

School of h¥drogeological Modelling & Project-related

trat*e*gies

Model Calibration and UA with PEST

17/05/2021 Rev.1

John Doherty

John Doherty, PhD, is the author of PEST and its supporting utility software suites. He is a selfemployed consultant at Watermark Numerical Computing, he has held positions with the National Centre for Groundwater Research and Training, Flinders University, Australia, and with University of Queensland, where he has undertaken research and supervised PhD students. He started his career as an exploration geophysicist, then moved to environmental modelling. He has since worked in the government, private and tertiary sectors. His research interests include the continued development of software and methodologies for solution of inverse problems using environmental models, quantification of model predictive uncertainty, and appropriate use of models in the decision-making context. He is currently active part of the GMDSI initiative. He is now part of the of the Scientific Committee of SYMPLE.

Francesca Lotti

Francesca Lotti, Ph.D, is a consultant hydrogeologist and partner at Kataclima srl. She has nearly 20 years of experience in field investigations and numerical modelling with MODFLOW and FEFLOW of contaminated sites, mines, geothermal systems, etc. She collaborates with research institutions and international companies. From 2001 to 2014 she was research fellow at the University of Tuscia, she is adjunct professor at the University of Camerino since 2008, supervisor of many students/PhD/interns, trainer at professional courses and lecturer at the II level Master "Caratterizzazione e tecnologie per la bonifica dei siti inquinati" at the University of Rome "Sapienza".



Giovanni Formentin

Giovanni Formentin is an environmental engineer and partner at Tethys srl. He has been working for 19 years as a consultant and researcher in the fields of hydrogeology and water management. He applies groundwater flow and transport models to water resources management and remediation of contaminated sites, in Italy and abroad. He has been teaching groundwater modelling with Modflow and Feflow as well as model calibration at universities in Milan (Politecnico) and Naples (Federico II).



School of h**Y**drogeological Modelling & Project-related rat*e*gies

Model Calibration and UA with PEST

17/05/2021 Rev.1

Course programme

Lesson 1 (1+3 hrs)

Presentation of the real-world case, a contaminated site in Milan. Exercise

Building of the real-world case model. Creation of the numerical model with MODFLOW-6: setting of boundary conditions, the grid, properties, observation points.

Lesson 2 (1 hour)

Introduction

- What is calibration?
- The PEST Roadmaps: getting oriented in the PEST manuals and related material

Lesson 3 (1 hour)

Structure of files

- MODFLOW input/output files
- PEST input/output files •

Lesson 4 (2+3 hrs)

Traditional Parameter Estimation

- Well-posed inverse problem
- Manual regularization

Exercise

Sensitivity analysis and zone calibration of parameters in the previously created model. Critical evaluation of results.

Lesson 5 (2+3 hrs)

Highly parameterized inversion

- Subspace regularization singular value decomposition
- Tikhonov regularization •
- Pilot points as a spatial parameterization • device

Exercise

Pilot point calibration of parameters in the previously created model. Critical evaluation of results

Lesson 6 (2 hrs)

Uncertainty analysis (part 1)

- Bayes equation
- Worst case analysis
- Using geostatistics for prior uncertainty analysis
- **Rejection Sampling**
- Markov chain Monte Carlo •
- Linear uncertainty analysis

Lesson 7 (2 + 4 hrs)

Uncertainty analysis (part 2)

- Null space Monte Carlo
- Ensemble smoother
- Direct predictive hypothesis testing
- Data space inversion

Exercise

Hands-on exercise on uncertainty analysis applied to the previously calibrated model.

Lesson 8 (1 hrs)

Decisions and Modelling

- Dealing with model defects
- Formulation of an appropriate objective function
- The role of model validation
- Metrics through which decision-support modelling should be judged
- When to calibrate and when not to calibrate

Lesson 9 (1 hrs)

An overview of PEST++

- Design philosophy •
- **Current capabilities**
- Codes, documentation and support

Lesson 10 (2 hrs)

An overview of model-partner software provided through the PEST and PEST++ suites

- Optimization •
- Optimization under uncertainty •
- **Review of optimal PEST settings** •

Lesson 11 (2 hrs)

Case Histories

These will focus not so much on modelling details, as on the relationship between modelling and management/decision-making. Questions to be answered are: "was it the best modelling choice to support the decisions that needed to be made?" and, "if it weren't, what would have been a better choice?"