#### SpringerBriefs in Applied Sciences and Technology

Rachid Ababou · Juliette Chastanet · Jean-Marie Côme · Manuel Marcoux · Michel Quintard



Uncertainty Analyses in Environmental Sciences and Hydrogeology Methods and Applications to Subsurface Contamination



## **SpringerBriefs in Applied Sciences and Technology**

SpringerBriefs present concise summaries of cutting-edge research and practical applications across a wide spectrum of fields. Featuring compact volumes of 50 to 125 pages, the series covers a range of content from professional to academic.

Typical publications can be:

- A timely report of state-of-the art methods
- An introduction to or a manual for the application of mathematical or computer techniques
- A bridge between new research results, as published in journal articles
- A snapshot of a hot or emerging topic
- An in-depth case study
- A presentation of core concepts that students must understand in order to make independent contributions

SpringerBriefs are characterized by fast, global electronic dissemination, standard publishing contracts, standardized manuscript preparation and formatting guidelines, and expedited production schedules.

On the one hand, **SpringerBriefs in Applied Sciences and Technology** are devoted to the publication of fundamentals and applications within the different classical engineering disciplines as well as in interdisciplinary fields that recently emerged between these areas. On the other hand, as the boundary separating fundamental research and applied technology is more and more dissolving, this series is particularly open to trans-disciplinary topics between fundamental science and engineering.

Indexed by EI-Compendex, SCOPUS and Springerlink.

Rachid Ababou · Juliette Chastanet · Jean-Marie Côme · Manuel Marcoux · Michel Quintard

# Uncertainty Analyses in Environmental Sciences and Hydrogeology

Methods and Applications to Subsurface Contamination



Rachid Ababou Institut de Mécanique des Fluides de Toulouse (IMFT) Toulouse. France

Jean-Marie Côme GINGER Lyon, France

Michel Quintard Institut de Mécanique des Fluides de Toulouse (IMFT) Toulouse. France Juliette Chastanet GINGER Lyon, France

Manuel Marcoux Institut de Mécanique des Fluides de Toulouse (IMFT) Toulouse, France

ISSN 2191-530X ISSN 2191-5318 (electronic) SpringerBriefs in Applied Sciences and Technology ISBN 978-981-99-6240-2 ISBN 978-981-99-6241-9 (eBook) https://doi.org/10.1007/978-981-99-6241-9

© The Author(s), under exclusive license to Springer Nature Singapore Pte Ltd. 2023

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Singapore Pte Ltd. The registered company address is: 152 Beach Road, #21-01/04 Gateway East, Singapore 189721, Singapore

Paper in this product is recyclable.

#### Acknowledgments

This book is based in part on previous research work performed in the framework of the ESPER project, funded by ADEME, the French environmental protection agency (Grant award number 1672C0022). The authors wish to acknowledge contributions from graduate students and junior researchers at the Institute of Fluid Mechanics in Toulouse: R. Leroux (IMFT post-doc) on fuzzy and possibilistic approaches; Y. Soumane (IMFT master student 2018-2019) on the 3D analytical model and ESPER-1 probabilistic package. The first author also thanks Pr. K. Alastal (IMFT visiting scientist 2019–2020) for additional help on MATLAB implementation of the 3D analytical model, and Pr. N. El Moçayd (UM6P) for his useful 2022 comment on Sobol indices versus Polynomial Chaos.

### **Contents**

1	Introduction, Objectives				
2	Ove	rview o	f Uncertainty Propagation Methods	3	
	2.1	Appro	aches to Uncertainty	3	
	2.2	Monte	Carlo Simulations (with or Without a Metamodel)	4	
		2.2.1	Direct Monte Carlo Simulations	4	
		2.2.2	Indirect Monte Carlo Simulations via a Metamodel	5	
		2.2.3	Summary on Direct Versus Indirect Monte Carlo		
			Simulations	6	
	2.3	Joint S	Sets of Parameters, Cross-Correlations, Design		
		of Exp	periments	6	
		2.3.1	Sampling and Uncertainty Propagation for Each Input		
			Parameter (One-By-One)	7	
		2.3.2	Joint Uncertainty Propagation for a Parameter Set		
			$\{P_1,P_2,\ldots,P_K\}$	9	
	2.4	Applio	cations to Risk Assessment in Field Pollution	13	
	2.5 Causes and Sources of Uncertainty		s and Sources of Uncertainty	14	
	2.6	Uncer	tainty Propagation: Output "Criteria"	16	
	Refe	erences		17	
3	Dov	iow of I	Probabilistic Versus Fuzzy Approaches to Uncertainty		
3			n in Geosciences	19	
			bilistic Characterization of Uncertainty	19	
	5.1	3.1.1	Univariate Probabilistic Characterization (Single	19	
		3.1.1		20	
		3.1.2	Parameter)	20	
		3.1.2		25	
		2 1 2	or More Uncertain Parameters)	25	
		3.1.3	Estimating a Covariance or Correlation from a Data	21	
	D. C		Sample	31	
	Rete	rences		- 3/1	

viii Contents

4	Fuzzy Set Characterization of Uncertainty (Fuzzy Variables)		
	4.1	Fuzzy Sets, Fuzzy Numbers, Fuzzy Logic and Arithmetic	35
		4.1.1 Fuzzy Sets, Fuzzy Numbers, Membership Functions,	
		and α-Cuts	35
		4.1.2 Fuzzy Logic and Fuzzy Arithmetic Rules in Models	36
	4.2	From Fuzzyness to "Possibility" (Fuzzy + Probabilistic)	38
		4.2.1 Fuzzy Probability Bounds: Possibility (Upper CDF),	
		Necessity (Lower CDF)	39
		4.2.2 Intermediate CDF's via α-Cuts (Confidence Levels	
		and Intervals)	42
		4.2.3 Random + Fuzzy Uncertainty: IRS Algorithm	40
		for Propagating Possibilistic CDFs	43
		4.2.4 Comparative Review: Softwares and Uncertainty	47
	D.f.	Propagation	47
	Refe	erences	50
5	App	olications of Uncertainty Analyses on Simplified Models	53
	5.1	Introduction: Models with Uncertain Parameters (Classification)	53
	5.2	Decay Kinetics with Uncertain Decay Parameter	54
		5.2.1 Introduction to the First Order Decay Kinetics Model	54
		5.2.2 Exact Explicit Analytical Expression of C(t)'s	
		Probability Law	55
	<b>~</b> ~	5.2.3 The Mean Concentration Curve C(t)	56
	5.3	Taylor Expansion Around the Mean: MVFO Method	
	5.4	and Application to Corrosion Pits	57
	5.4	Coupled 1D Model of Contaminant Migration and Source	62
		Dissolution	02
		via a Metamodel	64
		5.4.2 Possibilistic Analysis of 1D Contaminant Migration	04
		with IRS	69
	Refe	erences	71
			, -
6		dications of Uncertainty Analysis to 3D Subsurface	
		tamination Problems	73
	6.1	Application of Uncertainty Analysis to 3D Contaminant	
		Advection—Dispersion from a Decaying Source (Quasi-Analytical ESPER-1 Model)	74
			/4
		6.1.1 Model Equations: PDE, Geometry, Boundary and Initial Conditions	74
		6.1.2 The Quasi-analytical Solution C(x, y, z, t) and M(t)	78
		6.1.3 Visualizations of the Solution C(x, y, z, t) and M(t)	79
		6.1.4 Monte Carlo Analyses of 3D Analytical Model (ESPER1	19
		Package)	80
	6.2	Uncertainty Analysis of 3D Solute Migration and Source	30
	٠ <b>.</b> ــ	Attenuation in a Polluted Site (MODFLOW-SURFACT)	84
			٠.

Contents ix

	6.2.1	The Modflow-Surfact Code and Model Equations	85
	6.2.2	Main Hydrogeologic Characteristics of the Polluted Test	
		Site	88
	6.2.3	Uncertainty Analysis: Metamodeling Procedure	
		for the Field Site	88
	6.2.4	Results: Probabilistic Characterization of Output	
		Criterion (Critical Time)	92
	References		93
7	Discussion	and Conclusions	95

#### Chapter 1 **Introduction, Objectives**



The different alternatives for managing a contaminated site are based on a cost/benefit balance that requires predictive modeling to assess mass depletion and duration of contamination source in the subsurface. For instance, the ESPER<sup>1</sup> project (Evaluation and Sensitivity of models for Predicting the depletion and Remediation of organic contamination sources in subsurface) was aimed at developing a methodology and a software tool for facilitating the incorporation of uncertainty and sensitivity analyses into such subsurface contamination models.

Let us first clarify from the outset the term "uncertainty propagation."

Mathematical methods of uncertainty analyses can be viewed as "uncertainty propagation" methods, in the sense that they can "propagate" (or "carry") the uncertainty from the input parameters to the outputs of the model. The model may be analytical: a simple example is the first order decay model  $C(t) = C_0 \exp(-\lambda t)$ . Or it can be a more complex quasi-analytical model containing special functions and simple integrals. Or else, it can be a fully discretized space-time numerical model such as the MODFLOW-SURFACT<sup>TM</sup> code. It can also be, possibly, a polynomial "meta-model" ("surrogate model") derived from the initial model. The metamodel is essentially an input/output response function, derived from the original model, and which can be used to simplify the uncertainty propagation process (as will be explained later).

This book reviews and illustrates various approaches and methods for uncertainty analysis, and presents various models (from simple to complex) to illustrate these uncertainty analyses, including some model-specific results, and also, site-specific results, from the ESPER project in particular.

This book is organized as follows. After the present introduction, the next chapter (Chap. 2) covers different methods for carrying out uncertainty analysis, starting with an overview of different approaches and concepts. Chapter 3 develops a comprehen-

<sup>&</sup>lt;sup>1</sup> The ESPER project was funded in part by ADEME, the French environmental protection agency.