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Assimilating modelled dissolved inorganic nitrogen loads to monitored data using component-wise iterative ensemble Kalman inversion

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Abstract: Understanding the fate of dissolved inorganic nitrogen (DIN) sourced from land-based runoff is an important element in the development of strategies for managing water quality on the Great Barrier Reef (GBR). Direct measurement of the generation and transport of DIN from the landscape is impractical at large scale so most of the burden is deferred to water quality models (WQMs) that simulate catchment processes. Although WQMs are subject to uncertainty as most environmental models are, until recently WQMs designed to quantify nutrient, sediment and pesticide loads being discharged into the GBR lagoon have been deterministically calibrated with no reference to uncertainty. To properly assess the reliability and performance of WQMs they must be able to produce probabilistic predictions that correctly represent model uncertainty and Bayesian inference is an appealing framework for achieving this.

Although the principles of Bayesian inference can be succinctly expressed as Bayes' theorem, $f(\mathrm{M},\phi|\mathrm{d}) \propto f(\mathrm{d}|\mathrm{M},\phi) f(\mathrm{M},\phi)$, where M represents the model parameters, ϕ are parameters of the likelihood probability density function (pdf) and d some measured data, its application for WQMs can be challenging. In all but the most trivial cases, there is no practical way of symbolically deriving the posterior $f(\mathrm{M},\phi|\mathrm{d})$. In the absence of an analytical representation of the posterior, one may resort to Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) methods for sampling from the posterior. Although these stochastic processes are a *tour de force* that can yield high quality results, they require a large number of model evaluations to converge to an equilibrated solution.

Iterative ensemble Kalman inversion (IEKI) encompasses a family of algorithms, such as the ensemble randomized maximum likelihood method and ensemble smoother with multiple data assimilations that offer an efficient method for gradually propagating error statistics via an ensemble of model outputs to connect samples from the prior to an ensemble of posterior samples. The major advantage of these schemes is that they consume a fraction of the model evaluations that would be required otherwise and scale favorably with the dimensionality of the inverse problem. A major drawback of the ensemble methods in the current context is that in their formulation, they require that the likelihood $f(\mathrm{d}|\mathrm{M},\phi)$ is Gaussian and that the covariance, ϕ, is known. Unfortunately, measurement error statistics for water quality measurements used to inform the WQM calibration are difficult to derive and quite often unavailable. On the other hand, MCMC and SMC methods can infer the parametric likelihood given the data.

The authors recently introduced the component-wise IEKI (CW-IEKI) which hybridizes MCMC and IEKI by iteratively updating the model parameters, M, using an ensemble step followed by an MCMC step to adjust the likelihood parameters, ϕ. Since the MCMC step requires no further model evaluations, the algorithm offers efficiency comparable with conventional ensemble methods with the added benefit of likelihood parameter inference.

This paper presents the application of the CW-IEKI method to the problem of identifying parameters of a catchment scale DIN model. The results are discussed and found to compare satisfactorily to SMC on a number of model performance metrics.

Keywords: *Bayesian inference, Ensemble smoother, Sequential Monte Carlo sampling, Markov chain Monte Carlo sampling, Water quality model, Dissolved inorganic nitrogen.*

1. INTRODUCTION

Catchment water quality models (WQMs) have been aptly referred to as "over-parameterised, uncertain mathematical marionettes" (Wade et al., 2008). Typically, WQM epistemic uncertainty due to model structural deficiencies is compounded by noisy and sparse water quality monitoring data for quantification of model performance. Despite this, WQMs are valuable tools for supporting catchment management and policy. Fully informed decisions arising from WQM modeling results require not only the acknowledgment but also the quantification of the uncertainty inherent in the model's predictions

In most cases, model performance can be optimised by assimilating measurements from the field into the WQM to identify model parameters that provide the best possible description of the dynamical system and its uncertainty. Of the various options available, formulating the assimilation problem in a Bayesian inference framework is both a very popular and satisfying approach. Within the Bayesian *ansatz*, prior model parameters are conditioned on observed data to obtain the posterior probability using Baye's theorem which is simply expressed as

$$f(\mathrm{M}|\mathrm{d}) \propto f(\mathrm{d}|\mathrm{M})f(\mathrm{M}),$$

where M are the model parameters and $f(\mathrm{M})$ is the prior parameter probability density function (pdf). Measurement data, d, is incorporated via the likelihood term $f(\mathrm{d}|\mathrm{M})$. In the context of the WQM, the likelihood can be represented as

$$f(\mathrm{d}|\mathrm{M}) = f\big(\mathrm{d} - \mathrm{G}(\mathrm{M})\big) = f(\epsilon),$$

where $\mathrm{G}(\mathrm{M})$ is the model output using parameters M which means that something has to be known about the pdf of the measurement error, ϵ. If ϵ is known *a priori*, ensemble-based data assimilation methods such as iterative ensemble smoothers (IESs) can efficiently yield high quality approximations of the Bayesian posterior in many situations. Unfortunately, useful estimates of ϵ are rarely associated with water quality measurement data. Moreover, in the presence of imperfect models such as WQMs, ϵ doesn't entirely capture the likelihood since it ignores uncertainty due to model structural error.

Exact Bayesian inference can be carried out using Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) methods to sample from the posterior pdf including the parameters of the likelihood distribution, thus overcoming the limitation of the IES approach. However, MCMC can be a computationally expensive sampler due to the large number of model runs required to reach convergence, particularly when a large number of parameters are to be estimated. Even SMC sampling which can be considerably more robust than MCMC samplers and can also exploit parallel computing architecture (Dai et al., 2022) may still be of limited practicality for models with long computation times.

Recently, Botha *et al.* (2022) introduced the component-wise iterative ensemble Kalman inversion (CW-IEKI) method which seeks to bridge the gap between IES and Bayesian inference by allowing elements of ϵ to be inferred during the ensemble smoother iterations in a manner that adds negligibly to the computational costs.

This paper presents a case study of CW-IEKI applied to the problem of solving the inverse problem of identifying uncertain parameters of a catchment scale model for estimating dissolved inorganic nitrogen (DIN) stream loads. It is demonstrated that CW-IEKI results compare favorably with those obtained from SMC sampling. Assessment of the model performance by examining how well posterior predictive estimates represent measured loads indicate the CW-IEKI model satisfactorily forecasts DIN loads beyond the calibration period and very closely emulates the SMC results. This study extends earlier work investigating the use of IEKI methods for the uncertainty analysis of rainfall-runoff models and agricultural systems simulations (Bennett, 2021; Vilas et al., 2021).

2. METHODS

2.1. Component-Wise Iterative Ensemble Kalman Inversion

CW-IEKI can be thought of as an ensemble smoother that iteratively updates an ensemble of N_e parameter realisations of vector length N_m using the following equation given a vector of observations of length N_d:

$$\Delta\mathrm{M} \;=\; \mathrm{C}_{MD}\big(\mathrm{C}_{DD} + \alpha\Gamma(\phi)\big)^{-1}(\mathrm{D}_{uc} - \mathrm{D}).$$

Here, M is an $N_m \times N_e$ ensemble of model parameters and D is the $N_d \times N_e$ matrix of model outputs $\mathrm{G}(\mathrm{M})$. D_{uc} is an $N_d \times N_e$ perturbed measurement matrix whose rows are unconditioned samples of the measurement noise with covariance $\Gamma(\phi)$, and α is an inflation parameter that serves to temper the parameter step size. Using the zero-mean anomaly matrices $\Delta_M = (\mathrm{M} \ominus \overline{\mathrm{M}})/\sqrt{N_e - 1}$ and $\Delta_D = (\mathrm{D} \ominus \overline{\mathrm{D}})/\sqrt{N_e - 1}$ where $\overline{\mathrm{M}}$ and $\overline{\mathrm{D}}$ are the matrix means, the approximate sensitivity matrices can be constructed as $\mathrm{C}_{MD} = \Delta_M \Delta_D^{\mathrm{T}}$ and $\mathrm{C}_{DD} = \Delta_D \Delta_{\mathrm{D}}^{\mathrm{T}}$. Note, $\ominus$ is the broadcast subtraction operator. For the purposes of this paper, α is simply set to N_a, the number of assimilation iterations.

The innovation of the CW-IEKI is the way in which the measurement covariance is handled. The application of the canonical ensemble smoother with multiple data assimilation algorithm (Emerick and Reynolds, 2013) relies on the covariance Γ being known. By making the reasonable assumption that the model parameters M and the elements ϕ of Γ, can be treated independently, it is possible to use Bayesian inference to estimate ϕ at each iteration allowing Γ to evolve in a tempered fashion. In principle, the complexity of the structure of $\Gamma(\phi)$ is arbitrary with N_ϕ parameters but for the present case $\Gamma(\phi) = \phi \mathrm{I}$ with $N_\phi = 1$, where the $N_d \times N_d$ identity matrix, I, is used.

Algorithm 1 outlines the pseudocode for the CW-IEKI procedure showing the component-wise updating of M and ϕ at each assimilation step. It is worth noting that because ϕ is conditioned on M and the previously assembled D ensemble of model outputs, it requires no further evaluation of $\mathrm{G}(\cdot)$.

Algorithm 1 CW-IEKI

Input: $\mathrm{M}^f \in \Re^{N_m \times N_e}$, $\phi^f \in \Re^{N_\phi \times N_e}$ $d_{obs} \in \Re^{N_m \times 1}$; N_e sample drawn from the model parameter prior, N_e samples drawn from the error covariance parameter prior and the observation data vector

Output: The ensemble estimate of the Bayesian posterior of M and ϕ

Choose the number of assimilation steps, N_a, and inflation factors such that $\sum_{i=1}^{N_a} \frac{1}{\alpha_i} = 1$

$\mathrm{M}_0 \leftarrow \mathrm{M}^f$, $\phi_0 = \phi^f$; initialise M and ϕ

for $i = 1,\ldots, N_a$ **do**

$\mathrm{D}_{uc}^j \leftarrow d_{obs} + \sqrt{\alpha_i}\Gamma\left(\phi_{i-1}^j\right)^{1/2} z_d$ **;** perturb the observation vector for each ensemble member where $z_d \sim \mathcal{N}\left(0, \mathrm{I}_{N_d}\right)$

$\mathrm{D}_i^j \leftarrow \mathrm{G}\left(\mathrm{M}_{i-1}^j\right)$ **;** build ensemble of model outputs

$\Delta_{M,i} \leftarrow (\mathrm{M}_{i-1} \ominus \overline{\mathrm{M}_{i-1}})/\sqrt{N_e - 1}$

$\Delta_{D,i} \leftarrow (\mathrm{D}_i \ominus \overline{\mathrm{D}}_i)/\sqrt{N_e - 1}$

$\mathrm{C}_{MD,i} \leftarrow \Delta_{M,i}\Delta_{D,i}^{\mathrm{T}}$

$\mathrm{C}_{DD,i} \leftarrow \Delta_{D,i}\Delta_{D,i}^{\mathrm{T}}$

$\mathrm{M}_i^j \leftarrow \mathrm{M}_{i-1}^j + \mathrm{C}_{MD,i}\left(\mathrm{C}_{DD,i} + \alpha_i \Gamma\left(\phi_{i-1}^j\right)\right)^{-1}\left(\mathrm{D}_{uc}^j - \mathrm{D}_i^j\right)$; update the ensemble of model parameters

$\phi_i^j \leftarrow f\left(\phi \middle| \mathrm{M}_i^j, \mathrm{D}_i^j\right)$; MH-MCMC update of ϕ_i^j conditional on M_i^j and D_i^j

end for

$M \leftarrow M_{N_a}$

$\phi \leftarrow \phi_{N_a}$

The superscript *j* denotes the *j*th realisation from the respective ensemble.

The reader is referred to Botha *et al.*, (2022) for a detailed presentation of the derivation and application of CW-IEKI.

2.2. Study area

Despite representing only 2% of the total GBR catchment area, discharge from waterways in the Mackay-Whitsunday Natural Resource Management (NRM) region is estimated to contribute approximately 11% of the average annual GBR DIN load. About 13% of the DIN load is exported through the Pioneer River (Figure 1) (Packett et al., 2014).

The Pioneer catchment covers approximately 1573 square kilometres. The main waterway is the Pioneer River which is supplemented by smaller waterways including Cattle Creek. The main land uses are grazing (32%), forestry (22%), and sugarcane (22%). Most anthropogenic dissolved inorganic nitrogen (DIN) loads come from sugarcane with smaller contributions from urban and sewage treatment plants (Folkers et al., 2014).

2.3. Catchment water quality model

The WQM model used in this study is part of a larger suite of models that have been developed for the Paddock to Reef Integrated Monitoring, Modelling and Reporting Program (P2R) (Carroll et al., 2012) which provides the framework for evaluating and tracking progress towards achieving GBR water quality targets outlined in the Reef 2050 Water Quality Improvement Plan (Queensland, 2018). The models have been described in detail elsewhere (McCloskey et al., 2021a, 2021b), but essentially DIN is modelled two ways in the Pioneer catchment model. Agricultural Production Systems Simulator (APSIM) (Shaw et al., 2013) paddock scale agricultural models are used to estimate DIN generation and transport into the wider catchment from sugarcane landuse areas. Two delivery ratio parameters that describe the mean attenuation of total load generated from the paddock relative to that which appears at the monitoring point are considered here. *seep_dr* is the leached DIN delivery ratio and *surf_dr* is the surface runoff delivery ratio. The DIN loads generated from the remaining landuses are treated using a simple Event Mean Concentration/Dry Weather Concentration (EMC/DWC) approach. In all, the 11 parameters listed in Table 1 in section 3 are calibrated.

2.4. Loads data

Estimates of dissolved ammonium (NH_4) and oxides in nitrogen (NO_X) daily total loads at the Dumbleton Pump on the Pioneer River Station (Fig. 1) from July 2006 to June 2018 have been aggregated up to monthly total DIN loads (DIN = NH_4 + NO_X) resulting in a 144 month timeseries used for this study. The observed load estimates are based on monitoring data collected through the Great Barrier Reef Catchment Loads Monitoring Program (GBRCLMP) whose data provides the point of truth to validate loads predicted by the P2R Catchment models (Turner et al., 2013). The 144 samples have been partitioned into two subsets; data from the first 96 months of the timeseries were used for the calibration, and the remaining 48 monthly samples were used for validation.

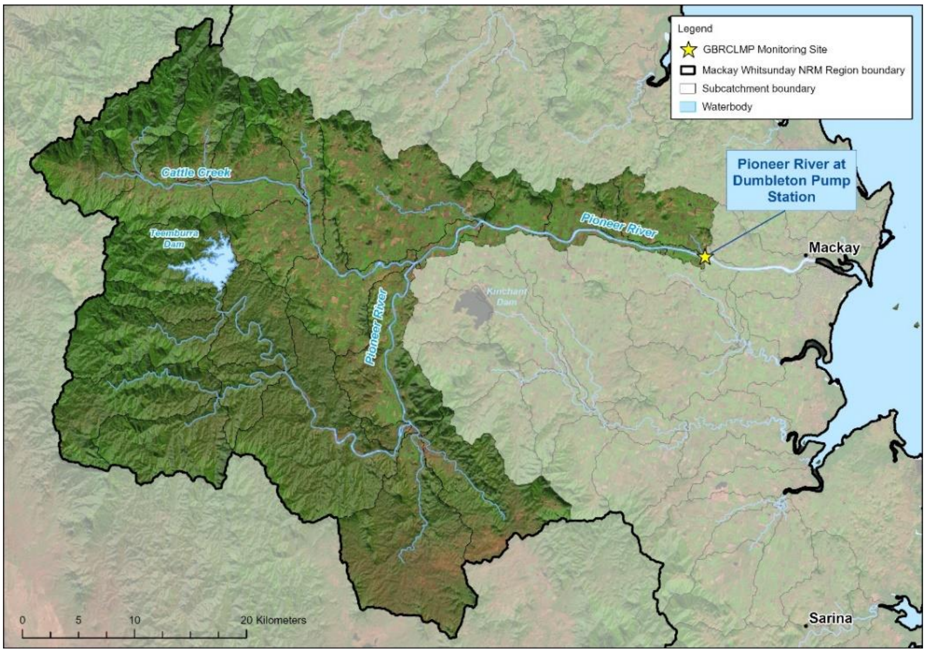

Figure 1. The Pioneer River catchment showing the location of the Dumbleton Pump Station upstream of the city of Mackay and the Cattle Creek tributary.

2.5. CW-IEKI and SMC-Bayes implementation

Bayesian inference implemented using likelihood tempering SMC sampling (denoted SMC-Bayes) and CW-IEKI proceeded from truncated normal priors $\mathcal{N}(\mu, \sigma^2, a, b)$ on the model parameters where μ is the mean, σ is the standard deviation and a and b are the lower and upper truncation limits. Referring to Table 1, for each parameter, μ is set to the midpoint of the range, a and b are the lower and upper range values, and σ is determined such that the span of the range is four standard deviations, *i.e.* $\sigma = (b - a)/4$. Parameter values were rescaled into a unit hypercube and then logit transformed. A half normal distribution, $|\mathcal{N}(0, 10^2)|$ was used for the prior on the noise parameter ϕ. Both the model output and observational data were square root transformed to allow for error heteroscedasticity. CW-IEKI and SMC-Bayes results presented in Section 3 are based on 1000 samples from their respective posteriors. 12 assimilation steps of the CW-IEKI required 12000 model runs compared to approximately 374000 model runs for an analogous sequence of SMC-Bayes likelihood tempering steps.

3. RESULTS AND DISCUSSION

CW-IEKI and SMC-Bayes marginal prior and posterior densities of the model and noise parameters are shown in Figure 2. A statistical summary of the prior and posterior pdf's is also provided in Table 1.

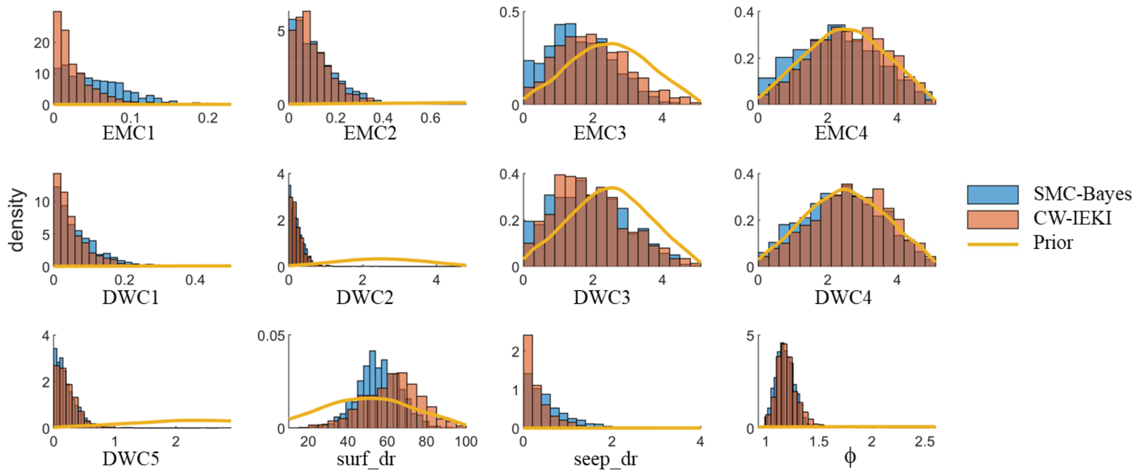

Figure 2. SMC-Bayes and CW-IEKI marginal prior and posterior density plots for eleven DIN model parameters and the noise noise parameter, ϕ.

Table 1. Posterior means and standard deviations (std) from SMC-Bayes and CW-IEKI samples for each of the parameters for the full model. The mean and standard deviations of the parameter prior pdf's can be derived from the parameter range as described in Section 2.5.

Parameter	Landuse	Range	SMC-Bayes		CW-IEKI	
			mean	std	mean	std
EMC1	Forestry, Conservation	0.0 – 5.0 mg/L	0.06	0.04	0.03	0.03
DWC1		0.0 – 5.0 mg/L	0.07	0.06	0.06	0.06
EMC2	Grazing	0.0 – 5.0 mg/L	0.12	0.09	0.11	0.09
DWC2		0.0 – 5.0 mg/L	0.22	0.17	0.23	0.26
EMC3	Urban, Cropping	0.0 – 5.0 mg/L	1.63	0.91	2.01	1.01
DWC3		0.0 – 5.0 mg/L	1.89	1.05	1.93	1.04
EMC4	Horticulture, Other	0.0 – 5.0 mg/L	2.27	1.15	2.60	1.09
DWC4		0.0 – 5.0 mg/L	2.43	1.12	2.66	1.10
DWC5	Sugarcane	0.0 – 5.0 mg/L	0.20	0.16	0.24	0.23
surf_dr		0.0 – 100.0 %	55.82	10.82	62.42	14.49
seep_dr		0.0 – 100.0 %	0.55	0.51	0.36	0.44

On examination, it is clear that the CW-IEKI and SMC-Bayes posterior pdfs are characteristically comparable. Parameters related to urban, cropping and horticulture, other landuses are not well identified. This is due to the small landuse areas for these categories which results in a diminutive contribution to the variance of the model response associated with these parameters. For the remaining parameters, there are some small divergences between the CW-IEKI and Bayes densities. Further insight into the relative performance of each method can be gained through the analysis of their respective posterior predictive distributions.

Figure 3 shows the posterior predictive densities using CW-IEKI and SMC-Bayes. Once again both methods yield similar results from inspection.

Various performance measures can be used to quantitatively compare the performance of the two models with respect to each other. Table 2 lists several statistics that address the performance of both the probabilistic model and a point estimate model that is given by the median value of the posterior predictive density. The P-factor is the percentage of measured data enveloped by the 95% credible interval and can be thought of as an indicator of the model reliability. The R-factor is a measure of the width of the 95% credible interval band and is calculated as the average 95% credible interval width divided by the standard deviation of the observation data. The average continuous-ranked probability score (CRPS) is a useful metric for quantifying the precision and accuracy of ensemble predictions (Hersbach, 2000). Lower performance results are indicated by the higher values of CRPS. The root mean square error-observations standard deviation ratio (RSR), Nash-Sutcliffe coefficient (NSE) and percent bias (PBIAS) are commonly used metrics for assessing performance of point-estimate hydrological and water quality models (Moriasi et al., 2007).

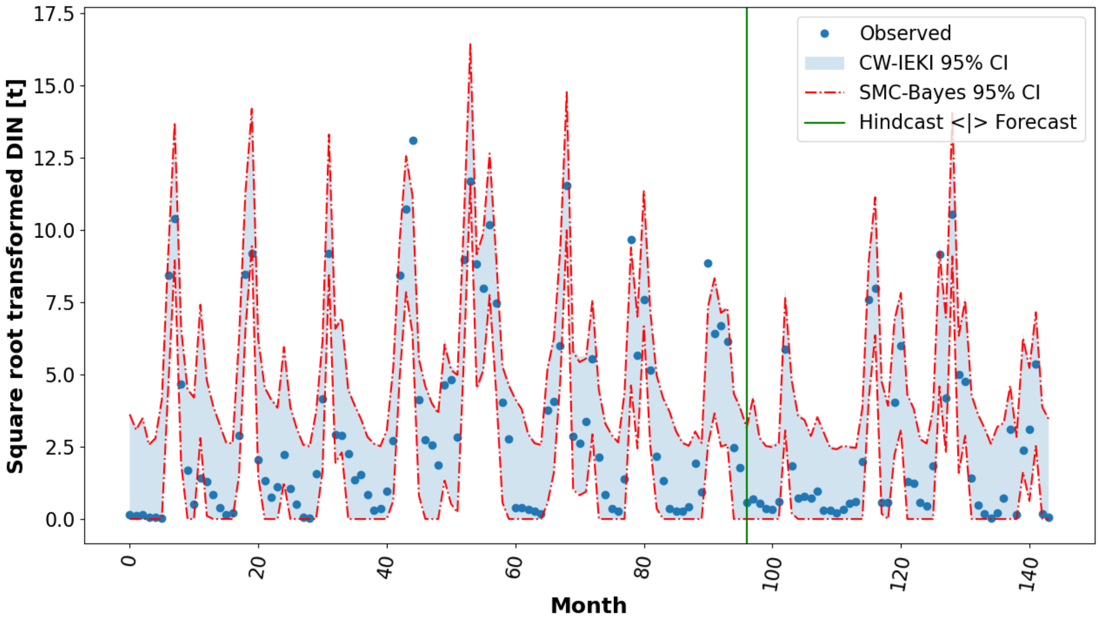

Figure 3. Comparison of the observed DIN loads data to the 95% central credible intervals (CI) for the posterior predictive distribution of the model fitted to this data. The models were fitted using CW-IEKI and SMC-Bayes (red dashed line). Data points to the left of the vertical green line were used for model fitting and those to the right for validation. The y-axis has been transformed for improved perspective.

Table 2. Performance summary statistics of calibration and uncertainty analysis for calibration, forecast and combined data periods for CW-IEKI and SMC-Bayes methods.

	CW-IEKI			SMC-Bayes		
Statistic	**All**	**Calibration**	**Forecast**	**All**	**Calibration**	**Forecast**
P-factor	94.4	93.8	95.8	93.1	91.7	95.8
R-factor	0.94	1.05	0.73	0.90	1.00	0.70
CRPS	4.92	6.10	2.56	4.93	6.13	2.55
RSR	0.44	0.47	0.31	0.44	0.46	0.32
NSE	0.81	0.78	0.90	0.81	0.79	0.90
PBIAS	-0.88	-2.11	4.11	-2.69	-3.65	1.19

In all cases, the P-factor is close to the theoretically expected value for the 95% CI. As an indicative reference point, depending on the situation an R-factor of <1.5 (Abbaspour et al., 2015) would be desirable so the *sharpness* of the 95% CI seems to be satisfactory by comparative standards. Moriasi *et al*. suggest the $0.0 \leq RSR \leq 0.5$, $0.75 \leq NSE \leq 1.00$ and $PBIAS < \pm 25$ gives a performance rating of "very good" for monthly DIN load models (Moriasi et al., 2007).

4. CONCLUSIONS

CW-IEKI and SMC-Bayes provide similar behavior based on all the performance metrics considered here. This is a single catchment scale DIN model case study, but several other environmental modelling case studies presented elsewhere have also demonstrated that CW-IEKI can substitute as a computationally efficient alternative to both MCMC and SMC for static Bayesian models of the form $\mathcal{N}\big(G(M), \Gamma(\phi)\big)$ where M and ϕ are unknown, and when $G(M)$ is expensive to compute (Botha et al., 2022). In the present case, a 31 fold efficiency dividend was achieved when comparing SMC inference to CW-IEKI, as summarised in Section 2.5.

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