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Applying PEST (Parameter ESTimation) to improve parameter estimation and uncertainty analysis in WaterCAST models

Ellis, R.J. [1], **Doherty, J.** [2], **Searle, R.D.** [1] **and Moodie, K.** [1]

[1] *Queensland Department of Environment and Resource Management, Australia*
2 Watermark Numerical Computing, Queensland, Australia
Email: robin.ellis@derm.qld.gov.au

In addition to requesting water quality models that contain a robust and reliable calibration, clients and stakeholders are increasingly demanding some measure of model uncertainty. The estimation of parameter values for water quality models like WaterCAST can be a difficult task for modellers, especially for large and complex models. The uncertainty surrounding the resulting parameter values, and the predictions from the model that use these values, is hard to quantify and communicate to a broad audience. The methodologies investigated by this study aim to more adequately satisfy the clients driving the production of these models.

A model-independent parameter estimation program, PEST, has been used to calibrate the basic rainfall-runoff and constituent generation models contained in a complex WaterCAST project representing the Fitzroy River Catchment in central Queensland, Australia. The calibrated parameter values have been calculated through a supervised approach which incorporates both Tikhonov and subspace techniques of mathematical regularisation, maintaining a high degree of modeller satisfaction and confidence. The calibration process considers all of the complex interactions possible within the subcatchment-node-link network, meaning that optimised parameter values are immediately suitable for application to the model.

One of the PEST tools employed in this process provides assistance in applying singular value decomposition. This assistance significantly reduced the number of model runs needed to achieve a satisfactory calibration. The same assistance was then used to attempt the unsupervised calibration of 100 random parameter sets in a Monte Carlo style approach. A high level of model run efficiency of the re-calibration process is achieved through using null space projection of random parameter fields to replace solution space components with those estimated through the previous calibration exercise. A total of 50 of these random parameter sets were able to have the statistical objective function minimised by PEST to within 0.5% of that achieved with the supervised calibration. These 50 calibrated parameter sets allow a quantifiable analysis of the uncertainty surrounding both the range of parameter values that provide a satisfactory calibration, and the range of model predictions that each of these parameter sets leads to. The same techniques were also applied to sediment generation processes in a sub-region of the Fitzroy catchment.

By calibrating model parameters within the WaterCAST environment, rather than in a secondary environment like the Rainfall Runoff Library, the calibration was able to consider all internal interactions. This has resulted in a statistical fit of predictions to observations that is a clear improvement (average coefficient of efficiency for daily flow at 20 locations increased from 0.50 to 0.79, average percent flow volume difference at 20 locations reduced from 91% to 15%). This calibration also satisfies the modellers need for an acceptable visual fit. Estimates of sediment generation from the WaterCAST model are accompanied by uncertainty estimates that most encapsulate the variability seen in a sporadic and variable observation data set.

Keywords: *Parameter estimation, uncertainty, regularisation, null space*

1. INTRODUCTION

Water quality models are being used by government, community groups and land managers to investigate the impacts of issues such as climate change and land management on water quality. Ultimately water quality model 'owners' want to utilise a modelling environment that is intuitive in design, easy to manipulate and navigate, and readily interpretable by a variety of users. However, as the investments and decisions arising from the analysis of these water quality models increase in size and importance, the model 'owners' are legitimately demanding that the model should also contain communicable measures of uncertainty.

The estimation of appropriate parameter values for any model can be a complex process for surface water models. In most surface water models the hydrologic process is represented by one or more rainfall-runoff models, converting climate inputs to runoff and ultimately stream flow. In most cases these rainfall-runoff models are calibrated by comparing modelled and observed stream flow at one location, with 'nesting' of observation points throughout the stream network handled only by multiple, independent calibrations. The modelled stream flow at these locations will be the culmination of the runoff and stream flow from many upstream contributing rainfall-runoff and flow routing models, and the complex interactions between these contributors should be considered in the calibration process. The same ethos can be applied to the calibration of constituent generation models, such as land use based soil erosion estimates.

A model-independent parameter estimation program, PEST (Doherty 2009), has been used to calibrate the basic rainfall-runoff and constituent generation models contained in a complex WaterCAST (Argent *et al*. 2008) project representing the Fitzroy River Catchment in central Queensland, Australia. The mathematical regularisation employed allows use of prior knowledge and user expertise in the calibration process, and retainment of parameterisation detail that reflects system detail in the model. This calibration technique also enables a subsequent, quantifiable, analysis of uncertainty. This technique of uncertainty analysis has been utilised mostly in groundwater applications, however its use in surface water applications is increasing, with recent progress by Tonkin and Doherty (2009) forming the basis of the uncertainty analysis conducted in this project.

2. STUDY AREA

The Fitzroy River Catchment covers an area of approximately 140, 000 km^2 in central Queensland, Australia (figure 1). The Fitzroy River flows to the Great Barrier Reef, and is therefore seen as a significant region in terms of water quantity and quality. This is a region of diverse climate and land management regimes, however most land management would be classified as extensive grazing, with some conservation areas, cropping, coal mining and minor horticulture also present. Rainfall is highly variable with much of the region being semi-arid but subject to occasional monsoonal rainfall and floods. The Fitzroy Catchment is also topographically diverse, and the soils and landscapes also variable.

To investigate hydrologic parameter estimation and uncertainty the Fitzroy River Catchment was represented in a WaterCAST scenario by 396 subcatchments (figure 1). These subcatchments were the result of an automated WaterCAST Digital Elevation Model (DEM) process, with additional subcatchments placed to allow representation of major water storages within the stream network. Each subcatchment had 7 'Functional Units' nominally assigned based on land use. Each functional unit instance was assigned a SIMHYD rainfall-runoff model (Chiew *et al*. 2002), each link in the node-link network was assigned a Laurenson non-linear flow routing model (Laurenson and Mein 1997), except for 12 links where a water storage model was applied (storage geometries and characteristics from the Fitzroy Basin Resource Operations Plan (Dept. Natural Resources and Water 2006)). A calibration period from 1st January 1985 to 31st December 2005 was selected. Climate inputs for rainfall-runoff models were sourced from the SILO Data Drill (SILO 2004).

For constituent generation (total suspended solids – TSS) parameter estimation and uncertainty analysis, a smaller region within the Fitzroy Catchment was studied. This 40, 000 km^2 'Beckers' area comprises most of the Dawson River Valley (figure 1), and is represented in the WaterCAST project by 119 subcatchments. A calibration period from 1st January 1986 to 31st December 2005 was selected.

3. METHODS

3.1. Whole of Fitzroy Hydrologic Parameter Estimation

The study area was broken into 20 calibration ‘regions’ according to the subcatchments contributing to the 20 gauging stations with daily flow observations (figure 1). Throughout these regions the WaterCAST entities of subcatchments, functional units, links and nodes continued to operate as discrete units, however models belonging to similar ‘types’ were grouped for PEST assessment. This method of parsimony implies uniformity within, but not between, calibration regions. Each SIMHYD model presented to PEST had 7 parameters available for adjustment. Each Laurenson non-linear flow routing model had 2 parameters available for adjustment. Parameter ranges were limited to those recommended in the relevant user guides.

Figure 1. Fitzroy River Catchment with flow observation points (gauging stations) and subcatchments indicated. Subcatchments are shaded by calibration ‘region’, with the ‘Beckers’ study area also indicated.

Observed daily flow totals were extracted from NR&W’s corporate data base environment ‘Hydstra Surface Water Database’. A baseflow separation algorithm (Boughton 1993) was applied to the observed daily flow, with the resulting baseflow ‘observations’ also used in calibration (algorithm source Grayson *et al*. 1996).

In solution of the inverse problem of model calibration, Tikhonov regularisation (Tikhonov and Arsenin 1977) was implemented by PEST as a means of providing numerical stability and of assimilating user expertise in the calibration process. ‘Preferred values’ were assigned to all parameters during the calibration process, and PEST was instructed to deviate from those estimates only to the minimum extent required to achieve a good fit between model outputs and flow measurements. It is assumed that the rainfall-runoff and flow routing models have a physical basis, and that the individual parameters are related to some real world phenomena (Doherty and Johnston 2003). Thus the ‘preferred values’ incorporate prior knowledge and expert opinion, and the acknowledgement of these in the calibration process is highly valued by modellers.

A PEST utility program, Time Series Processor (TSPROC), was used as a post-model processor to compare modelled flow outputs with observed data in a 60-part multi-component objective function. This objective function was comprised of the weighted, sum of squared residuals for daily flows, daily ‘baseflows’, and monthly volume accumulations at each calibration gauging station. The combination of various flow ‘functions’ in an objective function was shown to give satisfying ‘fits’ in small scale trials, and may also help to avoid the optimisation problem of ‘local minima’.

Inter group weightings were adjusted to ensure that the 60 observation groups initially made an equal contribution to the total objective function. This weighting strategy was employed to ensure that the resulting calibration considered observations from each gauging station equally, as inherent flow magnitudes are substantially different throughout the catchment.

Model calibration was implemented using the ‘SVD-Assist’ scheme implemented in PEST (Tonkin and Doherty 2005). Using this methodology a total of 120 ‘super parameters’ were defined as linear combinations of the 880 base parameters that are actually adjusted during the calibration process. These super parameters were defined on the basis of singular value decomposition (SVD) of a global sensitivity matrix computed on the basis of preferred parameter values to span the ‘calibration solution space’. Using this methodology, only

120 model runs were required per optimisation iteration, in spite of the fact that values were optimised for all 880 model parameters, and that Tikhonov constraints are applied to these base parameters.

The parameter set from the 4th optimization iteration was selected as the 'calibration' parameter set, as the 'fits' were satisfying to the modeller without too much deviation from the 'preferred' values. The objective function reduced from an initial value of 60,000 to 29,833.

3.2. Whole of Fitzroy Uncertainty Analysis

100 random sets of the 880 parameters employed by the model were then generated, with parameter values gained from the calibration used to 'centre' the random distribution within the literature recommended parameter ranges. Using the 'Null Space Monte Carlo' functionality available in PEST (Tonkin and Doherty 2009), these were modified such that they respected calibration constraints. This involved:

- Calibration and solution null spaces were defined based on SVD of the global sensitivity matrix.
- Each random parameter set was projected onto these spaces.
- The solution space component was removed and replaced by that of the calibrated parameter set.
- SVD-Assisted adjustment of the solution space component was then undertaken using the methodology described above.

Using SVD-Assist and 120 'super parameters', 50 of the 100 null space projected random parameter sets achieved an objective function value of 30,000 or less (within ~ 0.5% of the 'calibrated' objective function value) in a single optimisation iteration. The outcome of this procedure was a set of 50 parameter fields whose 'fit' was almost as good as that of the originally calibrated parameter field. All of these were considered to be reasonable in terms of the processes that they represent, but all of which were significantly different. The 50 parameter sets that achieved this near-calibration, and the model predictions from these parameter sets, form the basis of our quantified uncertainty analysis. The parameter sets and predictions can be subjected to probabilistic analysis, the outcomes of which can range from simple estimates of predictive mean and standard deviation, to more complex non-parametric analysis based on predictive frequency and cumulative frequency distributions. In this paper graphical representations have been selected.

3.3. 'Beckers' Hydrologic Parameter Estimation and Uncertainty

In modelling this subregion of the total Fitzroy model domain, rainfall-runoff (SIMHYD) models representing 6 functional units within 7 calibration regions were calibrated against daily observed flow data at 7 gauges (refer figure 2), for the period 1986 - 2005. Preferred parameter values were supplied to PEST based on local knowledge and previous research, and both Tikhonov and SVD-Assisted methods of regularisation were employed. PEST was instructed to use 35 'super parameters' to represent linear combination of the 429 parameters available. A 21 part, equal initial contribution objective function was formed using residuals from daily flow, monthly volume and exceedence times. Daily flow observations (and their paired model outputs) were weighted individually in a manner that emphasised low flow values.

After a calibrated parameter set was derived, a Null Space Monte Carlo process was conducted on 300 random parameter sets, with 133 of these 'realisations' achieving satisfactory 'calibration' at an average cost of about 15 runs per calibrated parameter field.

3.4. 'Beckers' Total Suspended Solids (TSS) Parameter Estimation and Uncertainty

To calibrate the Event Mean Concentration / Dry Weather Concentration (EMC/DWC) parameter values for each functional unit, daily TSS concentration (mg/L) observations were processed for the period 1986 – 2005 at each of the 7 calibration gauging stations. Where multiple observations occurred on any day, an average concentration value was calculated. The number of daily TSS concentration observations was sparse, with temporal and spatial distribution sporadic. Of the 346 daily average TSS observations used, the average number of observations at each site was only 50 (with a minimum of 6 and a maximum of 86).

A single set of two EMC/DWC parameters were estimated during this stage. These comprised a single EMC and DWC value applied to 'Grazing Open' land throughout the entire catchment. Fixed ratios between values for these parameters and those for other land uses were assumed. Different values for these parameters were estimated in 134 separate calibration exercises, one for each member of the 133 calibration-constrained random hydrology parameter sets, and one for the original calibrated parameter set.

The outcome of this process was a suite of 134 parameter sets for both hydrologic and water quality model components, all of which are very different, and none of which can be rejected as a possible catchment wide hydraulic property characterisation. Model predictions have been made with all of them, thereby allowing exploration of the uncertainty of those predictions.

4. RESULTS

4.1. Whole of Fitzroy Hydrology

Statistically the 'calibrated' parameter set yields flow predictions that provide a good match between observed and modelled flows at 20 locations throughout the catchment. Figures 2 and 3 compare the statistical assessment of predictions made from the calibrated parameter set with predictions using parameter sets (relevant to each calibration region) gained from the Rainfall Runoff Library (Podger 2004). The parameter sets from the RRL made use of a variety of optimisation techniques, and considered daily flow and total volume components, however the RRL environment can not account for the effects of flow routing and water storages. The PEST derived calibration parameter set was able to consider all of these interactions throughout the 20 regions simultaneously.

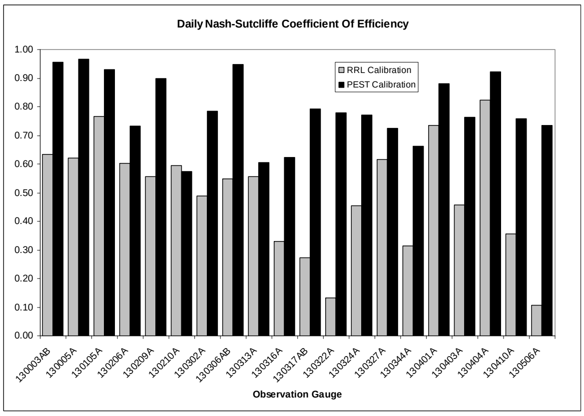

Figure 2. Coefficient of Efficiency for daily flow predictions at 20 observations locations throughout the Fitzroy Catchment.

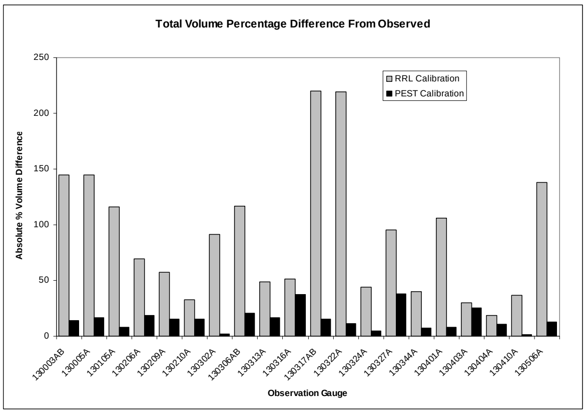

Figure 3. Total volume difference between predicted and observed flow at 20 observations locations throughout the Fitzroy Catchment.

Also of importance to modellers is the visual 'fit' when predicted flows are shown with observed. Figure 4 illustrates a visual comparison for the PEST derived calibration.

The range of values for each parameter throughout the 50 calibrated realisations can be represented graphically to indicate the range and distribution of each particular parameter within a quantified uncertainty assessment environment; figure 5 demonstrates this. In this case the assessment environment consists of 50 randomly produced parameter sets that each statistically satisfy the calibration objective function. The sensitivity of the optimisation objective function to changes in each parameter value is easily ascertainable from PEST. The magnitude of the sensitivity, whilst not shown here, can be interpreted as an indication of the likelihood that a change in this parameter will de-calibrate the model.

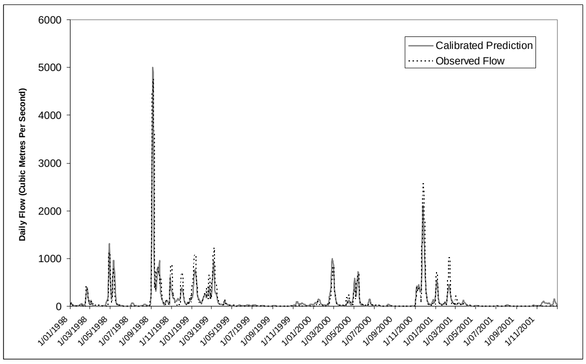

Figure 4. Comparison of predicted daily flow with observed daily flow at gauging station 130003AB for 1998 – 2001.

The uncertainty surrounding model predictions can also be analysed using the 50 calibrated realisations of parameter sets. For any intended analysis the model outputs gained from using each of the parameter sets can be used to represent the range and distribution of model predictions within a quantified assessment environment. Figure 6 illustrates how this may be done graphically, probabilistic analysis could also be conducted if project deliverables require this.

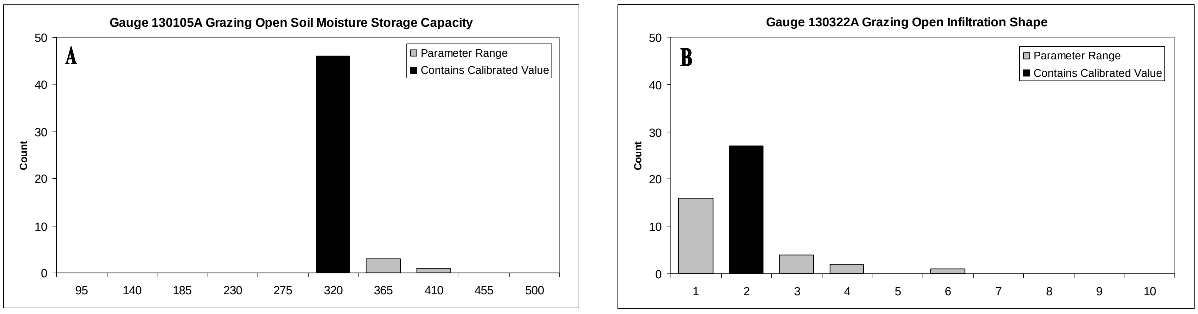

Figure 5. Frequency histograms representing the range of values for individual parameters within 50 calibrated realisations of parameter sets, categories that include the parameter value from the initial regularised calibration have a darker shading. Parameters represented range from a 'high' objective function sensitivity (A) to low objective function sensitivity (B).

The fact that observed flows were not always within calculated predictive uncertainty ranges shown in figure 6 is of some concern. Obviously, these ranges are not broad enough. The figure suggests that the Null Space Monte Carlo process should have allowed further parameter variability than was actually allowed (for example by specifying a higher objective function threshold at which calibration is deemed to occur, or by allowing broader pre-calibration probabilities for some or all parameters), or that features such as rainfall uncertainty within different parts of the catchment contribute more to the uncertainty of model predictions than does parameter uncertainty.

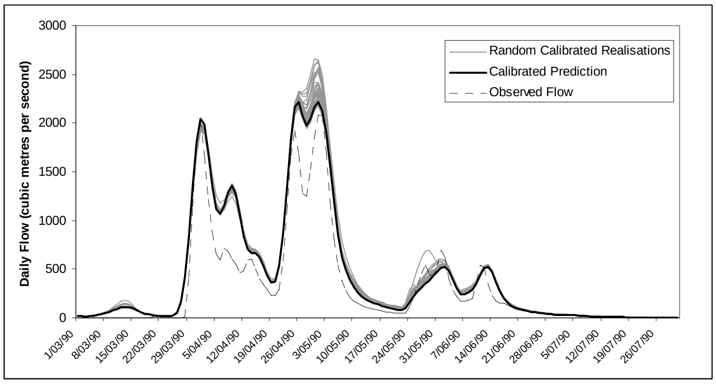

Figure 6. Model predicted daily flow (and observed daily flow) for gauge 130003AB for the period March – July 1990, including predictions from 50 calibrated parameter set

4.2. 'Beckers' Total Suspended Solids

Using null space projection a total of 133 random parameter sets that satisfied the calibration objective functions, considering both hydrology and TSS generation, were produced. As with the whole of Fitzroy hydrology analysis, the range and distribution of each parameter throughout the 133 realisations of parameter sets can be analysed and communicated. Figure 7 illustrates how model predictions (from the calibrated parameter sets and each of the realisations) of TSS concentration (and ultimately TSS load) at a given location may be graphically presented. Tabular summaries and statistics can also be utilised in this analysis and communication process. The fact that observed TSS levels are within predictive confidence bands is pleasing to note.

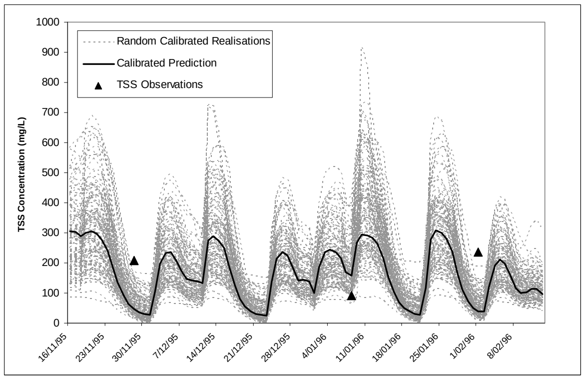

Figure 7. Daily model predictions of TSS concentration at gauge 130324A between November 1995 and March 1996. Model predictions are made from the calibrated parameter set and 133 random parameter sets that also satisfy the calibration objective function.

5. CONCLUSIONS

By calibrating model parameters within the WaterCAST environment, rather than in a secondary environment like the Rainfall Runoff Library, the calibration was able to consider all internal interactions.

This has resulted in a statistical fit that is a clear improvement. Calibrating parameters in such a way currently requires the use of optimsation software, such as PEST. The use of Tikhonov regularisation and singular value decomposition means that PEST, when used in this manner, will employ less complete model runs than other comparative techniques. The predictive analysis provided by PEST's Null Space Monte Carlo capability also provides a quantitative assessment of parameter and prediction uncertainty.

The use of Tikhonov regularisation to adhere closely to a supplied set of 'preferred' parameter values has forced the modellers to more critically review the existing data and knowledge pertaining to the system being represented. The modellers can also be satisfied that this knowledge has been considered in the calibration process The use of SVD-Assist and 'super parameters' has informed the modellers about parameter sensitivity in a way that was previously unavailable in this environment. The application of null space projection to random parameter sets has allowed a quantifiable range of parameters and model predictions to be rapidly produced and assessed for uncertainty analysis. While predictive uncertainty may have been underestimated in one of the examples presented above, the method can easily allow for greater uncertainty simply through 'loosening' calibration constraints and by allowing for greater parameter variability than was allowed.

This uncertainty analysis technique introduces a degree of subjectivity into the process. The modeller must supply estimates of likely parameter distributions prior to the production of random parameter sets. Also, to minimise the computational burden of multiple random parameter set re-calibration the modeller may decide under-estimate the dimensionality of the null space when setting up the null space projection process through which multiple calibration-constrained parameter sets are obtained. In doing so, the potential for parameter and predictive variability may be reduced (at the same time that computational efficiency is increased). This is likely to have occurred in the hydrologic analysis of the whole Fitzroy Catchment presented in this study. However, despite these subjectivities and simplifications, the resulting uncertainty analysis is transparent, quantifiable, readily communicable and applicable at the scale at which this type of water quality model informs land management decisions.

REFERENCES

Argent, R.M., Brown, A., Cetin, L.T., Davis, G., Farthing, B., Fowler, K., Freebairn, A., Grayson, R., Jordan, P.W., Moodie, K., Murray, N., Perraud, J-M, Podger, G.M., Rahman, J., Waters, D. (2008) WaterCAST User Guide, eWater CRC, Canberra.

Boughton, W.C. (1993). A hydrograph-based model for estimating water yield of ungauged catchments. Institute of Engineers Australia National Conference. Publication. 93/14, 317-324.

Chiew, F.H.S, Peel, M.C., and Western, A.W. (2002). Application and testing of the simple rainfall-runoff model SIMHYD. In: Mathematical Models of Small Watershed Hydrology and Applications (Editors: V.P. Singh and D.K. Frevert), Water Resources Publication, Littleton, Colorado, pp. 335 -367.

Department of Natural Resources and Water (2006). Fitzroy Basin Resource Operations Plan. Queensland Department of Natural Resources and Water, Brisbane, Australia.

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

Doherty, J. (2009). PEST: Model-Independent Parameter Estimation. Watermark Numerical Computing, Brisbane, Australia. http://www.sspa.com/pest

Grayson, R.B., Argent, R.M., Nathan, R.J, McMahon, T.A., and Mein, R.G. (1996). Hydrological Recipes – Estimation Techniques in Australian Hydrology. Cooperative Research Centre for Catchment Hydrology.

Laurenson, E.M. and Mein, R.G. (1997). RORB – Version 4, Runoff routing program - User Manual, second edition, Department of Civil Engineering, Monash University / Montech Pty. Ltd., Melbourne.

Podger, G., (2004). RRL Rainfall Runoff Library users guide. Cooperative Research Centre for Catchment Hydrology. Available from http://www.toolkit.net.au

SILO (2004). The SILO Data Drill. Queensland Department of Natural Resources and Mines. Available from http://www.longpaddock.qld.gov.au/silo.

Tikhonov, A.N, and Arsenin, V.Y. (1977). Solutions of Ill-posed Problems. V.H. Winston and Sons.

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.

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