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# The Double Constraint Inversion Methodology

## Equations and Applications in Forward and Inverse Modeling of Groundwater Flow

Springer

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# Preface

> Progress is the battle with the experts.
>
> Peter Schlumbohm

> Why another book with mathematical equations? I have already a book with these embellishments.
>
> Anonymous geologist

> This realization that the key to the understanding of Nature lay within an unassailable mathematics was perhaps the first major breakthrough in science.
>
> Sir Roger Penrose

This work deals with the mathematical and applied aspects of the double constraint methodology to estimate the parameters that play a role in groundwater flow and is intended to serve students and practitioners by bridging the gap between basic hydrogeology and inverse groundwater modeling. Groundwater is world's largest freshwater source, but sound and sustainable exploitation remains a challenge. For the development and management of groundwater resources, a proper knowledge of the physical and mathematical laws and their parameters governing the state and movement of groundwater is essential. In the last decades, substantial progress has been made in inverse groundwater modeling, so that not only forward modeling, but also inverse modeling has become an essential tool for groundwater resources management. However, a good knowledge of basic mathematical principles of groundwater flow is essential to understand numerical models. Often such knowledge is lacking in traditional academic programs like civil engineering or geology. Hence, this work attempts to synthesize the mathematics of groundwater flow to give insight in the physics of the relevant parameters that characterize the porous formations through which groundwater flows. In this respect, this work provides in-depth information for geophysicists, hydrogeologists, and engineers pursuing Bachelor, Masters, and Ph.D. degrees, as well as for groundwater practitioners and consultants who intend to become skillful and competent modelers.

In addition, petroleum reservoir engineers and basin modelers will find ample inspiration to support their exploration and production-related modeling activities.

The inspiration for this work came from two sources. In the 2000s, the idea to apply the double constraint methodology to assist in the application of conventional data assimilation techniques was born in the oil and gas department of Netherlands Organisation for Applied Scientific Research TNO. Conventional data assimilation techniques are smoothing the subsurface permeability field in the flow models in such a way that geologists do no longer recognize their carefully constructed geological models. To mitigate the over-smoothing without destroying the models' match with measured pressures and flow rates, the double constraint methodology was one of the proposed methods. In the 1980s and 1990s, there was a unique experiment at TNO: managing director Prof. Frans Walter and his successor Dr. Hessel Speelman were encouraging petroleum engineers and scientists of the oil and gas department as wells as hydrogeologists and geoscientists of the groundwater department to join forces in research and development, preferably in cooperation with universities. Subjects of common interest were modeling and uncertainty analysis. Among the many initiatives, research related to inverse modeling was initiated in close cooperation with the Department of Hydrology and Hydraulic Engineering of the Vrije Universiteit Brussel (VUB). Although TNO discontinued this experiment by end of the 1990s (from a commercial point of view, the petroleum market differs too much from the water market), the VUB team—Ph.D. students and supervisors—continued this research by developing mathematical proofs and models and performing case studies.

The reason why the double constraint methodology was initiated and continued at the VUB was that this methodology fits well as a research topic in its Water Resources Engineering Program for M.Sc. and Ph.D. students. This program, in which the Katholieke Universiteit Leuven (KU Leuven) has complementary tasks, is devoted to teaching and supervising water-related topics and is basically intended for international students, mostly from developing countries. The program has been running for a couple of decades and has close to a thousand graduates, working as researchers, consultants, academics, and practitioners all over the world. All students follow among others a course in groundwater hydrology, while electives as groundwater modeling have as ultimate goal to be proficient in modeling.

The students come from different backgrounds with diverse academic degrees in engineering, geological sciences, or environmental sciences. Engineers may have a profound knowledge of the mathematical–physical laws of conservation and movement, but often lack insight in specific properties and settings of groundwater-bearing formations and how these affect the equations describing groundwater flow. For earth scientists, it is usually the opposite as they have a good knowledge about geological conditions and processes, but often lack insight in the mathematical–physical aspects of describing flow and transport.

This above typical example of training students shows that better links are needed between basic geology/groundwater hydrology and groundwater modeling. The double constraint methodology, which is firmly based on the mathematical–physical laws of conservation and movement, as is amply explained and exemplified in this work, provides a link between “geologists” and “modelers.” We therefore believe that this work contributes to a better understanding of groundwater flow theory, thus providing a greater and more realistic insight into what groundwater models can do and how they should be applied in practice.

Finally, we want to express our thanks to Dr. Anna Trykozko from the Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw, Poland. She played an important role in the initial phase of the development of the double constraint methodology, especially regarding stability and the question how to avoid negative conductivities. In addition, she has considerably improved this book, not only regarding text on stability and negative conductivities, but also regarding text on numerical over-estimation and the related difference between calibration and imaging.

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# Chapter 1
# Introduction: Setting the Scene

Groundwater flow models are necessary tools to understand a groundwater system, to make predictions about the system's response to a stress, or to design and support management interventions and decisions. In groundwater flow modeling, we generally distinguish two types of problems:

(i) The *forward* problem, in which the parameters (e.g., hydraulic conductivities) are specified, as well as the appropriate boundary and initial conditions.
(ii) The *inverse* problem, in which not all parameters are specified. Instead, additional boundary conditions, more than required for a forward problem, are imposed.

Inverse problems are common to many fields of sciences, such as geophysical and medical imaging, meteorological forecasting, petroleum reservoir engineering, and hydrology. Each time when we need to determine unknown properties of a system from the observations of a response of that system, inverse models come into play. Usually, the unknown properties are physical parameters characterizing the model and their values are determined by systematically adjusting them while checking the match between the model outputs and the observed parameters.

Groundwater flow models are based on the following two mathematical basic equations:

(i) The water balance equation: a partial differential equation describing the physical law of mass conservation—mass cannot be created or destroyed in the groundwater flow field.
(ii) The momentum balance equation: a partial differential equation describing the physical law of conservation of momentum. In most practical cases, the low Reynolds number of groundwater flow allows simplification of the law of conservation of momentum to Darcy's law: Flow rate is equal to hydraulic conductivity times head gradient.

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