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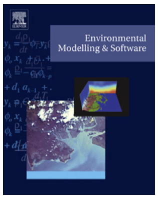

An iterative approach to multi-objective engineering design: Optimization of engineered injection and extraction for enhanced groundwater remediation☆

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ABSTRACT

This study contributes an iterative problem reformulation technique for multi-objective evolutionary algorithm (MOEA) decision support. Problem formulations consist of objectives, decision variables, and constraints, and directly influence the results generated by the MOEA. Typically, design problems are optimized based on a single problem formulation established *a priori*. In this paper, we demonstrate an approach to perform iterative optimization using problem formulations updated from analyses of results from prior rounds of optimization, which often reveal design components not initially considered. To demonstrate the approach, we consider a novel groundwater remediation technique, Engineered Injection and Extraction (EIE), which has never been optimized in the literature. Iterative problem reformulation enabled the MOEA to generate EIE solutions with better performance than the heuristically-developed solution used in prior work.

1. Introduction

Multi-objective evolutionary algorithms (MOEAs) have emerged as a powerful tool for engineering design optimization (Deb, 2001; Tan et al., 2005; Coello Coello et al., 2007; Zhou et al., 2011). They are used for many water resources engineering applications (Nicklow et al., 2010; Reed et al., 2013), model calibration (Efstratiadis and Koutsoyiannis, 2010), and processing data (Bandyopadhyay et al., 2014). Two properties of MOEA decision support contribute to their popularity. First, complex simulation models can be directly embedded within MOEAs. Therefore, instead of trying to create a linear programming (LP) representation of a complex system, the simulation model can be used to directly map system decision variables to outputs. Second, MOEAs are used to develop the tradeoffs between multiple conflicting objectives in a single algorithm run. By allowing decision makers to view the tradeoffs between their objectives, MOEAs avoid conceptual issues with aggregating multiple objectives together (Franssen, 2005).

This study contributes to prior work demonstrating the use of MOEAs to solve water resources management problems, an increasingly popular topic over the last few decades (Maier et al., 2014). Our specific water resources management problem of interest is groundwater remediation. Many previous studies have successfully used MOEAs to solve groundwater problems (Ritzel and Eheart, 1994; Yoon and Shoemaker, 1999; Maskey et al., 2002; Bayer and Finkel, 2004; Reed and Minsker, 2004; Kollat and Reed, 2006; Singh and Minsker, 2008; Reed et al., 2007); however for many of the case studies considered, the study focus was to develop and improve algorithms or to demonstrate the suitability of an algorithm to a particular problem (Maier et al., 2014). In our work, we focus on a different need: creating problem formulations for realistic engineering design problems to enable MOEAs to successfully solve these problems. To demonstrate our approach, we use a complex problem in the groundwater literature known as Engineered Injection and Extraction (EIE) (Mays and Neupauer, 2012) which is used to enhance contaminant degradation during groundwater remediation. We describe EIE in detail in Section 2.

MOEA optimization requires that the design problem be defined using a problem formulation, which includes objectives, decision variables, and constraints. Selecting a problem formulation is a critical part of the optimization process since the solutions

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generated by the algorithm directly reflect the chosen problem formulation (Kasprzyk et al., 2012; Woodruff et al., 2013). Objectives are used to quantify system performance, and often represent the goals of stakeholders. Decision variables represent actions that a decision maker or designer can perform. Constraints represent limitations imposed on the designed system, such as restrictions due to regulations or budget. Once the problem formulation is created, the MOEA is used to develop solutions that balance the objectives while adhering to the constraints. During the MOEA search, the concept of Pareto optimality is used to define tradeoffs. Informally, solutions are Pareto optimal if performance with respect to a given objective cannot be increased without degrading performance in a second objective (Cohen and Marks, 1975).

The use of a single, fixed problem formulation is common in MOEA studies. We can consider the aforementioned groundwater studies as examples. Early investigations by Yoon and Shoemaker (1999) compared the abilities of evolutionary algorithms, direct search methods, and derivative-based methods to optimize the design of a bioremediation system based on a single problem formulation, which included the objectives of minimizing cost and maximizing performance. Ritzel and Eheart (1994) optimized the design of a groundwater containment system based on a single problem formulation, which included decisions like the number of wells to install, where to install them, and how much to pump from each with the objectives of minimizing the cost and maximizing reliability. Maskey et al. (2002) and Bayer and Finkel (2004) used fixed problem formulations to optimize groundwater containment problems similar to the problem of Ritzel and Eheart (1994) to compare the performance of different evolutionary algorithms. Reed and Minsker (2004) have considered fixed problem formulation to optimize long-term groundwater monitoring network design, balancing the frequency of sampling events and the amount of sampling locations (and their associated costs) with the accuracy of contaminant concentration estimates and interpolated concentration maps. Kollat and Reed (2006) used the same topic, long-term groundwater monitoring design, as a test problem for comparing the performance of four different MOEAs based on a fixed problem formulation.

Although fixed problem formulations are common in MOEA studies, there is a need to determine how to best adapt the problem formulation to cater to realistic problems, as suggested in the position paper by Maier et al. (2014). Outside of MOEA studies, we have some examples of adapting the problem formulation. For instance, in fundamental problem-structuring literature, researchers have shown that adapting problem formulations is necessary to accommodate changing stakeholder preferences and system conditions, especially in the context of long range planning. For instance, Zeleny (1989) suggests that objectives, decisions, constraints, and problem representations are never fixed, but rather are in “continuous flux,” being reformulated as decision makers and analysts learn more about their system and problem. In this paradigm, objectives for the study can be discovered as a result of the planning process itself (Hitch, 1960). Similarly, literature in problem structuring methods attempts to combat the idea that the problem formulation is often assumed to be “established in advance and consensual” (Rosenhead, 1996).

In the problem-structuring literature, many researchers have developed approaches to iterative problem reformulation; however, these studies have not been conducted in the context of multi-objective optimization. Zeleny (1981) iteratively modified a linear program based on what the analyst learned while solving the problem. Turcanu et al. (2008) developed problem formulations in the context of multi-criteria decision aid by synthesizing evaluation criteria (i.e. objectives), and ranking those criterion according to the relative importance expressed by decision makers. Their approach is demonstrated for a theoretical nuclear emergency management scenario: the management of contaminated milk following a radioactive release. Gregory et al. (2012) demonstrate how problem structuring methods can be used to develop recovery plans for endangered species. Considerations for recovery planning are identified, a possible a solution is proposed, the proposed solution is analyzed according to an established framework, and the framework is improved upon iteratively based on the analysis.

The use of multiple problem formulations has recently been explored in the context of MOEAs, but little work has been conducted to iteratively adapt the problem formulation. Woodruff et al. (2013) optimized the design of aircraft product lines using problem formulations devised based on three different approaches. Given the large number of problem objectives, two of the approaches optimized formulations with aggregated objectives, while the other approach optimized a formulation with ten objectives. Zechman et al. (2013) constructed alternative problem formulations in order to generate distinct sets of nondominated solutions for wicked problems, defined as social and cultural problems which are difficult to solve due to incomplete data and diverse, often subjective, stakeholder opinions. The study showed that distinct sets of nondominated solutions can provide flexibility for decision-making in cases of wicked problems. Kasprzyk et al. (2012) developed a framework to guide the decision maker selection of water supply planning portfolios, where a portfolio represents the problem formulation in a design problem to optimize management strategies for municipal water resources. Since most variables associated with water management are uncertain, the framework uses sensitivity analysis on decision variables to inform problem formulation selection, resulting in solutions that perform robustly under a variety of conditions. An additional type of sensitivity analysis that explores robustness in deeply uncertain parameters can also be added to this process, as shown in Kasprzyk et al. (2013).

The objectives of this paper are to introduce an adaptive problem formulation approach for MOEAs and apply it to a complex design problem in groundwater remediation. The design problem, termed Engineered Injection and Extraction (EIE) (Mays and Neupauer, 2012), is used to enhance contaminant degradation during groundwater remediation. A complete explanation of the design problem is provided in Section 2. In previous work, a solution to this design problem was developed heuristically (Mays and Neupauer, 2012), but in this paper, we optimize the design of the groundwater remediation strategy using an MOEA. Using the previous work as a guide, we developed an initial problem formulation, which represented our best conception of the problem given the information available at that time. Optimizing with this initial formulation yielded inadequate optimization results, which motivated the development of an approach to learn more about the problem by iteratively reformulating the problem statement.

2. Engineered injection and extraction

In this study, we optimize the design of engineered injection and extraction sequences to enhance contaminant degradation during groundwater remediation. The cost to remediate all contaminated sites in the U.S. was recently estimated as $110 billion to $127 billion (NRC, 2013), which indicates the pressing need to develop and improve effective groundwater remediation strategies. One form of groundwater remediation is *in situ* chemical oxidation, where a treatment chemical is injected into the contaminated aquifer to degrade the groundwater contaminant *in situ*. The success of *in situ* chemical oxidation depends on the degree to which the injected treatment chemical can be spread throughout the region of contaminated groundwater, since contact of these reactants is necessary for degradation reactions to occur. EIE is a novel

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