

# Optimal design for problems involving flow and transport phenomena in saturated subsurface systems

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## Abstract

Estimation problems arise routinely in subsurface hydrology for applications that range from water resources management to water quality protection to subsurface restoration. Interest in optimal design of such systems has increased over the last two decades and this area is considered an important and active area of research. In this work, we review the state of the art, assess important challenges that must be resolved to reach a mature level of understanding, and summarize some promising approaches that might help meet some of the challenges. While much has been accomplished to date, we conclude that more work remains before comprehensive, efficient, and robust solution methods exist to solve the most challenging applications in subsurface science. We suggest that future directions of research include the application of direct search solution methods, and developments in stochastic and multi-objective optimization. We present a set of comprehensive test problems for use in the research community as a means for benchmarking and comparing optimization approaches.

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## 1. Introduction

Modeling of fluid flow and contaminant transport in subsurface porous medium systems has become commonplace [128]. These simulations continue to advance our general understanding of transport phenomena and are increasingly used as a basis for managing subsurface systems. Such management may involve identifying model parameters [84,132], planning data collection programs [14,80], or designing and operating engineered systems [66]. Within this general class of problems, design problems associated with fluid flow and species transport in subsurface systems are especially important [102].

Broadly speaking, design problems for these applications fall into the general class of constrained, non-linear, stochastic, multi-objective optimization problems (CNSMOP)—an especially challenging class of appli-

cation. The stochastic nature of these problems results directly from our imperfect knowledge of model parameters, auxiliary conditions, or in some cases even the fundamental form of the model that governs transport phenomena in typical heterogeneous porous medium systems [101]. The multi-objective aspect of these problems arises, for example, from a conflicting desire to minimize cost and maximize reliability of a design [116].

Most efforts to date for subsurface optimization problems have been some simple subset of the general class of CNSMOP problems. This is largely because of the complexity and computational demands of solving this general class of problems and partly because of the evolving nature of stochastic optimization. Over the last two decades, groundwater quality control and remediation have been the focus of optimization efforts in the subsurface literature [3–8,12,13,43,45,66,74,79,80,82,83,87,90,92,93,102,106,110,113,118,133,134,147]; in particular, the design of pump-and-treat (PAT) systems is the most frequent application considered [3–7,10,12,13,23,74,79,83,87,90,92,93,118,121].

The objectives of this work are (1) to provide a common conceptual framework for subsurface design

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