

A Particle Filter for Efficient Recursive BATEA Analysis of Hydrological Models

Amanda K. Newman

BE (Hons-1)

*A thesis submitted for the degree of
Doctor of Philosophy*



THE UNIVERSITY OF
NEWCASTLE
AUSTRALIA

June 2016

STATEMENT OF ORIGINALITY

The thesis contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by any other person, except where due reference has been made in the text. I give consent to the final version of my thesis being made available worldwide when deposited in the University's Digital Repository, subject to the provisions of the Copyright Act 1968.

Amanda K. Newman

STATEMENT OF AUTHORSHIP

I hereby certify that the work embodied in this thesis contains a published paper/s/scholarly work of which I am a joint author. I have included as part of the thesis a written statement, endorsed by my supervisor, attesting to my contribution to the joint publication/s/scholarly work.

The publication/s/scholarly work consists of two conference papers, listed below.

Newman A., Kuczera G. and Kavetski D., (2012), ‘Towards a Recursive Bayesian Total Error Analysis Framework’, *34th Hydrology and Water Resources Symposium*, Sydney, Engineers Australia

Newman A., Kuczera G. and Kavetski D., (2015), ‘Application of particle filtering methods to a conceptual rainfall-runoff model’, *36th Hydrology and Water Resources Symposium*, Hobart, Engineers Australia

Prof. George A. Kuczera
Supervisor

ACKNOWLEDGEMENTS

This thesis has only been made possible through the support and advice of family, friends and colleagues.

To my supervisors, George Kuczera and Dmitri Kavetski, thank you for all your support, assistance, guidance and patience. In particular, thank you George for being so willing to work with and around my vision problems – your willingness to do so has been invaluable.

To my fellow PhD candidates, thank you for your friendship, support, advice and the fun escapes. Thank you also to the academic staff within the Water & Environmental Engineering group for your interest, encouragement and the opportunities for experience you have provided. A special thanks to Dr. Dominik Jaskierniak for allowing me to access your computing resources while you were on holidays. Thank you also to the administrative staff in the School of Engineering.

To my parents, Margaret and Geoff, and my sister Heather, thank you for always being interested in my research. Keith, thank you for your love, patience and understanding during the past 6 ½ years; I appreciate you allowing me to acquire your desktop computer for running my simulations. Without the support and encouragement the four of you have provided, this work would not have been possible.

TABLE OF CONTENTS

Abstract	xxvi
Chapter 1: Introduction	1
1.1 Motivation	1
1.2 Objectives of Thesis	2
1.3 Outline of Thesis	3
Chapter 2: Hydrological Modelling and Calibration	7
2.1 Overview of the CHM System	9
2.2 The Structure of CHMs	11
2.3 Calibration of CHMs	13
2.4 Challenges of Calibration	15
2.5 Representations of Error	17
2.5.1 Aggregated error approach	18
2.5.2 Decompositional error approach	20
2.6 Concluding Remarks	21
Chapter 3: The Bayesian Total Error Analysis Framework	23
3.1 What is the BATEA Framework?	23
3.2 Applying BATEA to CHMs	32
3.3 Current Implementation of the BATEA Framework	35
3.4 Recursive Formulation of the BATEA Framework	39
Chapter 4: Recursive Estimation Methods	43
4.1 The State-space Model	43
4.1.1 The CHM as a state-space model	44
4.1.2 Bayesian recursive estimation of the state-space model	49
4.1.3 Equivalence of BATEA inference and Bayesian recursive estimation of the state-space model	50
4.2 Kalman Filter Solutions to the State-space Model	52

4.2.1 The Kalman filter.....	52
4.2.2 The extended Kalman filter	54
4.2.3 The unscented Kalman filter	55
4.2.4 The ensemble Kalman filter	57
4.2.5 Summary of Kalman filtering solutions	59
4.3 Particle Filter Solutions to the State-space Model	59
4.3.1 Sequential Importance Sampling.....	60
4.4 Overcoming the Shortcomings of SIS	64
4.4.1 Kernel approximations	65
4.4.2 Using MCMC to refresh particles	69
4.5 Gap Analysis	81
Chapter 5: Recursive BATEA Inference.....	85
5.1 The Generic Particle Filter Algorithm	85
5.2 Dealing With Constraints: The Role of Truncated Distributions	88
5.2.1 The truncated distribution.....	89
5.2.2 The truncation constant, the importance ratio and the MCMC acceptance probability.....	90
5.2.3 Example – generating uniform samples from a Gaussian proposal	91
5.3 Importance Sampling Step: Selection of a Robust Proposal.....	96
5.4 The MCMC Regeneration Step: Approximating the Posterior-prior.....	102
5.4.1 Parametric approximation to the posterior-prior	104
5.4.2 Kernel approximation	105
5.4.3 Selection of the preferred approximation method	105
5.5 Constructing the Kernel Approximation.....	107
5.5.1 The kernel density	108
5.5.2 Bandwidth selection	111
5.5.3 Problems with the kernel approximation.....	113

5.6 The Adopted Approximation to the Posterior-prior.....	116
5.7 Selection of MCMC Regeneration Proposal.....	117
5.7.1 Regeneration of latent states only.....	117
5.7.2 Regeneration of latent states and time-invariant parameters.....	119
5.7.3 Recommended proposals.....	123
5.8 Proposed Particle Filter.....	124
5.9 Concluding Remarks.....	126
Chapter 6: Design of Numerical Experiments to Evaluate the Particle Filter	127
6.1 Experimental Design.....	128
6.1.1 Generation of synthetic datasets.....	128
6.1.2 Assessment of approximations to the posterior-prior.....	128
6.1.3 Case study performance metrics.....	129
6.2 Selection of a Representative CHM.....	137
6.3 Selection of Error Models.....	141
6.4 The Datasets.....	144
6.5 The Case Studies.....	147
Chapter 7: Evaluation of Regeneration Schemes and Posterior-prior Approximations	149
7.1 Comparison of Approximations to the Posterior-prior and Selection of Regeneration Rule.....	150
7.1.1 Reference particle filter solution.....	152
7.1.2 Independent Gaussian posterior-prior approximation.....	154
7.1.3 Correlated Gaussian posterior-prior approximation.....	158
7.1.4 Epanechnikov kernel approximation to the posterior-prior using Scott bandwidth.....	164
7.1.5 Epanechnikov kernel approximation to the posterior-prior using Silverman bandwidth	169

7.1.6 Gaussian kernel approximation to the posterior-prior using Scott bandwidth.....	172
7.1.7 Gaussian kernel approximation to the posterior-prior using Silverman bandwidth.....	174
7.1.8 Conclusions: approximation of the posterior-prior	176
7.2 Guidance on the Selection of the Regeneration Rule	178
7.3 Sensitivity of PF-ESc Filter to Regeneration Threshold.....	183
7.4 Comparison of Different MCMC Proposals to Regenerate Parameters ...	206
7.4.1 Regeneration of θ and x_{t-1}	207
7.4.2 Regeneration of θ assuming the posterior-prior θ and x_{t-1} are independent	209
7.4.3 Regeneration of θ assuming the posterior-prior θ and x_{t-1} are correlated	212
7.4.4 Comparison of regeneration approaches	215
7.5 Concluding Remarks	218
Chapter 8: Proof of Concept Evaluation	223
8.1 Inferring Time-invariant Model Parameters	224
8.1.1 Diagnostics for <i>CAP</i>	225
8.1.2 Diagnostics for <i>BFI</i>	228
8.1.3 Diagnostics for <i>KB</i>	229
8.2 Inferring Structural Error	232
8.3 Processing Corrupted Forcing	249
8.4 Inferring Error Model Parameters	258
8.5 The Full BATEA Analysis.....	264
8.5.1 Inference of the time-invariant parameters.....	264
8.5.2 Inference of the structural errors	299
8.5.3 Inference of the discharge.....	313
8.5.4 Inference of rainfall	321

8.5.5 Features of the joint parameter and latent posterior	326
8.5.6 Concluding remarks: recursive BATEA analysis.....	331
8.6 A Qualitative Comparison of Batch and Recursive BATEA.....	333
8.7 Concluding Remarks	336
Chapter 9: Conclusions	339
9.1 Development of the Recursive BATEA Framework	339
9.2 Performance of the Recursive BATEA Framework	343
9.3 Future Work	345
9.3.1 Further testing of the kernel approximation to the posterior-prior	345
9.3.2 Further examination of regeneration rules.....	346
9.3.3 Extension of the recursive BATEA framework to different model structures	346
9.3.4 Testing inference of rainfall error model parameters	348
9.3.5 Application of the recursive BATEA framework to real data case studies.....	348
9.4 Concluding Remarks	349
References.....	351

LIST OF ALGORITHMS

Algorithm 4.1: Assimilation of observations using the SIS filter.....	63
Algorithm 4.2: Sampling from a kernel approximation.....	67
Algorithm 4.3: Particle MCMC (Andrieu, Doucet & Holenstein 2010; Duckworth 2012) with Metropolis-Hastings algorithm (Chib & Greenberg 1995).....	72
Algorithm 4.4: Resample-move filter (Berzuini & Gilks 2001; Gilks & Berzuini 2001) with sampling from a Markov transition kernel performed using the Metropolis-Hastings algorithm (Chib & Greenberg 1995).....	73
Algorithm 4.5: Particle-DREAM (Vrugt et al. 2013).	75
Algorithm 4.6: SMC ² (Chopin, Jacob & Papaspiliopoulos 2013).	77
Algorithm 4.7: Particle filter proposed by Moradkhani, DeChant and Sorooshian (2012).	79
Algorithm 5.1: The generic particle filter.	86
Algorithm 5.2: The Metropolis-Hastings algorithm (Chib & Greenberg 1995).....	87
Algorithm 5.3: Sampling from the Epanechnikov kernel.	109
Algorithm 5.4: Proposed particle filter.	125
Algorithm 6.1: Generation of synthetic data replicate.	128
Algorithm 7.1: Generation of a representative synthetic dataset.	179
Algorithm 7.2: Procedure for selection of regeneration rule by quick assessment.....	182
Algorithm 7.3: Procedure for selection of regeneration rule by full assessment.	183
Algorithm 9.1: Proposed particle filtering algorithm.....	341

LIST OF FIGURES

Figure 1.1: Major components of the thesis and their linkage.....	3
Figure 2.1: The CHM system.....	10
Figure 2.2: Common building blocks of CHMs: (a) reservoir, (b) lag function, (c) splitting junction and (d) union junction.	11
Figure 2.3: Schematic of the AWBM, after Boughton (2004).....	13
Figure 2.4: Sources of uncertainty (shaded) within the CHM system.	18
Figure 3.1: The BATEA perspective on sources of uncertainty (shaded) within the CHM system.....	32
Figure 3.2: CPU time to generate 10,000 MCMC samples from the BATEA posterior of GR4J as a function of the calibration data length (Kuczera et al. 2010a)....	37
Figure 4.1: Particle representation of a density.....	59
Figure 4.2: Illustration of a kernel approximation to a density.....	66
Figure 4.3: The effect of bandwidth on the kernel approximation – large bandwidth (black dotted), small bandwidth (blue solid).....	67
Figure 5.1: Relationship between the μ , σ and truncation constant of the Gaussian distribution bounded over the region $[0,1]$	93
Figure 5.2: Comparison of density estimates from generated Markov chains.....	94
Figure 5.3: Approximations to a correlated bivariate lognormal distribution: (top) series of independent Gaussians; (centre) correlated Gaussian; and (lower) a kernel approximation.....	106
Figure 5.4: The effect of bandwidth on the kernel approximation – large bandwidth (black dotted), small bandwidth (blue solid).....	111
Figure 5.5: Comparison of bandwidth scale factors.	113
Figure 6.1: A sample ensemble time-series plot for a time-invariant parameter.....	130
Figure 6.2: A sample marginal histogram plot.	132
Figure 6.3: Interpretation of the predictive QQ plot adapted from Laio and Tamea (2007) and Thyer et al. (2009).	135
Figure 6.4: A sample standardised bias plot and the corresponding QQ plot.....	137

Figure 6.5: Schematic of the AWBM, after Boughton (2004).....	138
Figure 6.6: True rainfall and ET series for all datasets (upper panel). True response for datasets DQP05 and DQP20 (lower panel).	145
Figure 6.7: Partial autocorrelation coefficients for SS_t and BS_t for the 26 DQS datasets.	146
Figure 7.1: Ensemble time-series for the PF-N filter (no parameter regeneration).	153
Figure 7.2: Precipitation density estimates for the PF-N filter (no parameter regeneration) at selected observations.....	154
Figure 7.3: Streamflow ensemble time-series for the PF-N filter (no parameter regeneration).....	154
Figure 7.4: Ensemble time-series for the PF-IG filter with regeneration rule A100. ...	155
Figure 7.5: Streamflow time-series for the PF-IG filter with regeneration rule A100..	156
Figure 7.6: Streamflow time-series for the PF-IG filter with regeneration rule C50....	156
Figure 7.7: Ensemble time-series for the PF-IG filter with regeneration rule C50.	157
Figure 7.8: Comparison of 100,000 samples from the independent Gaussian approximation (black) to the 1,000,000 PF-N posterior samples (red) for observation 2.	158
Figure 7.9: Ensemble time-series for the PF-CG filter with regeneration rule A100...	159
Figure 7.10: Streamflow time-series for the PF-CG filter with regeneration rule A100.	160
Figure 7.11: Ensemble time-series for the PF-CG filter with regeneration rule C50. ..	161
Figure 7.12: Streamflow time-series for the PF-CG filter with regeneration rule C50..	162
Figure 7.13: Precipitation density estimates for the PF-CG filter with regeneration rule C50 at selected observations.	162
Figure 7.14: Comparison of 100,000 samples from the Gaussian approximation (black) to the 1,000,000 PF-N posterior samples (red) for the observation 2.	163

Figure 7.15: Ensemble time-series for the PF-ESc filter with regeneration rule A100..	164
Figure 7.16: Streamflow time-series for the PF-ESc filter with regeneration rule A100.	165
Figure 7.17: Streamflow time-series for the PF-ESc filter with regeneration rule C50.	165
Figure 7.18: Ensemble time-series for the PF-ESc filter with regeneration rule C50....	166
Figure 7.19: Precipitation density estimates for the PF-ESc filter with regeneration rule C50 at selected observations.	167
Figure 7.20: Comparison of 100,000 samples from the Epanechnikov kernel approximation using Scott (1979) bandwidth (black) to the 1,000,000 PF-N posterior samples (red) for observation 2.....	168
Figure 7.21: Marginal posterior slice of KB and BS at observation 2 illustrating approximation of densities with a curved axis.	169
Figure 7.22: Ensemble time-series for the PF-ESm filter with regeneration rule A100.	170
Figure 7.23: Ensemble time-series for the PF-ESm filter with regeneration rule C50..	171
Figure 7.24: Ensemble time-series for the PF-GSc filter with regeneration rule A100.	173
Figure 7.25: Ensemble time-series for the PF-GSc filter with regeneration rule C50...	174
Figure 7.26: Ensemble time-series for the PF-GSm filter with regeneration rule A100.	175
Figure 7.27: Ensemble time-series for the PF-GSm filter with regeneration rule C50..	176

Figure 7.28: Example ensemble time-series plots of CAP illustrating (a) excessive regeneration (CS4-P20 replicate 1 with regeneration rule A100); and (b) acceptable regeneration where the filter mean does not converge to the true parameter (CS9-P20 replicate 20 and regeneration rule given in Table 8.1).	181
Figure 7.29: Comparison of inference of rainfall event 34.....	187
Figure 7.30: Comparison of inference of rainfall event 100.....	188
Figure 7.31: Comparison of inference of rainfall event 251.....	189
Figure 7.32: CAP time-series for regeneration rules A10 to A70.....	191
Figure 7.33: CAP time-series for regeneration rules B10 to B70.....	192
Figure 7.34: CAP time-series for regeneration rules C10 to C70.....	193
Figure 7.35: CAP time-series for regeneration rules K10 to K70.....	194
Figure 7.36: Marginal histogram of CAP at observation 50.....	197
Figure 7.37: Marginal histogram of CAP at observation 100.....	198
Figure 7.38: Marginal histogram of CAP at observation 150.....	199
Figure 7.39: Marginal histogram of CAP at observation 200.....	200
Figure 7.40: Marginal histogram of CAP at observation 250.....	201
Figure 7.41: Marginal histogram of CAP at observation 300.....	202
Figure 7.42: Marginal histogram of CAP at observation 350.....	203
Figure 7.43: Marginal histogram of CAP at observation 400.....	204
Figure 7.44: Partial streamflow time series for joint regeneration of θ and x_{t-1}	208
Figure 7.45: Ensemble time series for joint regeneration of θ and x_{t-1}	209
Figure 7.46: Partial streamflow time series for regeneration of θ assuming independence from x_{t-1}	211
Figure 7.47: Ensemble time series for regeneration of θ assuming independence from x_{t-1}	212
Figure 7.48: Ensemble time series for regeneration of θ allowing for correlation with x_{t-1}	214

Figure 7.49: Partial streamflow time series for regeneration of θ allowing for correlation with x_{t-1}	214
Figure 7.50: Inference of rainfall during selected rainfall events. Regeneration approach: (a) regeneration of θ and x_{t-1} , (b) assume independence between θ and x_{t-1} , (c) assume correlation between θ and x_{t-1}	216
Figure 7.51: Distribution of CAP at selected observations. Regeneration approach: (a) regeneration of θ and x_{t-1} , (b) independent θ and x_{t-1} , (c) correlated θ and x_{t-1}	217
Figure 8.1: Predictive QQ plot of CAP after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	226
Figure 8.2: Standardised bias of CAP after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	226
Figure 8.3: Predictive QQ plot of BFI after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	228
Figure 8.4: Standardised bias of BFI after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	229
Figure 8.5: Predictive QQ plot of KB after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	230
Figure 8.6: Standardised bias of KB after assimilation of observation 400. Case study: (a) CS4-P20; (b) CS5; (c) CS6-P05; (d) CS6-P20; (e) CS9-P05; and (f) CS9-P20.	231
Figure 8.7: Marginal parameter histogram plot for CS9-P20 replicate 14 after assimilation of observation 300.....	232
Figure 8.8: Predictive QQ plot of SS_t for CS1. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	234

Figure 8.9: Standardised bias of SS_t for CS1. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	234
Figure 8.10: Predictive QQ plot of BS_t for CS1. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	234
Figure 8.11: Standardised bias of BS_t for CS1. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	235
Figure 8.12: Predictive QQ plot of BS_t for CS3. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	236
Figure 8.13: Predictive QQ plot of SS_t for CS3. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	236
Figure 8.14: Standardised bias of SS_t for CS3. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	237
Figure 8.15: Predictive QQ plot of SS_t for CS5. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	238
Figure 8.16: Standardised bias of SS_t for CS5. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	238
Figure 8.17: Predictive QQ plot of BS_t for CS5. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	238
Figure 8.18: Standardised bias of BS_t for CS5. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	239
Figure 8.19: Predictive QQ plot of BS_t for CS6. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	240
Figure 8.20: Predictive QQ plot of SS_t for CS6. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	240

Figure 8.21: Standardised bias of SS_t for CS6. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	241
Figure 8.22: Predictive QQ plot of SS_t for CS7. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	242
Figure 8.23: Standardised bias of SS_t for CS7. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	242
Figure 8.24: Predictive QQ plot of BS_t for CS7. Observation: (a) 100, (b) 200, (c) 300 and (d) 400.	242
Figure 8.25: Predictive QQ plot of SS_t for CS8. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	244
Figure 8.26: Standardised bias of SS_t for CS8. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	244
Figure 8.27: Predictive QQ plot of BS_t for CS8. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	245
Figure 8.28: Predictive QQ plot of SS_t for CS9. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	246
Figure 8.29: Standardised bias of SS_t for CS9. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	247
Figure 8.30: Predictive QQ plot of BS_t for CS9. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	247
Figure 8.31: Standardised bias of BS_t for CS9. Observation: (a) 100, (b) 200, (c) 300 and (d) 400 for input series P05 and (e) 100, (f) 200, (g) 300 and (h) 400 for input series P20.	248

Figure 8.32: Rainfall inference at observation 33 (top) and 184 (bottom) for replicate 2. Inference problem: (a) CS2-P05 (known CHM parameters), (b) CS2-P20 (known CHM parameters), (c) CS4-P05 (unknown CHM parameters), and (d) CS4-P20 (unknown CHM parameters).....	251
Figure 8.33: Rainfall inference at selected observations for replicate 2. Inference problem: (a) CS2-P05, (b) CS2-P20.	251
Figure 8.34: Predictive QQ plot of rainfall for CS2. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	253
Figure 8.35: Standardised bias of rainfall for CS2. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	254
Figure 8.36: Predictive QQ plot of rainfall for CS4. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	255
Figure 8.37: Standardised bias of rainfall for CS4. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	255
Figure 8.38: Predictive QQ plot of rainfall for CS3. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	256
Figure 8.39: Predictive QQ plot of rainfall for CS6. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	256
Figure 8.40: Predictive QQ plot of rainfall for CS8. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	257
Figure 8.41: Predictive QQ plot of rainfall for CS9. Observation: (a) 34, (b) 100, (c) 174 and (d) 251. Rainfall error model: (i) P05, and (ii) P20.....	257
Figure 8.42: Comparison of true (black solid) and mean filtered (red dashed) SS_t structural error density when: (a) SS_t is near a bound; and (b) truncation is insignificant.....	260
Figure 8.43: Predictive QQ plot of σ_{SS} at observation 400. Case study: (a) CS7, (b) CS8- P05, (c) CS8-P20, (d) CS9-P05 and (e) CS9-P20.....	260
Figure 8.44: Standardised bias of σ_{SS} at observation 400. Case study: (a) CS7, (b) CS8- P05, (c) CS8-P20, (d) CS9-P05 and (e) CS9-P20.....	261

Figure 8.45: Predictive QQ plot of σ_{BS} at observation 400. Case study: (a) CS7, (b) CS8-P05, (c) CS8-P20, (d) CS9-P05 and (e) CS9-P20.....	262
Figure 8.46: Standardised bias of σ_{BS} at observation 400. Case study: (a) CS7, (b) CS8-P05, (c) CS8-P20, (d) CS9-P05 and (e) CS9-P20.	263
Figure 8.47: Comparison of true (black solid), mean filtered CS9-P05 (red dashed) and mean filtered CS9-P20 (blue dot-dash) BS_t structural error density when: (a) BS_t is near a bound; and (b) truncation is insignificant.	263
Figure 8.48: Predictive QQ plot of CAP for CS9-P05 at selected observations.....	266
Figure 8.49: Predictive QQ plot of CAP for CS9-P20 at selected observations.....	267
Figure 8.50: Standardised bias of CAP at selected observations for CS9-P05.....	267
Figure 8.51: Standardised bias of CAP at selected observations for CS9-P20.....	268
Figure 8.52: CS9-P05 ensemble time-series for CAP replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	269
Figure 8.53: CS9-P20 ensemble time-series for CAP replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	270
Figure 8.54: CS9-P05 marginal histograms of CAP. Replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	271
Figure 8.55: CS9-P20 marginal histograms of CAP. Replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	272
Figure 8.56: Predictive QQ plot of BFI for CS9-P05 at selected observations.	274
Figure 8.57: Predictive QQ plot of BFI for CS9-P20 at selected observations.	275
Figure 8.58: Standardised bias of BFI at selected observations for CS9-P05.	275
Figure 8.59: Standardised bias of BFI at selected observations for CS9-P20.	276
Figure 8.60: CS9-P05 ensemble time-series for BFI replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	277
Figure 8.61: CS9-P20 ensemble time-series for BFI replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	278
Figure 8.62: Predictive QQ plot of KB for CS9-P05 at selected observations.....	280
Figure 8.63: Predictive QQ plot of KB for CS9-P20 at selected observations.....	280

Figure 8.64: Standardised bias of KB at selected observations for CS9-P05.	281
Figure 8.65: Standardised bias of KB at selected observations for CS9-P20.	281
Figure 8.66: CS9-P05 ensemble time-series for KB replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	282
Figure 8.67: CS9-P20 ensemble time-series for KB replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	283
Figure 8.68: Predictive QQ plot of σ_{SS} for CS9-P05 at selected observations.	285
Figure 8.69: Predictive QQ plot of σ_{SS} for CS9-P20 at selected observations.	286
Figure 8.70: Standardised bias of σ_{SS} at selected observations for CS9-P05.	286
Figure 8.71: Standardised bias of σ_{SS} at selected observations for CS9-P20.	287
Figure 8.72: CS9-P05 ensemble time-series for σ_{SS} replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	288
Figure 8.73: CS9-P20 ensemble time-series for σ_{SS} replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	289
Figure 8.74: Predictive QQ plot of σ_{BS} for CS9-P05 at selected observations.	291
Figure 8.75: Predictive QQ plot of σ_{BS} for CS9-P20 at selected observations.	292
Figure 8.76: Standardised bias of σ_{BS} at selected observations for CS9-P05.	292
Figure 8.77: Standardised bias of σ_{BS} at selected observations for CS9-P20.	293
Figure 8.78: CS9-P05 ensemble time-series for σ_{BS} replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	294
Figure 8.79: CS9-P20 ensemble time-series for σ_{BS} replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	295
Figure 8.80: Marginal posterior histograms at observation 400 for CS9-P05 replicate 7.	296
Figure 8.81: Marginal posterior histograms at observation 400 for CS9-P05 replicate 20.	297
Figure 8.82: Marginal posterior histograms at observation 400 for CS9-P20 replicate 1.	297

Figure 8.83: Marginal posterior histograms at observation 400 for CS9-P20 replicate 26.	298
Figure 8.84: Predictive QQ plot of SS_t for CS9-P05 at selected observations.	301
Figure 8.85: Predictive QQ plot of SS_t for CS9-P20 at selected observations.	301
Figure 8.86: Standardised bias of SS_t at selected observations for CS9-P05.	302
Figure 8.87: Standardised bias of SS_t at selected observations for CS9-P20.	302
Figure 8.88: CS9-P05 ensemble time-series for SS_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	303
Figure 8.89: CS9-P20 ensemble time-series for SS_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	304
Figure 8.90: Predictive QQ plot of BS_t for CS9-P05 at selected observations.	306
Figure 8.91: Predictive QQ plot of BS_t for CS9-P20 at selected observations.	307
Figure 8.92: Standardised bias of BS_t at selected observations for CS9-P05.	307
Figure 8.93: Standardised bias of BS_t at selected observations for CS9-P20.	308
Figure 8.94: CS9-P05 ensemble time-series for BS_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	309
Figure 8.95: CS9-P20 ensemble time-series for BS_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	310
Figure 8.96: Marginal posterior histograms at observation 75 for CS9-P20 replicate 26.	311
Figure 8.97: Marginal posterior histograms at observation 138 (2 observations after a quickflow event) for CS9-P20 replicate 26.....	312
Figure 8.98: Marginal posterior histograms at observation 400 for CS9-P20 replicate 26.	312
Figure 8.99: Predictive QQ plot of Q_t for CS9-P05 at selected observations.	315
Figure 8.100: Predictive QQ plot of Q_t for CS9-P20 at selected observations.	315
Figure 8.101: CS9-P05 ensemble time-series for Q_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	316

Figure 8.102: CS9-P20 ensemble time-series for Q_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	317
Figure 8.103: CS9-P05 ensemble time-series for Q_t between observations 150 and 250. Replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	319
Figure 8.104: CS9-P20 ensemble time-series for Q_t between observations 150 and 250. Replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.	320
Figure 8.105: Predictive QQ plot of P_t for CS9-P05 at selected observations.....	322
Figure 8.106: Predictive QQ plot of P_t for CS9-P20 at selected observations.	323
Figure 8.107: CS9-P05 marginal histograms for P_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	324
Figure 8.108: CS9-P20 marginal histograms for P_t replicate (a) 1, (b) 7, (c) 14, (d) 20, and (e) 26.....	325
Figure 8.109: Marginal posterior histograms at observation 35 for CS9-P05 replicate 26.	327
Figure 8.110: Marginal posterior histograms at observation 50 for CS9-P20 replicate 20.	328
Figure 8.111: Marginal posterior histograms at observation 93 for CS9-P05 replicate 20.	329
Figure 8.112: Marginal posterior histograms at observation 150 for CS9-P20 replicate 14.....	330
Figure 8.113: Marginal posterior histograms at observation 400 for CS9-P20 replicate 26.....	331

LIST OF TABLES

Table 4.1: Summary of combined particle and MCMC approaches.....	81
Table 5.1: Average variance ratio for the samples drawn from the kernel approximation. * indicates a value in equation (5.51) using the recommended bandwidth h	115
Table 6.1: True model parameters and prior distributions for the synthetic studies....	141
Table 6.2: Error model parameters used to generate the synthetic data.....	143
Table 6.3: Synthetic datasets.....	145
Table 6.4: Synthetic case studies.	148
Table 7.1: Regeneration trigger levels.	151
Table 7.2: Regeneration rules for sensitivity assessment of the PF-ESc filter.	184
Table 7.3: Regeneration frequency data for regeneration rules.	185
Table 7.4: Impoverishment measures for CAP for the PF-ESc and PF-N filters. The resolution is provided in brackets.....	196
Table 7.5: Time taken to assimilate the observed data series.	215
Table 8.1: Regeneration control parameters used for the case studies.	223
Table 8.2: Posterior parameter moments at observation 400. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates. Prior mean and standard deviation provided for comparison.....	225
Table 8.3: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS1.	234
Table 8.4: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS3.	237
Table 8.5: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS5.	239

Table 8.6: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS6.	241
Table 8.7: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS7.	243
Table 8.8: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS8.	245
Table 8.9: Posterior structural error moments at selected observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates of CS9.	248
Table 8.10: Posterior rainfall moments at selected quickflow observations. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates. True rainfall is provided for comparison.	252
Table 8.11: Posterior structural error standard deviation moments at observation 400. The mean and standard deviation (shown in brackets) of each statistic is the calculated from the filtered statistics of all replicates. Prior mean and standard deviation provided for comparison.	259
Table 8.12: Average and standard deviation (in brackets) of posterior filtered moments for CAP at selected observations. The prior is provided for comparison.	265
Table 8.13: Average and standard deviation (in brackets) of posterior filtered moments for BFI at selected observations. The prior is provided for comparison.	273
Table 8.14: Average and standard deviation (in brackets) of posterior filtered moments for KB at selected observations. The prior is provided for comparison.	279
Table 8.15: Average and standard deviation (in brackets) of posterior filtered moments for σ_{SS} at selected observations. The prior is provided for comparison.	284
Table 8.16: Average and standard deviation (in brackets) of posterior filtered moments for σ_{BS} at selected observations. The prior is provided for comparison.	290

Table 8.17: Average and standard deviation (in brackets) of posterior filtered moments for SS_t at selected observations. The statistics of the true SS_t are provided for comparison.	299
Table 8.18: Average and standard deviation (in brackets) of posterior filtered moments for BS_t at selected observations. The statistics of the true BS_t are provided for comparison.	305
Table 8.19: Average and standard deviation (in brackets) of posterior filtered moments for Q_t at selected observations. The statistics of the true Q_t are provided for comparison.	314
Table 8.20: Average and standard deviation (in brackets) of posterior filtered moments for P_t at selected observations. The true P_t are provided for comparison, with the number of replicates with observed quickflow.....	322

ABSTRACT

The Bayesian Total Error Analysis (BATEA) framework permits model calibration and prediction to be informed by estimates of data and model uncertainty, and allows assessment of the relative contribution of various sources of error to the total uncertainty within the conceptual hydrologic modelling system. However, full BATEA applications are presently limited to studies with relatively short record lengths. This is because batch calibration rapidly becomes computationally infeasible as the number of inferred input and/or model structural errors grows.

This thesis presents the development of a recursive implementation of the BATEA framework based on particle filtering techniques. Particle filtering techniques, traditionally used in automatic control and signal processing, are a group of sequential Monte Carlo methods which can be adapted to provide a robust recursive implementation of the BATEA framework within the non-linear and non-Gaussian conditions presented by conceptual hydrologic models. The particle filter developed in this thesis is designed to preserve the constraints and relationships between time-invariant parameters and latents which exist in most conceptual hydrologic models. This is achieved in a fully recursive manner through careful selection of appropriate Importance Sampling proposals, design and selection of Markov Chain Monte Carlo (MCMC) proposals which permit efficient regeneration of time-invariant parameters and the construction of an approximation to the Metropolis-Hasting acceptance probability which avoids the need for batch evaluation. The resulting particle filter is capable of efficiently performing an approximate recursive BATEA analysis for a conceptual hydrological model subject to observation, structural and parameter uncertainty with the parameters of both the error model and the hydrological model requiring inference. The performance of the approximate BATEA analysis technique is demonstrated with synthetic case studies ranging from well-posed to highly ill-posed problems and is shown to produce practically useful results at a small fraction of the computational effort required in batch calibration.