10	295	247	2	HG-MP-24	0.10	808	669	6
HG-MP-10	0.20	397	285	2	HG-MP-25	0.20	906	644	6
HG-MP-11	0.15	399	308	2	HG-MP-26	0.15	905	692	7
HG-MP-12	0.10	395	330	3	HG-MP-27	0.10	908	752	7
HG-MP-13	0.20	498	357	2	HG-MP-28	0.20	1008	716	7
HG-MP-14	0.15	499	385	3	HG-MP-29	0.15	1007	770	7
HG-MP-15	0.10	495	413	3	HG-MP-30	0.10	1009	835	8

The set of available pipe types and their corresponding costs can be found in Table 2.3. The planning horizon \mathcal{T} is composed of 24 time periods (corresponding to the hourly scenarios in a day). Additionally, a minimum pressure head of 20m is required in every demand node at every time period, and a maximum velocity of 2m/s is set for the water flow through every pipe in the network, at every time period. Demand nodes are divided into five categories (domestic, industrial, energy, public services, and commercial demand nodes), each with a corresponding base load and demand pattern. The base loads and demand patterns can be found in the EPANET input files of the instances (De Corte & Sørensen, 2014b). We remark that we do not use multi-period counterparts for the classic single-period instances available in the literature since these are relatively small (considering the number of pipes). Besides, De Corte and Sørensen (2016b) tested the algorithm with the classical instances and were able to reach the best-known solutions. Furthermore, the proposed approaches are directed to improve the capability of obtaining good quality solutions for more challenging larger instances.

Table 2.3: Information about the available pipe types.

Number	Diameter (in mm)	Roughness (unitless)	Cost (in EUR per m)	Number	Diameter (in mm)	Roughness (unitless)	Cost (in EUR per m)
1	20	130	9	9	200	130	116
2	30	130	20	10	250	130	150
3	40	130	25	11	300	130	201
4	50	130	30	12	400	130	290
5	60	130	35	13	400	130	290
6	80	130	48	14	500	130	351
7	100	130	50	15	600	130	528
8	150	130	61	16	1000	130	628

2.4.2 Tested approaches and settings

In this subsection we present the tested approaches and the preliminary experiments carried out to determine the parameters of the proposed techniques. We compared the following approaches:

- (a) the simulation based iterated local search metaheuristic of De Corte and Sörensen (2016a) (ILS);
- (b) our newly proposed enhanced simulation based iterated local search metaheuristic (ILS+), described in Section 2.3.

In the computational tests, each approach was executed ten times on each test instance for each of the time limits $time^{max} \in \{60, 180, 300, 600\}$ (in seconds). The best and average costs over these ten runs are reported in the following sections.

ILS was executed with the same parameter settings used in the authors' original work. The settings for ILS+ were determined based on preliminary computational experiments, which took into consideration around 10% of the instances, randomly chosen, with varying sizes and characteristics.

The following values were tested for each parameter:

- greediness factor: $\alpha \in \{0.05, 0.08, 0.10\}$;
- type reduction factor: $f \in \{1, 2, 4\}$;
- size of the pool of solutions: $\nu \in \{1, 2, 3\}$.

Based on the preliminary experiments, the selected configurations for the parameters were $\alpha = 0.05$, $f = 4$ and $\nu = 3$.

2.4.3 Computational results

Tables 2.4 and 2.5 summarize the performed computational results. We remind that the reported values for each combination of instance and time limit take into consideration ten runs of the corresponding approach. For each instance group, the reported best and average values are the average over the five instances in the group.

Table 2.4 reports the results for the instance groups with less than 500 pipes while Table 2.5 presents the results for those with more than 500 pipes. In each of these tables, the first two columns identify the instance group and the time limit (in seconds). The next two columns give, respectively, the best and average solutions achieved by ILS for the corresponding instance group. Due to their magnitude, the best and average values are presented using the scientific notation $value \times 10^6$, with four significant digits. The next six columns present the results for ILS+ and indicate how it compares against ILS. More specifically, the fifth and sixth columns indicate the best and average solutions for the corresponding instance group. The lowest values for best and average solutions are shown in boldface. The seventh and eighth columns indicate, respectively, the numbers of instances (out of the five in the instance group) the best and average values obtained by ILS+ were strictly better than those obtained by ILS. The last two columns represent the average gain, calculated for each instance as $100 \times \frac{z_{ILS+} - z_{ILS}}{z_{ILS}}$, achieved by ILS+ over ILS for best and average values, correspondingly.

Table 2.4 shows that for the instances with less than 500 pipes, ILS and ILS+ present quite similar results when it comes to the best encountered solutions. As it can be seen in the two last lines of the table, ILS+ presented improved best solutions for 156 out of the 300 combinations

and an average gain of only 0.5%. However, it is remarkable that ILS+ is more robust for these instances. To be more specific, ILS+ achieved improved average results for 227 out of the 300 combinations and an average improvement of 3.6%. As expected, considerably large gains were achieved for the more restricted time limits (e.g., with a time limit of 60 seconds, average gains of 12.4% and 8.1% were achieved, respectively, for instance groups HG-MP-2 and HG-MP-13).

Table 2.5 exhibits that ILS+ outperforms ILS for the instances with more than 500 pipes. The best and average results achieved by ILS+ are considerably better than those obtained by ILS for most of the instance groups. As it can be seen in the two last lines of the table, ILS+ presented improved best solutions for 228 out of the 300 combinations and an average gain of 8.4%. Additionally, it was able to obtain improved average solutions for 240 out of the 300 combinations and an average gain of 9.3%. The results evidence the fact that noticeable gains were achieved by ILS+ for all instance groups when considering the more restricted time limits.

Table 2.4: Results obtained by ILS and ILS+ for instances with less than 500 pipes.

Instance group	Time limit (seconds)	ILS		ILS+					
		Best (10 ⁶)	Avg (10 ⁶)	Best (10 ⁶)	Avg (10 ⁶)	#impr (Best)	#impr (Avg)	Gain (%) (Best)	Gain (%) (Avg)
HG-MP-1	60	0.345	0.358	0.336	0.341	3	3	2.7	5.0
	180	0.344	0.357	0.336	0.339	3	3	2.6	5.1
	300	0.343	0.357	0.335	0.339	3	3	2.5	5.2
	600	0.343	0.357	0.335	0.339	3	3	2.3	5.1
HG-MP-2	60	0.301	0.355	0.303	0.308	3	5	-0.9	12.4
	180	0.300	0.351	0.301	0.306	3	5	-0.3	12.1
	300	0.300	0.349	0.301	0.305	3	5	-0.5	11.9
	600	0.299	0.348	0.301	0.304	3	5	-0.6	11.8
HG-MP-3	60	0.388	0.413	0.387	0.389	2	5	0.3	5.6
	180	0.388	0.408	0.386	0.389	2	5	0.3	4.6
	300	0.388	0.407	0.386	0.389	2	5	0.3	4.6
	600	0.387	0.406	0.386	0.388	3	5	0.3	4.6
HG-MP-4	60	0.699	0.728	0.706	0.723	2	3	-1.0	0.6
	180	0.695	0.723	0.702	0.717	2	3	-1.1	0.6
	300	0.695	0.722	0.701	0.715	2	3	-0.9	0.7
	600	0.694	0.721	0.700	0.713	2	3	-0.9	0.9
HG-MP-5	60	0.748	0.810	0.740	0.759	3	4	1.0	6.4
	180	0.744	0.800	0.738	0.753	3	3	0.8	6.0
	300	0.742	0.796	0.738	0.751	3	3	0.5	5.7
	600	0.739	0.791	0.738	0.749	3	3	0.2	5.4
HG-MP-6	60	0.753	0.779	0.755	0.780	1	2	-0.4	-0.2
	180	0.750	0.775	0.752	0.773	1	2	-0.4	0.0
	300	0.749	0.774	0.751	0.771	1	2	-0.4	0.2
	600	0.741	0.771	0.749	0.766	0	2	-1.1	0.4
HG-MP-7	60	0.847	0.905	0.818	0.856	3	5	3.1	5.0
	180	0.823	0.883	0.799	0.839	4	5	2.6	4.6
	300	0.815	0.880	0.789	0.834	4	5	2.9	4.9
	600	0.811	0.875	0.787	0.830	4	5	2.7	4.9
HG-MP-8	60	0.871	0.954	0.858	0.904	3	3	1.3	4.9
	180	0.862	0.934	0.846	0.886	3	4	1.7	5.0
	300	0.859	0.931	0.843	0.880	3	4	1.7	5.3
	600	0.856	0.927	0.834	0.873	4	4	2.4	5.6
HG-MP-9	60	0.844	0.881	0.861	0.892	1	3	-2.1	-1.3
	180	0.833	0.863	0.840	0.869	1	3	-0.9	-0.6
	300	0.828	0.858	0.836	0.861	1	3	-1.0	-0.4
	600	0.826	0.854	0.825	0.854	3	4	-0.0	-0.1
HG-MP-10	60	0.827	0.893	0.802	0.845	5	5	2.9	5.5
	180	0.797	0.855	0.786	0.812	4	5	1.4	5.0
	300	0.793	0.849	0.782	0.807	4	5	1.3	5.0
	600	0.791	0.843	0.778	0.800	5	5	1.7	5.0
HG-MP-11	60	0.932	0.998	0.942	0.991	1	4	-1.1	0.6
	180	0.907	0.955	0.920	0.959	2	3	-1.5	-0.4
	300	0.904	0.948	0.912	0.945	2	3	-1.0	0.4
	600	0.896	0.941	0.905	0.932	2	4	-1.0	0.9
HG-MP-12	60	1.050	1.104	1.071	1.107	2	2	-1.8	-0.2
	180	1.024	1.069	1.048	1.067	1	3	-2.3	0.3
	300	1.019	1.061	1.040	1.059	1	3	-2.0	0.3
	600	1.014	1.053	1.033	1.050	0	4	-1.9	0.4
HG-MP-13	60	1.321	1.419	1.214	1.301	5	5	8.0	8.1
	180	1.189	1.274	1.174	1.221	3	5	1.3	4.2
	300	1.174	1.247	1.164	1.204	3	5	0.9	3.5
	600	1.161	1.226	1.155	1.184	3	5	0.6	3.5
HG-MP-14	60	1.166	1.257	1.125	1.177	3	4	2.4	5.4
	180	1.089	1.141	1.093	1.121	3	3	-0.6	1.5
	300	1.064	1.121	1.075	1.106	2	2	-1.3	1.1
	600	1.056	1.106	1.070	1.095	2	3	-1.5	0.9
HG-MP-15	60	1.222	1.314	1.180	1.240	4	4	3.3	5.5
	180	1.162	1.220	1.132	1.186	3	4	2.3	2.6
	300	1.149	1.196	1.127	1.177	3	4	1.7	1.2
	600	1.139	1.176	1.118	1.164	3	4	1.6	0.6
Total					156/300	227/300			
Average (%)							0.5	3.6	

Table 2.5: Results obtained by ILS and ILS+ for instances with more than 500 pipes.

Instance group	Time limit (seconds)	ILS		ILS+					
		Best (10 ⁶)	Avg (10 ⁶)	Best (10 ⁶)	Avg (10 ⁶)	#impr (Best)	#impr (Avg)	Gain (%) (Best)	Gain (%) (Avg)
HG-MP-16	60	1.821	2.007	1.619	1.701	5	5	11.3	15.3
	180	1.523	1.666	1.542	1.610	3	3	-1.0	3.7
	300	1.487	1.610	1.527	1.584	2	3	-2.4	2.0
	600	1.463	1.575	1.499	1.560	2	3	-2.2	1.4
HG-MP-17	60	1.913	2.096	1.718	1.903	4	4	9.6	8.7
	180	1.623	1.764	1.667	1.802	4	4	-3.5	-2.5
	300	1.595	1.717	1.655	1.766	3	4	-4.6	-3.4
	600	1.573	1.689	1.632	1.715	4	4	-4.5	-2.1
HG-MP-18	60	1.770	1.964	1.621	1.759	5	5	8.3	10.6
	180	1.507	1.637	1.560	1.627	1	3	-3.9	0.4
	300	1.480	1.597	1.537	1.601	1	2	-4.3	-0.4
	600	1.465	1.567	1.514	1.572	2	2	-3.7	-0.5
HG-MP-19	60	2.999	3.296	2.408	2.565	5	5	19.4	21.9
	180	2.253	2.473	2.193	2.354	3	5	2.8	4.6
	300	2.184	2.359	2.145	2.293	3	4	1.9	2.6
	600	2.144	2.297	2.093	2.220	3	4	2.5	3.1
HG-MP-20	60	2.928	3.211	2.215	2.409	5	5	22.7	23.7
	180	2.196	2.365	2.114	2.242	4	4	3.9	5.5
	300	2.095	2.232	2.046	2.156	4	4	2.5	3.7
	600	2.031	2.150	2.010	2.084	2	3	1.2	3.3
HG-MP-21	60	2.786	2.967	2.225	2.356	5	5	20.3	20.8
	180	2.243	2.385	2.134	2.207	5	5	4.9	7.5
	300	2.192	2.298	2.125	2.180	4	4	3.1	5.2
	600	2.157	2.246	2.108	2.151	4	4	2.3	4.3
HG-MP-22	60	4.358	4.758	3.144	3.401	5	5	27.4	28.0
	180	2.957	3.196	2.815	2.997	5	5	4.5	5.9
	300	2.798	2.965	2.707	2.885	5	5	3.2	2.5
	600	2.657	2.830	2.620	2.769	4	5	1.4	2.1
HG-MP-23	60	4.129	4.516	3.228	3.521	5	5	21.7	21.5
	180	2.950	3.263	2.883	3.121	4	4	2.2	4.1
	300	2.808	3.000	2.826	3.040	2	2	-0.8	-1.6
	600	2.734	2.856	2.683	2.917	2	2	1.7	-2.4
HG-MP-24	60	3.765	4.062	2.825	2.975	5	5	25.1	27.0
	180	2.759	2.923	2.649	2.792	4	3	4.0	4.7
	300	2.628	2.784	2.594	2.717	3	3	1.4	2.4
	600	2.573	2.690	2.517	2.618	3	3	2.1	2.6
HG-MP-25	60	7.440	7.827	4.856	5.306	5	5	34.6	32.3
	180	4.661	5.054	4.206	4.577	4	5	8.6	8.7
	300	4.211	4.507	4.012	4.347	3	3	3.6	2.8
	600	3.956	4.173	3.792	4.145	3	2	3.1	-0.1
HG-MP-26	60	6.836	7.257	4.635	4.952	5	5	32.0	31.4
	180	4.204	4.667	4.070	4.381	4	5	3.0	6.1
	300	3.846	4.225	3.889	4.242	1	2	-1.1	-0.5
	600	3.697	3.965	3.743	4.079	2	2	-1.2	-3.0
HG-MP-27	60	6.649	7.027	4.206	4.477	5	5	36.6	36.1
	180	4.164	4.471	3.791	4.015	5	5	8.5	9.8
	300	3.799	4.140	3.720	3.905	3	3	1.8	5.5
	600	3.665	3.926	3.679	3.808	3	3	-0.6	3.0
HG-MP-28	60	10.518	11.365	6.917	7.472	5	5	33.9	33.9
	180	6.212	6.598	5.102	5.563	5	5	17.9	15.5
	300	5.356	5.705	4.768	5.260	5	5	11.0	7.6
	600	4.838	5.141	4.670	5.047	5	4	3.5	1.9
HG-MP-29	60	11.624	12.385	7.162	7.679	5	5	38.4	38.1
	180	6.229	6.974	5.555	6.091	5	5	10.7	12.5
	300	5.444	5.845	5.304	5.710	3	3	2.5	2.3
	600	5.023	5.325	5.104	5.447	2	2	-1.6	-2.2
HG-MP-30	60	9.557	10.011	5.764	6.068	5	5	39.7	39.3
	180	5.613	6.097	4.562	5.096	5	5	18.5	16.0
	300	4.999	5.463	4.334	4.776	5	5	12.9	12.1
	600	4.557	4.992	4.215	4.474	5	5	7.4	10.0
Total Average (%)					228/300	240/300	8.4	9.3	

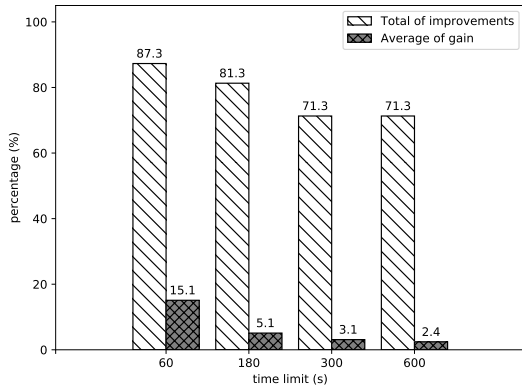
2.4.4 Graphical summary

A graphical summary of the computational results is depicted in Figure 2.2. The figure illustrates the improvements achieved by ILS+ over ILS, considering the individual instances rather than instance groups.

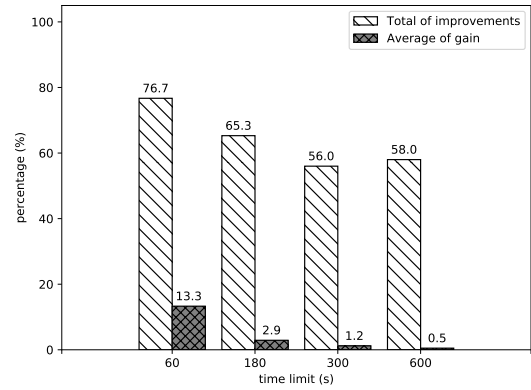
Considering all the 150 instances, Figure 2.2a shows that ILS+ improved the average solutions achieved by ILS for over 71.3% of them for all the tested time limits, and such improvement is more evidenced for the time limit of 60 seconds, for which improved solutions were obtained for 87.3% of the instances. The figure also shows that the average gain is considerably larger for the more restricted time limit of 60 seconds (15.1%) and progressively decreases as the time limit increases. Figure 2.2b shows that ILS+ encountered improved best solutions when compared to ILS for over 56.0% for all the considered time limits. ILS+ encountered improved best solutions for 76.7% of the instances when the time limit was set to 60 seconds. Similarly to what was observed for the average solutions, it can be seen that the average gain is considerably larger for the more restricted time limit (13.3%) and progressively decreases with the increase of the time limit.

Considering the 75 instances with less than 500 pipes, Figure 2.2c shows that ILS+ improved the average solutions achieved by ILS for over 73.3% of them with a similar behavior for all the tested time limits, for which improved solutions were obtained for percentages of the instances varying between 73.3% and 78.7%. The figure also shows that the obtained average gains were between 3.3% and 4.2% for all the tested time limits. Figure 2.2d shows that ILS+ encountered a very similar performance when compared to ILS. ILS+ encountered improved best solutions for 54.7% of the instances for the time limits of 60 and 600 seconds. However, for the time limits of 180 and 300 seconds ILS+ encountered improved best solutions for just 49.3%. Further, there is no considerably gain for any of the time limits, for which the average gains were obtained around 0.55%.

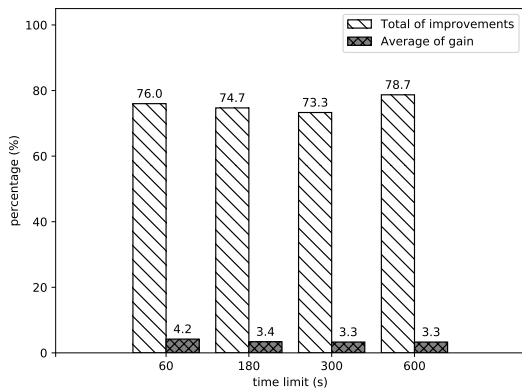
Considering the 75 instances with more than 500 pipes, Figure 2.2e shows that ILS+ improved the average solutions achieved by ILS for over 64.0% of them for all the tested time limits, and such improvement is more evident for the time limit of 60 seconds, for which improved solutions were obtained for 98.7% of the instances. The figure also shows that the average gain is considerably larger for the more restricted time limit of 60 seconds (25.9%) and progressively decreases as the time limit increases. Figure 2.2f shows that ILS+ encountered improved best solutions when compared to ILS for over 61.3% for all the considered time limits. It is remarkable the fact that ILS+ obtained improved best solutions for 98.7% of the instances when the time limit was set to 60 seconds. Similarly to what was observed for the average solutions, it can be seen that the average gain is considerably larger for the more restricted time limit (25.4%) and progressively decreases with the increase of the time limit.



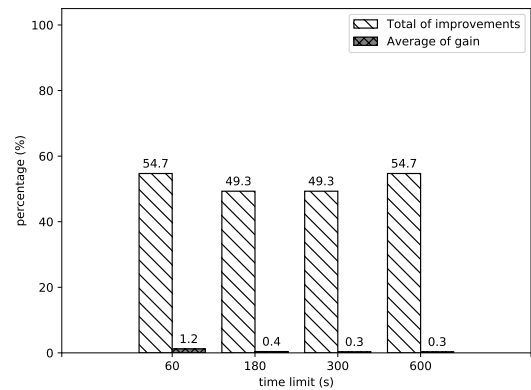
(a) Average cost considering all instances



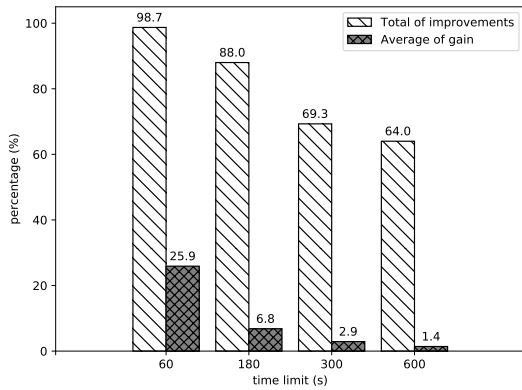
(b) Best cost considering all instances



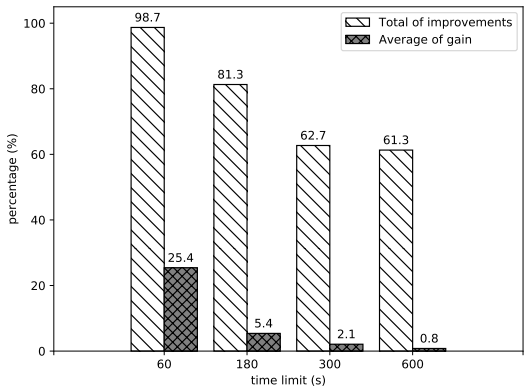
(c) Average cost considering the instances with less than 500 pipes



(d) Best cost considering the instances with less than 500 pipes



(e) Average cost considering the instances with more than 500 pipes



(f) Best cost considering the instances with more than 500 pipes

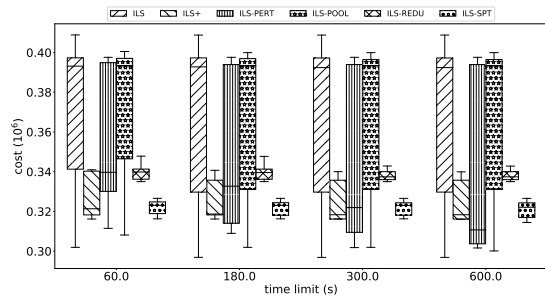
Figure 2.2: Graphical summary of the improvements achieved by ILS+ over ILS. The subfigures show the percentage of the instances for which ILS+ improved ILS, as well as the average gains of ILS+ over ILS. Subfigures (a) and (b) consider the average and best costs for all instances; Subfigures (c) and (d) examine the average and best costs for instances with less than 500 pipes; Subfigures (e) and (f) contemplate instances with more than 500 pipes.

2.4.5 Analyzing the impact of each individual novelty

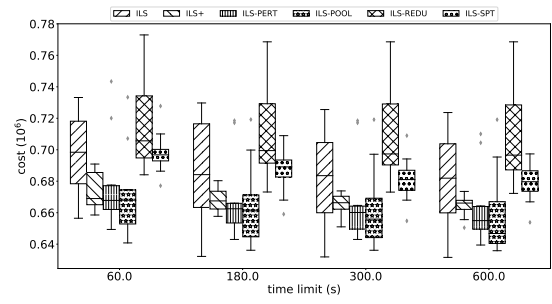
In this section, we analyze the impact of each of the proposed novelties individually on the obtained solution values and compare these with ILS and ILS+. Each of the tested novelties is defined as using a single improvement on top of ILS, namely: the aggressive reduction (ILS-REDU), the pool of solutions (ILS-POOL), the new perturbations (ILS-PERT), and the shortest path-based local search (ILS-SPT). We consider a subset of the instances described in Subsection 2.4.1, containing 10% of them, chosen randomly from varying instance groups. The settings are defined as in Subsection 2.4.2.

Figures 2.3-2.4 summarize the results. The values composing the boxplots for each instance and time limit represent ten runs of the corresponding approach. It is noteworthy that the enhancements achieved by the individual novelties on the obtained solutions are very diverse. ILS-PERT was able to reach a good performance in certain cases, and that behavior is possibly related to its ability to overcome local minima solutions encountered by the algorithm. ILS-REDU seldom allows considerable gains over ILS, especially when the allowed running time is increased. This is probably due to the nature of ILS-REDU, as it attempts to improve the convergence of the algorithm, quickly reaching hard-to-escape-from local minima solutions. It can allow, however, much faster convergence in some situations. ILS-POOL has a good performance, especially when considering instances with less than 500 pipes, showing the benefits of diversification. This is most likely related to the fact that it increases the possibility of exploring more diverse solutions. ILS-SPT has a great performance and seems to be the individual novelty that allows the most considerable reduction in the costs of the obtained solutions, corroborating our claim that the pattern compelled by the shortest path-based local search indeed allows reaching good quality solutions.

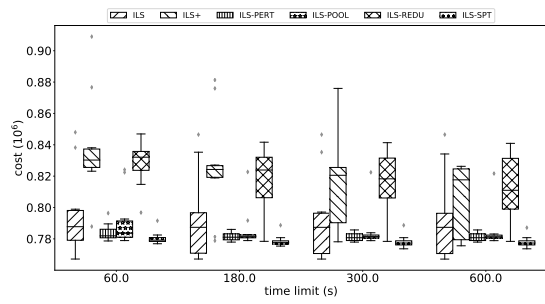
Most importantly, the figures allow us to observe that ILS+ presented the best overall performance, showing that the combination of the individual novelties is indeed valuable. Together they reach robustness and reduce the possible deficiency that each of them could present individually.



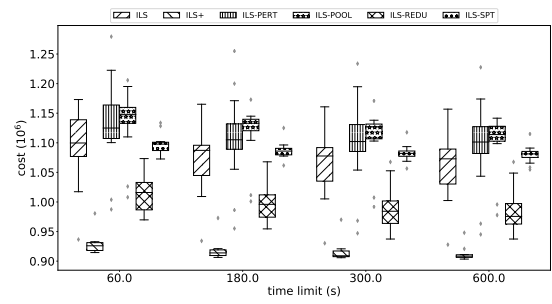
(a) HG-MP-2-1



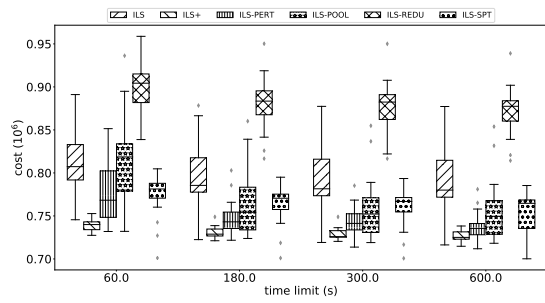
(b) HG-MP-4-3



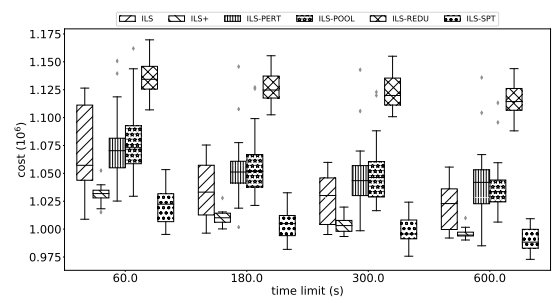
(c) HG-MP-6-5



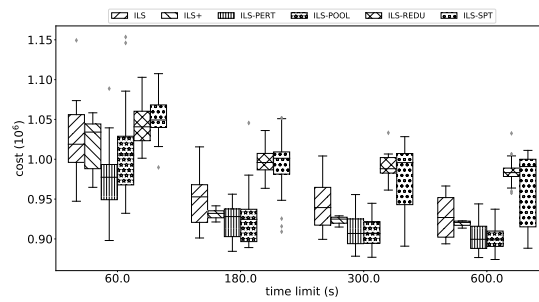
(d) HG-MP-8-5



(e) HG-MP-10-4

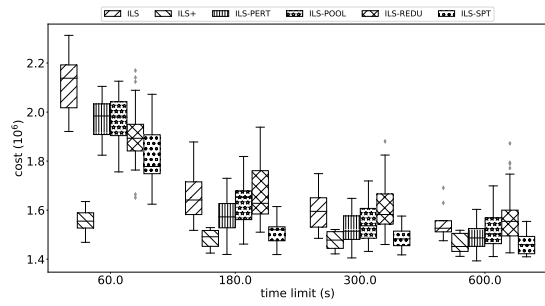


(f) HG-MP-12-4

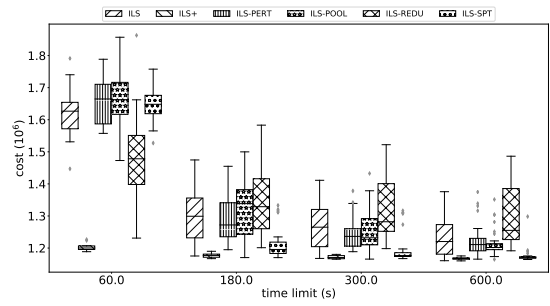


(g) HG-MP-14-5

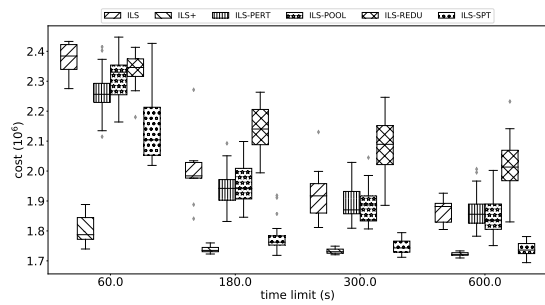
Figure 2.3: Impact of the individual novelties on the obtained solution costs considering instances with less than 500 pipes.



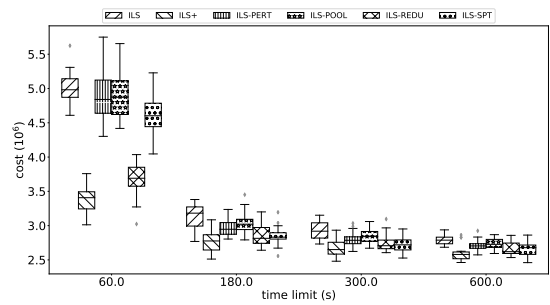
(a) HG-MP-16-1



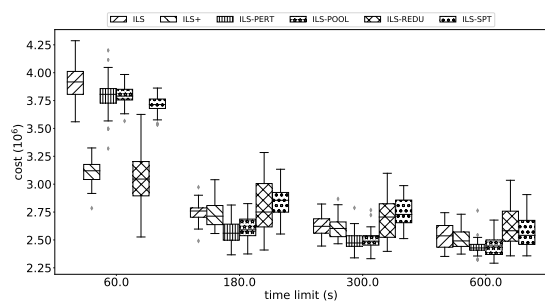
(b) HG-MP-18-2



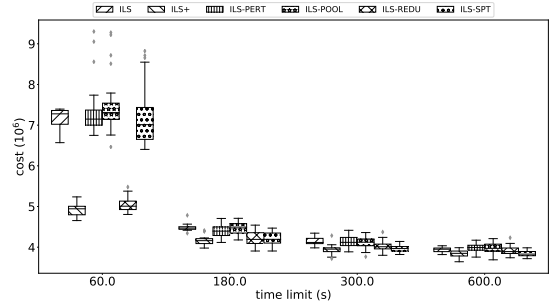
(c) HG-MP-20-2



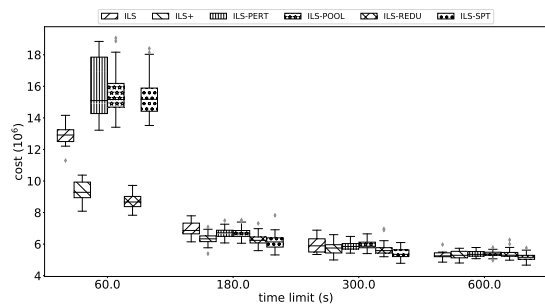
(d) HG-MP-22-2



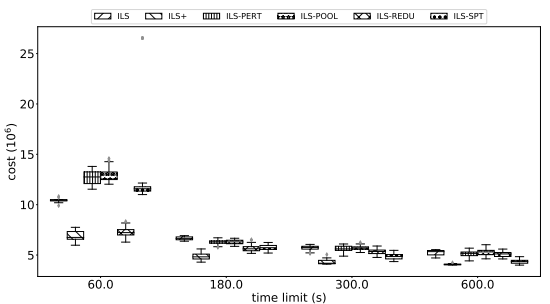
(e) HG-MP-24-4



(f) HG-MP-26-1



(g) HG-MP-28-1



(h) HG-MP-30-3

Figure 2.4: Impact of the individual novelties on the obtained solution costs considering instances with more than 500 pipes

2.4.6 Analyzing additional indicators for ILS and ILS+

In this section, we analyze the behavior of ILS and ILS+ when considering indicators such as the number of iterations, the number of calls to the hydraulic simulator, and the number of tested solutions. We consider the same set of instances used in Subsection 2.4.5. Besides, the settings are defined as in Subsection 2.4.2.

Table 2.6 summarizes the results. The first two columns indicate the instances and the allowed running times. For each combination of instance and allowed running time, ten executions of each approach were performed. The next columns report, for ILS and ILS+, the average number of iterations (i.e., number of executions of the while loop of lines 3-11 in Algorithm 8), the average number of calls to the hydraulic simulator, and the amount of tested solutions (including the average percentage of feasible solutions). Table 2.6 shows that both ILS and ILS+ present reasonably high numbers of iterations, hydraulic simulation calls, and tested solutions, and these values tend to decrease as the size of the instances increase, as expected. This indicates that the simulations do not seem to be a real bottleneck, and the main challenge lies in the search for good quality solutions. The table also shows that ILS+ consistently achieved higher values for all indicators but the percentage of feasible solutions. A possible explanation for that behavior is the faster convergence of ILS+. We remark that these indicators suggest that ILS+ presents a better efficiency in the search for good quality solutions when compared to ILS.

Table 2.6: Additional indicators for analyzing the behavior of ILS and ILS+.

Instance	Time (s)	ILS			ILS+		
		#iter (10 ³)	#hydr (10 ⁶)	#testedsol (10 ³) {Feas. rate (%)}	#iter (10 ³)	#hydr (10 ⁶)	#testedsol (10 ³) {Feas. rate (%)}
HG-MP-2-1	60	1.98	1.03	93.58 {21.05}	2.94	1.43	130.67 {14.01}
	180	6.05	3.08	281.25 {20.62}	8.89	4.26	390.09 {13.87}
	300	10.13	5.12	469.44 {20.44}	14.88	7.08	649.22 {13.91}
	600	20.36	10.23	940.06 {20.30}	30.08	14.11	1301.81 {13.99}
HG-MP-4-3	60	0.48	0.55	45.17 {25.52}	0.86	0.73	67.01 {16.24}
	180	1.54	1.59	135.79 {23.47}	2.71	2.16	204.17 {15.58}
	300	2.60	2.63	226.54 {23.19}	4.58	3.59	341.91 {15.48}
	600	5.26	5.24	453.77 {22.95}	9.27	7.17	687.18 {15.40}
HG-MP-6-5	60	0.48	0.60	55.61 {19.55}	0.74	0.75	82.88 {9.93}
	180	1.51	1.75	168.40 {17.77}	2.30	2.24	251.07 {9.37}
	300	2.54	2.90	281.20 {17.43}	3.87	3.73	419.44 {9.28}
	600	5.12	5.78	563.18 {17.20}	7.86	7.47	839.93 {9.31}
HG-MP-8-5	60	0.19	0.38	30.44 {28.05}	0.41	0.48	45.95 {16.93}
	180	0.66	1.07	92.29 {23.73}	1.28	1.42	140.89 {15.11}
	300	1.13	1.76	154.01 {22.86}	2.13	2.35	235.53 {14.66}
	600	2.31	3.48	309.22 {22.13}	4.26	4.68	472.42 {14.27}
HG-MP-10-4	60	0.09	0.30	20.42 {33.53}	0.16	0.36	26.46 {20.31}
	180	0.35	0.84	59.75 {28.09}	0.67	1.05	81.18 {18.81}
	300	0.62	1.38	99.01 {27.00}	1.19	1.74	136.39 {18.63}
	600	1.30	2.70	197.49 {26.17}	2.51	3.46	275.76 {18.53}
HG-MP-12-4	60	0.10	0.32	21.52 {33.00}	0.16	0.38	29.40 {16.40}
	180	0.34	0.90	64.42 {25.78}	0.56	1.15	90.33 {13.88}
	300	0.60	1.47	107.36 {24.35}	0.97	1.91	151.51 {13.40}
	600	1.24	2.88	214.53 {23.23}	1.98	3.81	305.25 {13.05}
HG-MP-14-5	60	0.05	0.23	15.85 {39.98}	0.10	0.28	24.27 {20.60}
	180	0.21	0.63	47.56 {30.75}	0.41	0.84	72.70 {18.15}
	300	0.38	1.02	79.10 {28.74}	0.73	1.40	121.74 {17.74}
	600	0.81	1.99	157.66 {27.52}	1.59	2.80	245.95 {17.57}
HG-MP-16-1	60	0.02	0.19	12.48 {40.48}	0.05	0.22	15.90 {26.35}
	180	0.11	0.51	36.53 {31.65}	0.23	0.64	50.66 {19.54}
	300	0.21	0.81	59.63 {29.31}	0.42	1.06	86.09 {18.04}
	600	0.46	1.55	117.08 {27.07}	0.90	2.10	175.24 {17.05}
HG-MP-18-2	60	0.02	0.22	12.07 {57.20}	0.06	0.24	16.09 {25.68}
	180	0.13	0.57	38.34 {36.48}	0.24	0.73	52.23 {18.42}
	300	0.24	0.93	64.03 {32.35}	0.43	1.21	89.46 {17.14}
	600	0.53	1.80	126.79 {29.51}	0.93	2.41	184.15 {16.28}
HG-MP-20-2	60	0.02	0.19	11.58 {48.46}	0.05	0.20	15.34 {28.77}
	180	0.10	0.49	36.59 {32.93}	0.22	0.59	50.05 {21.10}
	300	0.18	0.79	60.80 {30.07}	0.40	0.97	84.98 {19.65}
	600	0.41	1.51	120.49 {28.01}	0.84	1.93	172.46 {18.60}
HG-MP-22-2	60	0.01	0.15	8.99 {49.60}	0.02	0.15	10.97 {34.34}
	180	0.05	0.39	26.66 {38.72}	0.10	0.46	36.12 {22.89}
	300	0.11	0.61	43.85 {34.11}	0.20	0.76	61.01 {19.65}
	600	0.25	1.16	87.01 {29.09}	0.42	1.53	122.73 {17.09}
HG-MP-24-4	60	0.01	0.19	9.55 {67.53}	0.02	0.18	12.67 {31.75}
	180	0.06	0.47	30.88 {40.93}	0.11	0.53	41.71 {20.45}
	300	0.12	0.74	52.41 {33.76}	0.20	0.88	70.80 {17.96}
	600	0.28	1.43	105.26 {28.82}	0.45	1.77	144.00 {15.90}
HG-MP-26-1	60	0.01	0.15	7.95 {62.49}	0.01	0.15	10.25 {34.44}
	180	0.04	0.40	25.02 {41.21}	0.07	0.45	33.37 {22.07}
	300	0.08	0.63	42.85 {33.58}	0.13	0.75	56.64 {18.85}
	600	0.19	1.20	86.08 {28.35}	0.30	1.49	115.44 {15.95}
HG-MP-28-1	60	0.01	0.14	8.09 {49.06}	0.01	0.14	9.25 {40.30}
	180	0.03	0.36	23.54 {41.13}	0.05	0.39	29.84 {26.57}
	300	0.06	0.57	38.96 {36.31}	0.10	0.64	50.15 {22.54}
	600	0.15	1.05	75.97 {31.12}	0.23	1.26	99.87 {18.83}
HG-MP-30-3	60	0.01	0.15	8.23 {56.68}	0.01	0.14	10.01 {35.84}
	180	0.03	0.39	25.00 {42.29}	0.05	0.42	31.77 {25.74}
	300	0.06	0.61	42.42 {35.52}	0.10	0.71	52.62 {21.29}
	600	0.16	1.16	85.48 {29.18}	0.22	1.43	104.89 {16.93}

2.5 FINAL REMARKS

In this work, we addressed the water distribution network design (WDND) optimization problem and proposed a new enhanced simulation-based iterated local search (ILS) metaheuristic. Grounded on the structure of the problem, the proposed simulation-based ILS presents four main novelties: a local search strategy for smart dimensioning the pipes in shortest paths between reservoirs and high demand nodes, an aggressive pipe diameter reduction scheme based on varying factors to speed up convergence to good quality solutions, a concentrated perturbation mechanism to allow escaping from very restrained local optima regions, and a pool of solutions to allow a good balance between intensification and diversification.

The performed computational experiments have shown that the novelties embedded in our newly proposed simulation-based ILS allow improved performances when compared to a state-of-the-art simulation-based ILS. Furthermore, the results showed that our new approach presents a much faster convergence to good quality solutions and more robustness, as it obtained low costs solutions when allowing stricter time limits and achieved less deviation from the encountered best solutions when multiple executions were performed. Our approach found improved best solutions for 64.0% (384 out of 600) of the tests for the instance groups and improved average solutions for 77.8% (467 out of 600) of them. Remarkable improvements were achieved for the larger instance groups, for which these values were 76.0% (228 out of 300) for best solutions and 80.0% (240 out of 300) for average solutions. Furthermore, the average gains for the larger instances were in the order of 8.4% for best solutions and 9.3% for average solutions.

CONCLUSION

This chapter summarizes the main contributions of this master's thesis and discusses possible directions for future works. We proposed a simulated-based optimization approach for a nonlinear NP-hard optimization problem in the field of water resource, which hybridizes metaheuristics with a simulation model. Extensive computational experiments have shown that the proposed are effective and reported new best results for several tested instances.

The water distribution network design (WDND) problem studied in this master's thesis introduced a new enhanced simulation-based iterated local search (ILS) metaheuristic which further explores the structure of the problem in an attempt to obtain high quality solutions. The approach is able to improve over a state-of-the-art metaheuristic for most of the performed tests. Furthermore, it converges much faster to low cost solutions and demonstrates a more robust performance in that it obtains smaller deviations from the best known solutions. Our approach found improved best solutions for 64.0% for the instance groups where remarkable improvements were achieved for the larger instance groups, for which these values were 76.0% for best solutions. The results have shown that simulated-based optimization approaches is effective to deal with complex optimization problems and its use contributes to the development of effective algorithms. Lastly, the contents of Chapter 2 were submitted for publication in a relevant operational research journal (Martinho et al., 2020).

3.1 FUTURE WORKS

The strong point of the work is the investigation and identification of concepts about the structure of the problem that allow improvements in performance instead of the use of common random heuristics with generalized concepts. It would be interesting to investigate why some instances the algorithm is able to work much better than the state of the art, while in other instances the performance was similar or even without a good performance, finding more concepts in the structure and exploring them. The possibilities for improving the work include diversification through the use of solutions with possibly different characteristics. The improvement would investigate a more aggressive approach that would widely use this possibility without loss of performance compromise for large instances. In addition to adding machine

learning concepts to increase efficiency with the use of larger and more complex instances. Furthermore, all the findings in this direction can provide new insights into the development of robust algorithms and valid concepts that can leverage the effectiveness of such approaches.

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