Resume: John Doherty

Personal Details

Year of Birth:	1955
Nationality:	Australian
Education:	BSc. App. [Geophys] Hons I (University of Queensland, 1975) PhD [Physics] (University of Queensland, 1987)
Awards:	W. H. Bryan Prize (Geology), 1972 H. C. Richards Prize (Geology), 1973 University Medal, 1975 NGWA M. King Hubbert Award, 2009 WRR editors' choice award, 2011 (shared with other authors)

Present Employment

Director of Watermark Numerical Computing Pty. Ltd.

Activities include:

- Scientific and engineering programming.
- Development and construction of groundwater models for environmental, agricultural, water supply, remediation, mining and Coal Seam Gas applications.
- Maintenance, support and development of upgrades for PEST, a popular model-independent nonlinear parameter estimator used throughout the world for the calibration of environmental models of all kinds.
- Education in environmental modelling through direct advisory consultancies, and the leadership of modelling courses and workshops in Australia, Europe, the US and elsewhere; these are mainly focussed on the use of nonlinear parameter estimation methods in the calibration of environmental models, and in exploration of the uncertainty pertaining to predictions made by these models.
- Provision of services for the calibration of models used in the hydrological and environmental sciences. Contracts to date have included work with storm water and sewerage system models, forest production models, watershed models (including both quantity and quality aspects of surface water movement), groundwater flow and transport (including salt water intrusion) models, and multiphase multicomponent fluid flow models.
- The development of utility software to expedite the use of PEST with specific models.
- Development, in conjunction with personnel from U.S. Geological Survey, U.S. Environmental Protection Agency, U.S. Department of Energy and U.S. Army Corps of Engineers, of methodologies and software for application of nonlinear parameter estimation and predictive uncertainty analysis techniques in the surface water and ground water modelling contexts.

Professor, National Centre for Groundwater Research and Training, Flinders University

Activities include:

- Supervision of post-graduate students working on projects involving the development and application of state-of-the-art environmental model calibration and predictive uncertainty analysis software and methodologies.
- Development of public domain software to implement linear and nonlinear uncertainty analysis.

June to October 2001

Visiting Professor, University of Idaho, Idaho Falls.

Activities included:

- Development of software to facilitate the use of nonlinear parameter estimation methods in ground and surface water modelling.
- Application and testing of these methods in conjunction with personal from the U.S. Geological Survey and the U.S. Environmental Protection Agency.
- Provision of formal education in the use of nonlinear parameter estimation methods for calibration and predictive analysis of environmental models.

Previous Employment

1987 - 1991: Research Fellow, James Cook University of North Queensland.
1991 - 1995: Senior Groundwater Hydrologist, Queensland Department of Natural Resources.

Duties included:

- The construction and calibration of large, complex models simulating groundwater and surface water movement within irrigation areas.
- The development of groundwater-modelling-based procedures to assess salinity risks in dryland and irrigated agricultural areas.
- The development of translation software for transfer of data between models, Geographical Information Systems, databases, and visualisation/display packages.
- The enhancement of a Geographical Information Systems for use in the groundwater context.

1976 - 1979: Geophysicist, Geological Survey of Queensland.
1979 - 1985: Geophysicist, Water Division, Northern Territory Power and Water Authority.

Duties included:

- The undertaking of geophysical surveys for groundwater supply and environmental investigations; methods used included seismic refraction, resistivity, IP, EM and magnetics.
- The interpretation and reporting of data gathered on these surveys.
- The development of computer programs for forward and inverse modelling of earth response to different geophysical techniques.
- The design and construction of some surface and downhole instrumentation.
- The operation of a borehole logging system.

- Geological mapping and logging of drilling returns.

Research

1985 - 1987: PhD student, Physics Department, University of Queensland.

During this period I undertook research into the numerical simulation of the electromagnetic response of subsurface bodies to external magnetic and electrical excitation. This work culminated in a thesis exploring the use of the boundary element method in the "two-and-a-half dimensional" modelling context.

Commercial and Public Domain Software

1991: MODINV
A MODFLOW-specific parameter estimator. MODINV was used at over 250 sites worldwide.

1994: PEST
PEST is a model-independent nonlinear parameter estimator. It is presently used worldwide for the calibration of hydrological and other engineering/scientific models, and for interpretation of field data based on mathematical inversion. It is supported by a number of commercial modelling graphical user interfaces including Visual MODFLOW, Groundwater Vistas, GMS, PMWIN and BASINS.

1994: PEST Utilities for MODFLOW/MT3D Parameter Estimation
A set of utilities to facilitate the use of PEST with MODFLOW and MT3D.

1995: Groundwater Data Utilities
A suite of programs to undertake certain aspects of groundwater model pre- and postprocessing, and to facilitate data transfer between MODFLOW, MT3D, MICROFEM, PEST, SURFER, GIS and various visualisation/display packages.

1996: SENSAN: A Model-Independent Sensitivity Analyser
Uses the PEST model interface protocol for the construction of a model-independent sensitivity analyser.

1997: Parallel PEST
A version of PEST that dramatically reduces optimisation time by undertaking simultaneous model runs across a PC network.

1997: PEST GMS Utilities
A set of programs which facilitates the use of PEST with the popular "Groundwater Modelling System" developed by Brigham Young University.

1998: PEST98
A major upgrade for PEST, including the addition of user-intervention functionality.

1998: Utilities for use of PEST with HSPF

Written on behalf of the United States Environmental Protection Agency.

1999: PEST Surface Water Utilities
A suite of software tools developed to enhance the use of PEST in the calibration of surface water models.

1999: PEST2000
A major PEST upgrade including the addition of nonlinear predictive uncertainty analysis functionality.

1999: Composite IQQM/MODFLOW Model
MODFLOW96 was linked to IQQM, a basin-scale hydrologic and water management model developed by the New South Wales Department of Land and Water Conservation.

2000: PEST Interface to GMS Version 3.1
This was developed jointly with personnel from Brigham Young University.

2000: PEST-ASP
In late 2000 PEST was upgraded to include sophisticated regularisation capabilities to enhance its use in the calibration of complex distributed-parameter models in heterogenous settings ("ASP" stands for "Advanced Spatial Parameterisation").

2000: MF2PEST
MF2PEST is a MODFLOW2000-to-PEST dataset translator, allowing use of PEST as an enhancement to MODFLOW. This is complemented by MODFLOW-ASP, an enhanced version of MODFLOW-2000 that includes a PEST interface, the ability to parameterise a model domain using pilot points, and better handling of drying/re-wetting conditions.

2001: Pilot Point Utilities
A number of programs were added to the Groundwater Data Utility Suite that facilitate the use of PEST in MODFLOW and MT3D spatial parameterisation. Sophisticated, geostatistically-based, regularisation conditions are introduced to the parameterisation process, making use of PEST-ASP's advanced regularisation capabilities.

2001: TSPROC
TSPROC is a comprehensive time-series processor developed for use as an adjunct to PEST in the calibration of surface water models on the basis of many different kinds of measured and/or processed data.

2002-2003: Improvements to PEST
These include functionality for adaptive regularisation, compressed data storage, and other devices to improve the use of PEST in highly parameterised contexts. They also include drivers that allow PEST to avoid entrapment in local minima during surface water model calibration.

2003: MICA

MICA is a model-independent Markov Chain Monte Carlo program developed under contract from U.S. EPA for calculation of model predictive uncertainty in a Bayesian framework.

2004: Advanced Regularisation
In 2004 a unique hybrid regularisation methodology known as "SVD-Assist" was added to PEST. This was supported by the addition of a number of new programs to the PEST utility suite. Use of SVD-Assist realises great gains in the numerical stability of a regularised inverse problem, at the same time as it results in large efficiency gains.

2005 Advanced Model Predictive Error Analysis
Based on theory published in a number of scientific journals (see below), utility software was developed to carry out fast and efficient model predictive error analysis as an adjunct to regularised inversion. This software allows rapid analysis of the uncertainty range of model parameters, source terms and predictions that are compatible with a given suite of historical measurements of system state, and with the known or inferred level of geological heterogeneity prevailing in a study area. This technology is unique to PEST.

2006 Improvements to PEST
These included improvements to its regularisation capabilities, new algorithms for accommodation of poor model performance with respect to derivatives calculation, improved recording of history of the calibration process, incorporation of the LSQR solver for highly parameterised systems, and parallelised versions of the CMA and SCE global inversion engines as calibration alternatives to PEST.

2007 Null Space Monte Carlo
This required modifications to PEST and the development of a number of utility support software to allow rapid generation of multiple parameter realisations which, on the one hand, respect a user-specified stochastic distribution, while on the other hand provide a fit between model outputs and field data which is as good as that of the "calibrated model".

2009 Pareto Mode
A new mode of operation based on the exploration of the Pareto front was added to PEST. This was designed for use in highly parameterized contexts where expert-based subjective judgements must be used in determining optimality of imposition of regularization constrains during calibration, and optimality of imposition of calibration constraints during predictive uncertainty analysis.

Publications

PhD Thesis

Doherty, J., 1987. The use of surface integral equations in modelling for electrical prospecting. PhD Thesis, University of Queensland.

Journal and USGS Open File Report Publications

Banta, E.R., Poeter, E.P, Doherty, J. and Hill, M.C., 2006. JUPITER: Joint Universal Parameter IdenTification and Evaluation of Reliability – an Application Programming Interface (API) for Model Analysis. Techniques and Methods 6-E1. U.S. Geological Survey, Denver, CO.

Banta, E.R., Hill, M.C., Poeter, E., Doherty, J. and Babendreier, J., 2008. Building model analysis applications with the Joint Universal Parameter IdenTification and Evaluation of Reliability (JUPITER) API. *Computers & Geosciences* 34 (2008) 310–319

Christensen S. and Doherty, J., 2008. Using many pilot points and singular value decomposition in groundwater model calibration. *Calibration and Reliability in Ground Water Modelling: Credibility of Modelling.* Proceedings of MODELCARE, 2007, Copenhagen, Denmark. IAHS Publ.

Christensen, S. and Doherty, J., 2008. Predictive error dependencies when using pilot points and singular value decomposition in groundwater model calibration. *Advances in Water Resources*. Volume 31, Issue 4, April, pages 674-700.

Dausman, A.M., Doherty, J., Langevin, C.D., and Sukop, M.C., 2010. Quantifying data worth toward reducing predictive uncertainty. *Groundwater, 48 (5), 729-740*.

Dausman, A.M, Doherty, J., Langevin, C.D. and Dixon, J., 2009. Hypothesis testing of buoyant plume migration using a highly parameterized variable-density groundwater model. *Hydrogeology Journal* DOI 10.1007/s10040-009-0511-6.

Dixon, O. and Doherty, J., 1977. New interpretation methods for IP soundings. *ASEG Bulletin* Vol. 8, No. 3 pp 65-74.

Doherty, J., 1988. EM modelling using surface integral equations. *Geophysical Prospecting*, Vol. 36, No. 6.

Doherty, J., 1990. The interpretation of pump-test data from a disused underground mine. *Journal of Hydrology* Vol. 114, pp 109-123.

Doherty, J., 2001. A methodology for preventing the occurrence of dry cells in a three-dimensional MODFLOW model. *Ground Water,* Vol *39.*

Doherty, J., 2003. Groundwater model calibration using Pilot Points and Regularisation. *Ground Water*. Vol 41 (2): 170-177

Doherty, J., 2011. Modeling: picture perfect or abstract art? *Ground Water*, 49(4), 455-456.

Doherty, J. and Christensen, S., 2011. Use of paired simple and complex models in reducing predictive bias and quantifying uncertainty. doi:10.1029/2011WR010763.

Doherty, J., Fienen, M,N. and Hunt, R.J., 2010. Approaches to highly parameterized inversion: pilot-point theory, guidelines and research directions. *USGS Scientific Investigations Report 2010-5169.* Downloadable from http://pubs.usgs.gov/sir/2010/5168/

Doherty, J. and Hunt, R.J., 2009. Two statistics for evaluating parameter identifiability and error reduction. *Journal of Hydrology*. 366, 119-127.

Doherty, J., and Hunt, R.J., 2010. Response to comment on "Two statistics for evaluating parameter identifiability and error reduction". *Journal of Hydrology*. 380, 489-496.

Doherty, J., and Hunt. R.J., 2010. Approaches to highly parameterized inversion: a guide to using PEST for Groundwater-Model calibration. *USGS Scientific Investigations Report 2010-5169.* Downloadable from http://pubs.usgs.gov/sir/2010/5169/

Doherty, J. and Johnston, J.M., 2003. Methodologies for calibration and predictive analysis of a watershed model, *J. American Water Resources Association*, 39(2):251-265.

Doherty, J. 2008. Model predictive error: how it arises and how it can be accommodated. *Calibration and Reliability in Ground Water Modelling: Credibility of Modelling.* Proceedings of MODELCARE, 2007, Copenhagen, Denmark. IAHS Publ.

Doherty, J. and Skahill, B, 2006. An advanced regularization methodology for use in watershed model calibration. *Journal of Hydrology, 327 (3-4), pp564-577.*

Doherty, J. and Welter, D., 2010, A short exploration of structural noise, *Water Resour. Res*., 46, W05525, doi:10.1029/2009WR008377. ***WRR featured article.***

Eddebarh, A.-A, James, S.C., Doherty, G.A., Zyvoloski, G.A. and Arnold, B.W., 2007. A new saturated zone site-scale model for Yucca Mountain. *EOS Transaction* American Geophysical Union, 88, 52, H21C-0706.

Ellis, R.J., Doherty, J., Searle, R.D. and Moodie, K., 2009. Applying PEST (parameter ESTimation) to improve parameter estimation and uncertainty analysis in WaterCAST models. *in* RS Anderssen, RD Braddock & LTH Newham (eds), *18th World IMACS Congress and MODSIM09 International Congress on Modelling and Simulation*, Modelling and Simulation Society of Australia and New Zealand and International Association for Mathematics and Computers in Simulation, Cairns, Australia, pp. 3158-3164.

Fienen, M.N., Doherty, J.E., Hunt, R.J. and Reeves, H.W., 2010. Using prediction uncertainty analysis to design hydrologic monitoring networks: example applications from the Great Lakes Water Authority availability pilot project. *USGS Scientific Investigations Report 2010-5159*, 44p.

Gallagher, M.R. and Doherty, J. 2006. Parameter Estimation and Uncertainty Analysis for a Watershed Model, *Environmental Modelling and Software*, 22, 1000-1020.

Gallagher, M. and Doherty, J., 2007. Predictive error analysis for a water resource management model. *Journal of Hydrology*, 34(3-4), 513-533.

Gallagher, M. R., and Doherty, J., 2007. Parameter interdependence and uncertainty induced by lumping in a hydrologic model, *Water Resour. Res*., 43, W05421, doi:10.1029/2006WR005347.

Herckenrath, D., Langevin, C.D., and Doherty, J., 2011. Predictive uncertainty analysis of a salt water intrusion model using null space Monte Carlo. *Water Resour. Res*., 47, W05504. doi:10.1029/2010WR009342.

Hunt, R.J., Doherty, J, and Tonkin, M.J., 2007. Are models too simple? Arguments for increased parameterisation. *Ground Water* 45 (3), 254–262

Hunt, R.J. and Doherty, J., 2011. Interesting or important? Resetting the balance of theory and application. Guest editorial in *Ground Water* 49 (3), 301.

Hunt, R.J., Luchette, J., Shreuder, W.A., Rumbaugh, J., Doherty, J., Tonkin, M.J. and Rumbaugh, D., 2010. Using the cloud to replenish parched groundwater modeling efforts. Rapid Communication for *Ground Water*, doi: 10.1111/j.1745-6584.2010.00699

James, S.C., Doherty, J. and Eddebarh, A.-A., 2009. Post-calibration uncertainty analysis: Yucca Mountain, Nevada, USA. *Ground Water*. 47 (6), 851-869.

Keating, E., Doherty, J., Vrugt, J.A. and Kang, Q., 2010. Optimization and uncertainty assessment of strongly nonlinear groundwater models with high parameterization dimensionality. *Water Resources Research*, Vol 46, W10517, 18 pp., 2010 doi:10.1029/2009WR008584. ***Winner of the WRR editor's choice award for 2010.***

Kim, S.M., Benham,B.L. Brannan, K.M., Zeckoski, R.W. and Doherty, J., 2007, Comparison of hydrologic calibration of HSPF using automatic and manual methods, *Water Resources Research*, 43, W01402, doi:10.1029/2006WR004883.

McKenna, S.A., Doherty, J. and Hart, D.B., 2003. Non-Uniqueness of Inverse Transmissivity Field Calibration and Predictive Transport Modeling. *Journal of Hydrology*, 281(4) 265-282.

Moore, C. and Doherty, J., 2005. The role of the calibration process in reducing model predictive error. *Water Resources Research*. Vol 41, No 5. W05050.

Moore, C. and Doherty, J., 2006. The cost of uniqueness in groundwater model calibration. *Advances in Water Resources*. Volume 29, Issue 4, April, pages 605 – 623.

Moore, C., Wöhling, T., and Doherty, J., 2010. Efficient regularization and uncertainty analysis using a global optimization methodology. *Water Resources Research.* Vol 46, W08527, doi:10.1029/2009WR008627.

Tonkin, M. and Doherty, J., 2005. A hybrid regularised inversion methodology for highly parameterised models. *Water Resources Research*. Vol. 41, W10412, doi:10.1029/2005WR003995, 2005.

Tonkin, M., Doherty, J. and Moore, C., 2007. Efficient nonlinear predictive error variance for highly parameterized models. *Water Resour. Res.*, 43, W07429, doi:10.1029/2006WR005348.

Tonkin M., J. and Doherty, J., 2009. Calibration-constrained Monte Carlo analysis of highly parameterized models using subspace techniques, *Water Resour. Res.*, 45, W00B10, doi:10.1029/2007WR006678.

Tonkin, M.J., Hill, M.C., and Doherty, J, 2003, MODFLOW-2000, the U.S. Geological Survey modular ground-water model -- Documentation of MOD-PREDICT for predictions, prediction sensitivity analysis, and enhanced analysis of model fit: U.S. Geological Survey Open-File Report 03-385, 69 p.

Skahill, B. and Doherty, J., 2006. Efficient accommodation of local minima in watershed model calibration. *Journal of Hydrology*, 329 (1-2), pp122-139.

Wilsnack, M.M., Doherty, J.E. and Welter, D.E., 2010. A Pareto-based methodology for calibration and uncertainty analysis of gated culvert flows. *ASCE J. Irr. & Drain. Accepted for publication.*

Invited Presentations at Major Conferences

"Model Complexity: How Much is Too Much?" MODFLOW98 Conference, Golden, Colorado.

"Model Parameterisation and Predictive Uncertainty - Their Role in the Model Construction Process." Geological Society of America Annual Meeting, Denver, 1999.

"Groundwater Model Parameterisation – Space Age Technology or Science Fiction". MODFLOW-2001 Conference, Golden Colorado.

"Decreasing Expectations and Increasing Credibility in Groundwater Modeling". MODFLOW 2003 conference, Golden Colorado.

"Highly parameterised inversion in calibration and uncertainty analysis for complex models". AGU Fall Meeting, San Francisco, 2006.

"Model Predictive Error: How it Arises and How it can be Accommodated". ModelCare conference, Copenhagen, 2007.

"Models and Decisions: A Better Way". PEST Conference, Maryland, 2009.

"Model-based decision making: A new perspective". Doherty, J. E., S. C. James, and P. W. Reimus, *13th International High-Level Radioactive Waste Management Conference*, 1049-1058, Albuquerque, NM, 2011.

"Complexity and Simplicity – Combining the Strengths of Both". Invited presentation at Geological Society of America Annual Meeting, Minneapolis, 2011.

"Environmental Modelling – Encapsulating what we Know and Quantifying what we Don't". NCGRT Distinguished Lecture Series – presented at most Australian capital cities through 2011.