



# A Bayesian approach to model the trends and variability in urban stormwater quality associated with catchment and hydrologic parameters

Thamali Perera<sup>a,b,c</sup>, James McGree<sup>d</sup>, Prasanna Egodawatta<sup>a,e</sup>, K.B.S.N. Jinadasa<sup>f</sup>, Ashantha Goonetilleke<sup>a,e,\*</sup>

<sup>a</sup> Faculty of Engineering, Queensland University of Technology (QUT), GPO Box 2434, Brisbane, 4001 Queensland, Australia

<sup>b</sup> Department of Mathematics, University of Sri Jayawardenepura, Nugegoda, 10250, Sri Lanka

<sup>c</sup> Postgraduate Institute of Agriculture, University of Peradeniya, Peradeniya, 20400, Sri Lanka

<sup>d</sup> Faculty of Science, Queensland University of Technology (QUT), GPO Box 2434, Brisbane, 4001 Queensland, Australia

<sup>e</sup> Centre for the Environment, Queensland University of Technology (QUT), GPO Box 2434, Brisbane, 4001 Queensland, Australia

<sup>f</sup> Department of Civil Engineering, University of Peradeniya, Peradeniya, 20400, Sri Lanka

## ARTICLE INFO

### Article history:

Received 24 October 2020

Revised 14 February 2021

Accepted 17 March 2021

Available online 20 March 2021

### Keywords:

stormwater runoff

Bayesian hierarchical modelling

uncertainty analysis

stormwater quality

stormwater pollutant processes

## ABSTRACT

Stormwater runoff pollution has become a key environmental issue in urban areas. Reliable estimation of stormwater pollutant discharge is important for implementing robust water quality management strategies. Even though significant attempts have been undertaken to develop water quality models, deterministic approaches have proven inappropriate as they do not address the variability in stormwater quality. Due to the random nature of rainfall characteristics and the differences in catchment characteristics, it is difficult to generate the runoff pollutographs to a desired level of certainty. Bayesian hierarchical modelling is an effective tool for developing complex models with a large number of sources of variability. A Bayesian model does not look for a single value of the model parameters, but rather determines a distribution of the model parameters from which all inference is drawn. This study introduces a Bayesian hierarchical linear regression model to describe a catchment specific runoff pollutograph incorporating the associated uncertainties in the model parameters. The model incorporates catchment and rainfall characteristics including the effective impervious area, time of concentration, rain duration, average rainfall intensity and the antecedent dry period as the contributors to random effects.

© 2021 Elsevier Ltd. All rights reserved.

## 1. Introduction

Stormwater runoff is perceived as a major contributor to water quality degradation in the receiving water bodies in urban areas (Göbel et al., 2007; Goonetilleke et al., 2005; Sheng et al., 2006). Increased extent of impervious surfaces such as pavements and roofs in the urban environment accumulate significant loads of pollutants such as solids, nutrients, organic matter, metals and hydrocarbons during the dry weather period prior to a storm event (Goonetilleke et al., 2009; Gunawardana et al., 2011; Helmreich et al., 2010; Jayarathne et al., 2019; Liu et al., 2016). The reduction in stormwater infiltration and the increase in surface runoff subsequently wash-off high loads of accumulated pollutants during rain events and discharges into receiving water. These pro-

cesses impose adverse water quality and quantity consequences in urban areas.

It is commonly accepted that suspended solids (SS) are an extremely important indicator of water quality deterioration (Bilotta and Brazier, 2008). Also, most importantly, SS also provide a medium for the accumulation, transport and storage of other pollutants. These include toxic compounds such as heavy metals and hydrocarbons. Therefore, SS can be considered as a surrogate indicator of stormwater quality (Allenby et al., 2005; Gunawardana et al., 2011; Hsieh and Davis, 2005; Liu et al., 2010; Miguntanna et al., 2013; Sheng et al., 2006; Williamson and Crawford, 2011). Therefore, the understanding of SS behaviour during a rainfall-runoff event and subsequently being able to predict such behaviour meets an important need in urban water quality management.

A range of water quality models have been developed during the past decades using deterministic approaches. However, these have constraints due to limitations in data and not being able to

\* Corresponding author at: Faculty of Engineering, Queensland University of Technology, GPO Box 2434, Brisbane 4001, Australia.

E-mail address: [a.goonetilleke@qut.edu.au](mailto:a.goonetilleke@qut.edu.au) (A. Goonetilleke).

account for the variability associated with pollutant discharge pattern during a runoff event. Further, such models are based on data collected from a limited number of rainfall events (Fu et al., 2019; Haris et al., 2016; Obropta and Kardos, 2007; Tiefenthaler et al., 2000). Researchers have observed that large variability and uncertainty in stormwater quality during stormwater runoff discharge is largely dependent on rainfall, runoff and catchment characteristics (Memon et al., 2017).

It is important to have an in-depth understanding of the relationships which describe the pollutant concentration at different time periods during the resulting stormwater runoff event in order to formulate effective stormwater management strategies. Most commonly, stormwater runoff concentration has been modelled as an exponential decay function of the runoff volume or the available surface pollutant load (Bach et al., 2010; Qjin et al., 2016; Qjin et al., 2010). However, with the demand for large datasets and long-term records needed by deterministic models for model calibration and validation, probabilistic methods have proven efficient when compared to deterministic approaches (Wan et al., 2014; Daly et al., 2014).

Conventional statistical techniques such as multiple linear regression and ordinary least squares regression, estimates an interval for the likely value of a parameter and selects one of the point estimate (mean, median) for each in a model describing the relationship between stormwater quality and the influential variables. However, stormwater quality can, on average, vary depending on the nature of a rainfall event and catchment characteristics. Therefore, it is important to capture this variability when modelling. However, spatial and temporal variability of the parameters have not been discussed in-depth in past studies (Amiri and Nakane, 2009; Cristiano et al., 2017; Kang et al., 2010). Vogel et al. (2005) introduced a bivariate linear relationship between the log transformed pollutant concentrations and flow. Allenby et al. (2005) derived a stochastic model for estimating SS loads and its variability during rainfall events which allows for accounting for the uncertainty in the model variables. Even though, these models have used advanced statistical tools, they still demand extensive field investigations. Wan et al. (2014) extended an existing water quality model by adopting a Bayesian hierarchical approach for the modelling. The researchers examined the relationship between land use and land cover in relation to water quality and found that Bayesian regression approach is more reliable compared to simple regression for inferring the relative contribution of land use to water quality.

Bayesian hierarchical modelling approach has proven to be a powerful tool for providing probabilistic predictions with associated uncertainty. Most importantly, with limited number of field investigations, this approach facilitates the derivation of complex models that incorporate a large number of sources of variability by decomposing interactions of observed data into a set of simple conditional models (Wan et al., 2014). Guo et al. (2019) used a Bayesian hierarchical model structure to identify the key predictors of temporal variability and showed that streamflow is the most important determinant of temporal variability. However, they have not considered variability of site-specific conditions and their influence on water quality. This paper has considered both, the variability in site-specific conditions and hydrological conditions and their subsequent impact on the variability in stormwater concentration during a runoff event.

This study adopted the Bayesian hierarchical modelling approach to model the runoff pollutographs. The objectives of the study were: 1) to analyse the within event variability and between event variability of SS concentration; 2) to relate variability in SS concentration to selected catchment characteristics and rainfall characteristics and finally, 3) to derive catchment specific

runoff pollutographs by assessing the associated uncertainty due to the variability in rainfall-runoff characteristics.

## 2. Materials and Methods

### 2.1. Data Collection

Three urban catchments, namely, Coomera, Highland park, and the Brisbane domestic airport apron in Queensland State, Australia were selected for the data collection. Both, Coomera and Highland park are residential catchments and have three sub-catchments each. The airport apron is a completely impervious surface. Accordingly, the collected data was spread over seven different catchments having different physical characteristics. For the baseline catchment data, a desktop study was conducted to collate the required information such as total area and land cover including pervious and impervious surface fractions. Accordingly, catchment characteristics including the effective impervious area fraction, fractions of different types of impervious surfaces including roofs, roads and driveways and time of concentration of the catchment were selected for the analysis. Table S1 in Supplementary Information provides a summary of the key characteristics of each catchment.

Tipping bucket rain gauges were used to collect the rainfall data and data were recorded using a data logger. The data generated by the rain gauges were collated using a Campbell Scientific CR1000 data logger and transmitted via telemetry. A V-notch weir installed at the catchment outlet was used to measure the runoff volume. Accordingly, baseline rainfall and runoff variables widely cited in research literature in relation to stormwater quality studies, namely, rainfall depth, average and maximum intensity, runoff depth, runoff volume and antecedent dry period for the monitored events were determined. Altogether, 39 storm events having a complete collection of required rainfall-runoff data were used for the analysis. Table S2 in the Supplementary Information provides a summary of the collected rainfall data conveying the inter-site variability in the data.

SS concentration was considered as the indicator water quality parameter. To obtain stormwater quality data, automatic water quality samplers were installed at the catchment outlets. The samplers were triggered by rainfall depth and enabled discrete stormwater samples to be collected into 1 L plastic bottles during the rising limb and falling limb of the hydrographs resulting from rainfall events. The sampling could be extended up to 24 bottles depending on the rainfall duration. However, the frequency of sample collection varied depending on the rainfall duration and the runoff volume. Stormwater samples were then transported to the laboratory following stipulated standards (AS/NZS 5667.1:1998) and analysed for the SS concentration. SS was tested according to Test Method No. 2540C (APHA 2005).

### 2.2. Data Analysis

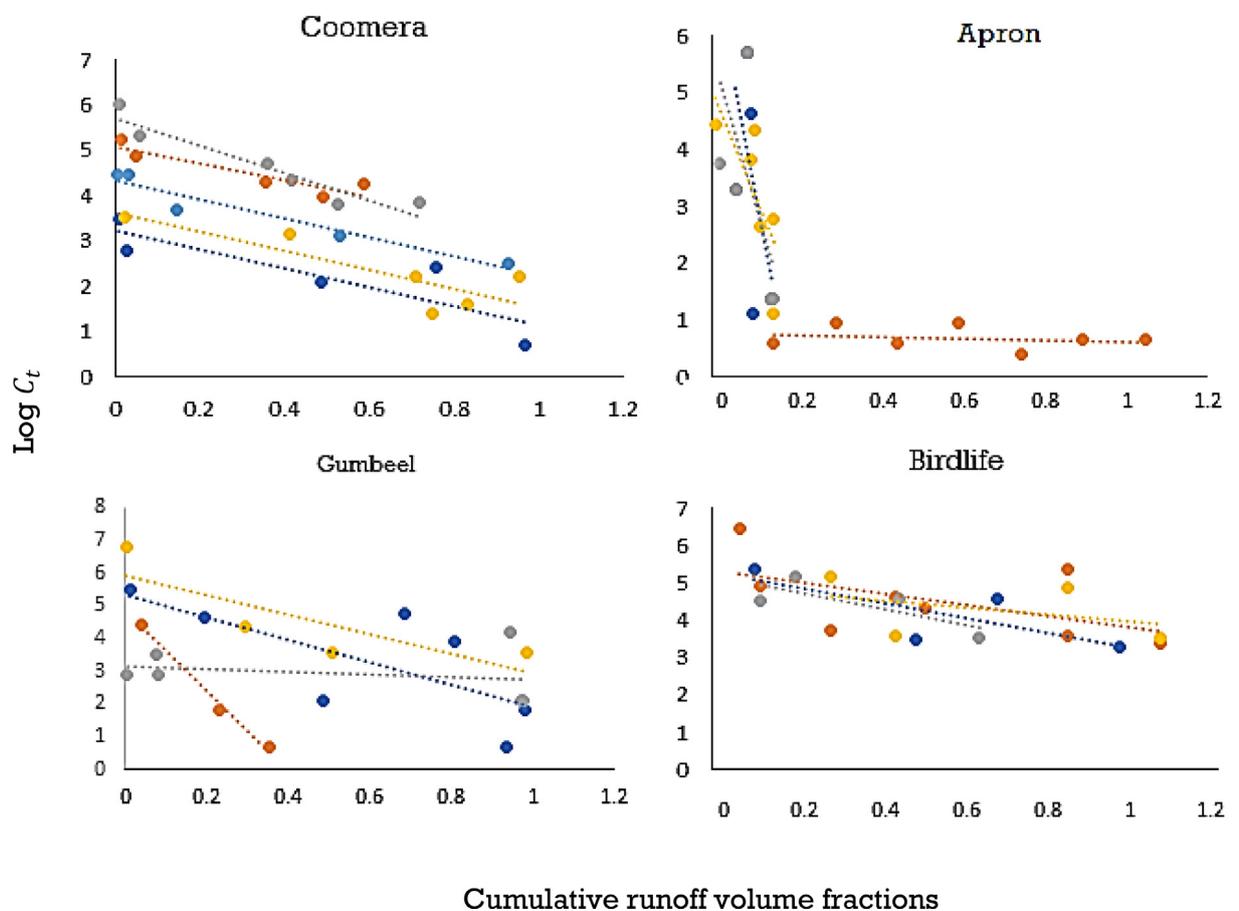
#### 2.2.1. Preliminary analysis

As the collected data were in different scales, all the data were standardised such that each variable has a mean of 0 and a standard deviation of 1 using the formula given below.

$$z = \frac{x - \mu}{\sigma} \quad (1)$$

Where,  $z$  is the standardised variable, and  $\mu$  is the mean and  $\sigma$  is the standard deviation of the unstandardised variable.

Exploratory data analysis was initially used to identify any collinearity between variables, and thereby facilitating the elimination of data redundancy. The resulting correlation matrices of catchment specific variables and event specific variables are given



**Fig. 1.** Distribution of SS concentration and the fitted linear models for each catchment. Note: runoff volume fractions were used instead the runoff volume for the visualization.

in Table S3 and Table S4, respectively, in the Supplementary Information. By considering the correlation coefficients between variables and the associated scatterplots, the effective impervious area (EIA), time of concentration (TC), antecedent dry period (ADP), rain duration (D) and the average intensity (AvgI) were selected for use in the model. Accordingly, the variables such as runoff depth (RoD), rainfall depth (RD) and maximum 5 min intensity (MaxI) were removed to avoid data redundancy. The data matrix used for the analysis is given in Table S5 in the Supplementary Information.

One of the primary objectives of this study was to analyse the variability in pollutant concentration during a runoff event. However, the discrete nature of the collected stormwater quality (SS concentration) data makes it difficult to analyse such variability. Water quality samples were not collected at equally spaced time intervals for individual rainfall events. Further, the frequency and the number of samples collected for each event varied due to variations in the duration of the runoff events. Therefore, it was important to reproduce the entire pollutograph using a common criterion eliminating limitations in the available data and the limited knowledge in the underlying processes.

### 2.3. Modelling methods

#### 2.3.1. Modelling the runoff pollutograph

Runoff concentration has generally been described via an exponential decay model. Based on the observed SS concentrations and work by past researchers, we described the concentration of SS via an exponential decay of the form given in Equation 2 (Borris et al., 2014; Brodie and Dunn, 2010; Charbeneau and Barrett, 1998;

Sartor and Boyd, 1972).

$$C_t = C_0 e^{-kV_t} \tag{2}$$

where,  $C_t$  is the concentration of SS in the runoff with respect to an accumulated runoff volume  $V_t$  of a rainfall event and  $C_0$  is a proportionality constant which is related to the pollutant concentration at the beginning of runoff. Here,  $k$  is the rate of decay of the pollutant concentration.

Even though, it has been hypothesized that  $k$  is a catchment specific parameter,  $k$  can fluctuate due to factors such as rainfall-runoff conditions (Al Ali et al., 2018; Kim et al., 2005). The validity of the selection of exponential decay form in the modelling was checked with the available data and the corresponding results are given in Table S6 in the Supplementary Information.

By taking the logarithmic transformation of Equation 2, Equation 3 can be obtained.

$$\ln C_t = -kV_t + \ln C_0 \tag{3}$$

Equation 3 yields a linear relationship between the runoff volume and natural logarithmic transformation of concentration. The natural log transformation can ensure minimizing measurement error associated with measuring the SS concentration during the runoff event and can be appropriately described via a normal distribution (Liu, 2011; Sharifi et al., 2011; Wan et al., 2014).

In the preliminary analysis, SS concentration data of each event was plotted, and linear models were fitted following Equation 3. Model fit for selected events at different catchments are illustrated in Fig. 1. Generally, a model in the form of Equation 3 is a fixed form which assumes that the observations are independent of each other given the predictor variables. However, it can be noted that

such independence does not hold for our data (Fig. 1) as the intercept and the slope of the model vary within and between the event and within and between the catchments they belong. This kind of dependence or clustering cannot be captured through a standard general linear model. What is needed is a model that allows each catchment to have its own intercept and slope (see Equation 3), but still contribute to the associated variability between rainfall events. This can be accommodated by including random effects into the model (say) for each catchment, and thus extending the model given in Equation 3 to a linear mixed effects model (Nakagawa and Schielzeth, 2013).

### 2.3.2. Linear mixed modelling (LMM)

LMM is an extension of linear modelling which takes into account the variations explained by the independent variables under consideration (fixed effects) and the variation not explained by the independent variables called the random effects (Winter, 2013). Random effects typically represent some grouping variable and allows the estimation of variance in the response variable within and among these groups (Harrison et al., 2018).

In terms of Equation 3, the deviation of the predictions from the measured values can be incorporated by adding an error term  $e$  which is a random variable representing random fluctuations in data as shown in Equation 4.

$$\ln C_t = -kV_t + \ln C_0 + e \quad (4)$$

However, there are multiple measurements for each catchment obtained from different runoff events. As mentioned above, these multiple measurements lead to a violation of the assumption of the independence of errors (Sorensen and Vasishth, 2015). Therefore, regression parameters ( $\ln C_0$ ,  $k$ ) vary between catchments and between events as demonstrated in Fig. 1. Different regression models can be fitted to the data from multiple events in the same catchment.

LMM can account for such variability by catchment and by event. Instead of fitting regression models separately, it can be assumed that the parameters follow a pre-determined statistical distribution (such as normal, lognormal, uniform) (Gelman and Hill, 2007; Pinheiro and Bates, 2000). A Bayesian structure facilitates the determination of the parameters in terms of distributions where a regression model fails to perform and thereby to assess the uncertainty in predictions arising from the inter-event and inter-site variability in the data. This avoids the requirement of fitting separate models for different events and different catchments (Sandoval et al., 2018).

Accordingly, Equation 4 can be modified by adding terms which represent catchment specific and event specific terms to the intercept and the slope, and this is referred to as a random effect model as given in Equation 5.

$$\ln C_t = (\ln C_0 + u_0 + w_0) - (k + u_1 + w_1)V_t \quad (5)$$

where  $u_0$  and  $w_0$  are the catchment and event specific random effects to the overall intercept and  $\ln C_0$ , and  $u_1$  and  $w_1$  are the catchment and event specific random slopes.

Further, these random variables ( $u_0$ ,  $w_0$ ,  $u_1$ ,  $w_1$ ) can be assumed to follow a known distribution (For example, normal distribution with mean zero and variances  $\sigma_{u0}^2$ ,  $\sigma_{w0}^2$ ,  $\sigma_{u1}^2$  and  $\sigma_{w1}^2$ , respectively). Accordingly, it is possible to incorporate the most appropriate combination of the fixed effects and random effects into the model based on the observed data by adopting formal model selection procedures.

### 2.3.3. Bayesian Modelling

Bayesian analysis derives the posterior distribution of the parameters given some data and prior beliefs about the distributions

of those parameters, and it is this distribution from which all inferences are based. Thus, to fit Bayesian models, a prior distribution needs to be defined. The prior distributions are usually defined based on expert knowledge or previously collected data. In cases where this is not available (as in this study), vague/flat priors are considered (Goddard, 2003). The resulting posterior distribution allows for calculating credible intervals of true parameter values for assessing the uncertainty in the predictions.

However, often there is no closed form solution to the posterior distribution. Therefore, approximating it or sampling from it directly can be difficult. This has led to the development of methods such as Markov chain Monte Carlo (MCMC) which provide approaches to sample from posterior distributions from a wide variety of Bayesian models. MCMC involves iteratively proposing values for the parameters, and accepting/rejecting these with a certain probability (Goddard, 2003). Accordingly, multiple chains were used to check whether each converge to the same stationary distribution. The subsequent chain of accepted parameter values was then used as a sample from the posterior distribution, once the chain had converged to a stationary distribution (which is assumed to be the posterior distribution). When performing an MCMC simulation, it is necessary to define the MCMC simulation parameters such as the number of samples to be derived, number of chains, thinning and burn-in. Thinning is the process of using only every  $k^{\text{th}}$  step of the chain for analysis, while all other steps are discarded with the goal of reducing autocorrelation and obtaining relatively independent samples. Thinning avoids bias in the standard error estimate of posterior mean (Harms and Roebroeck, 2018). Burn-in is the practice of ignoring samples at the initial stages of the MCMC algorithm as these are unlikely to be from the posterior distribution.

### 2.4. Linear mixed modelling with Bayesian Hierarchical model

The Bayesian model structure developed including random intercepts and random slopes used in the analysis is given below

$$\ln C_{jit} \sim N(\mu_{jit}, \sigma^2)$$

$$\mu_{jit} = \log C_{0ij} - k_{ij} V_t$$

$$\log C_{0ij} = \log C_0 + u_{0i} + w_{0j}$$

$$\log k_{ij} = \log k + u_{1i} + w_{1j}$$

$$i = 1 \dots \text{number of events}$$

$$j = 1 \dots \text{number of catchments}$$

$$t = 1 \dots \text{number of samples per event}$$

**Priors:**

$$\sigma^2 \sim IG(0.001, 1)$$

$$\log C_0 \sim N(0, 10)$$

$$w_{0j} \sim N(\log C_0, \sigma_{w0}^2), \sigma_{w0}^2 \sim IG(0.001, 1)$$

$$u_{0i} \sim N(\log C_0 + w_{0j}, \sigma_{u0}^2), \sigma_{u0}^2 \sim IG(0.001, 1)$$

$$w_{1j} \sim N(k, \sigma_{w1}^2), \sigma_{w1}^2 \sim IG(0.001, 1)$$

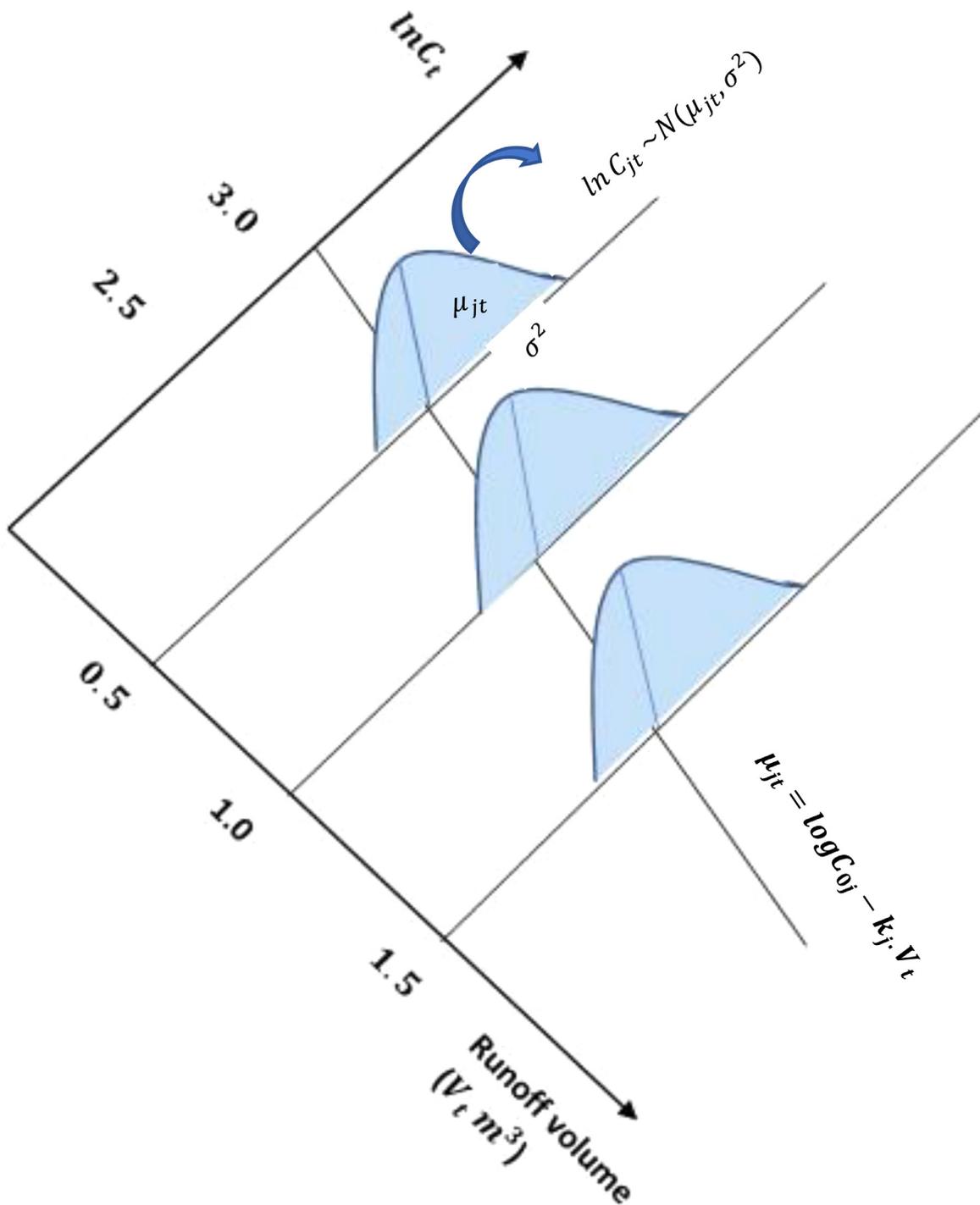


Fig. 2. An illustration of Bayesian definition of the variability in concentration for a typical event.

$$u_{1i} \sim N(\log k + w_{1j}, \sigma_{u1}^2), \sigma_{u1}^2 \sim IG(0.001, 1)$$

It was assumed that the logarithmic transformed concentration at time  $t$  of the event  $i$  at  $j$ th catchment,  $\ln C_{jit}$ , is normally distributed with mean  $\mu_{jit}$  and variance  $\sigma^2$ . Fig. 2 illustrates how the distributions have been defined for a typical rainfall event. Accordingly, the mean natural logarithmic concentration  $\mu_{jit}$  was defined as a linear mixed model with fixed effects  $C_0$ ,  $k$  and random effects  $u_{0i}$ ,  $u_{1i}$ ,  $w_{0j}$  and  $w_{1j}$  that accounts for the variability in rainfall characteristics and catchment characteristics. The relationship between  $\mu_{jit}$  and  $V_t$  is given by  $k_{ij}$ , which is the catchment and rain-

fall dependent slope parameter.  $k_{ij}$  is given as the overall parameter  $k$ , plus the variability associated with catchment and event accounted for via the random effect parameters  $w_{1j}$  and  $u_{1i}$ . Instead of using  $C_0$  and  $k$  directly, the logarithmic transformations of  $C_0$  and  $k$  were modelled to ensure these parameters remain positive.

Vague priors were defined for the parameters as given in the model structure. These vague priors were defined due to the lack of past information. Importantly, it was assumed that the rainfall events are nested within catchments as the same rainfall event cannot occur in two different catchments.

**Table 1**  
Bayesian model checking results for different models defined.

Model	Expected predictive error	Special Notes
1. $\mu_{jit} = \log C_0 - k_j \cdot V_i$	pD = 67857.7 and DIC = 68429.5	Each catchment has its own random slope $k_j$ , which is distributed around the overall slope parameter $k$ and $r_j$ and captures the variability associated with each catchment.
2. $\mu_{jit} = \log C_0 + u_{oi} - k_j \cdot V_i$	pD = 14805.9 and DIC = 15577.1	Event specific random intercept parameter, $u_{oi}$ has been included
3. $\mu_{jit} = \log C_0 + u_{oi} + w_{oj} - k_j \cdot V_i$	pD = 18876.5 and DIC = 19070.9	Catchment specific random intercept parameter, $w_{oi}$ has been included
4. $\mu_{jit} = \log C_0 + u_{oi} + w_{oj} + r_1 AvgI + r_2 D + r_3 ADP - k_j \cdot V_i$	pD = 14369.2 and DIC = 14574.8	Three rainfall parameters (AvgI, D, ADP) have been included. These variables were found to be influenced by the variability in the intercept.
5. $\mu_{jit} = \log C_0 + u_{oi} + w_{oj} + r_1 AvgI + r_2 D + r_3 ADP + c_1 TC + c_2 EIA - k_j \cdot V_i$	pD = 12946.2 and DIC = 13309.6	Two catchment specific parameters have been included.
6. $\mu_{jit} = \log C_0 + u_{oi} + w_{oj} + r_1 AvgI + r_2 D + r_3 ADP + c_1 TC + c_2 EIA - k_j \cdot V_i + u_{ij} + w_{1j}$	pD = 22442.4 and DIC = 22634.2	Two random slope parameters $u_{ij}$ and $w_{1j}$

Note: DIC info (using the rule, pD = var(deviance)/2).

**Table 2**  
Summary statistics of MCMC sampling for the selected model (model 5 in Table 1).

Parameter	mu.vect	sd.vect	2.5%	25%	50%	75%	97.5%	Rhat	n_eff
b[1]	4.145	1.472	1.775	3.099	3.985	5.022	7.413	1.002	1400
b[2]	2.797	0.787	1.416	2.247	2.729	3.290	4.514	1.003	930
b[3]	4.204	1.712	1.408	2.967	4.023	5.257	8.011	1.005	1200
b[4]	5.413	2.142	1.900	3.921	5.152	6.658	10.325	1.001	2400
b[5]	3.560	2.736	-0.753	1.534	3.191	5.257	9.776	1.001	2700
b[6]	4.359	1.743	1.433	3.127	4.195	5.464	8.147	1.001	3000
b[7]	2.399	2.569	-3.565	0.880	2.749	4.166	6.565	1.001	3000
b 0	0.146	0.325	-0.493	-0.084	0.145	0.371	0.771	1.001	3000
C1	0.718	2.237	-2.829	-0.828	0.416	2.027	5.837	1.001	2600
C2	0.162	0.295	-0.418	-0.043	0.156	0.359	0.742	1.002	1900
K	-0.015	0.727	-1.344	-0.537	-0.031	0.478	1.476	1.012	400
r[1]	0.156	0.729	-1.352	-0.337	0.158	0.671	1.475	1.012	520
r[2]	0.191	0.741	-1.331	-0.297	0.197	0.716	1.536	1.010	570
r[3]	0.064	0.757	-1.526	-0.440	0.078	0.600	1.419	1.009	470
r[4]	0.093	0.726	-1.375	-0.405	0.113	0.610	1.434	1.012	420
r[5]	-0.025	0.746	-1.578	-0.522	-0.005	0.497	1.325	1.011	410
r[6]	0.067	0.728	-1.409	-0.426	0.082	0.591	1.385	1.012	430
r[7]	0.020	0.728	-1.478	-0.472	0.037	0.545	1.357	1.012	380
r1	-0.054	0.233	-0.519	-0.208	-0.057	0.105	0.399	1.001	3000
r2	-0.111	0.132	-0.375	-0.200	-0.111	-0.022	0.149	1.001	3000
r3	0.144	0.120	-0.093	0.063	0.144	0.227	0.381	1.002	1100
Deviance	287.058	81.971	57.648	256.809	318.294	343.384	361.995	1.045	57

pD = 12946.2 and DIC = 13309.6.

The model was defined using the general structure of a Bayesian mixed model which was used in the subsequent analysis. Once the model was developed, it was necessary to select the most appropriate random effects and variables to include into the model for the data. Therefore, several models were developed with the inclusion of more random effects and exclusion of the random effects and compared using the deviance information criterion (DIC). DIC is a metric used to compare Bayesian models and is an estimate of expected predictive error (lower deviance is better) (Pooley and Marion, 2018).

For the MCMC convergence diagnostics, initially, summary statistics of the MCMC sampling were obtained for each of the model parameters including the mean, standard deviations and 95% upper and lower credible limits. Further,  $\hat{R}$  (Rhat) was obtained for each parameter, another diagnostic which is a measure of how well the Markov chains have mixed and should ideally have a value very close to 1 for the parameters of interest.  $\hat{R}$  refers to the potential scale reduction statistic, also known as the Gelman-Rubin statistic (Sorensen and Vasishth, 2015).

### 3. Results

#### 3.1. Model convergence and model selection

The model structure given in Section 2.4 describes the approach which was used to derive the relationship between the parameters. Accordingly, different models were defined, and posterior predictive checking was performed to check how well the models fit the data. For each MCMC simulation, 3 chains were used each with 12000 iterations and the first 2000 were discarded (burn in) because these first values depend strongly on the chosen initial values. Each 10<sup>th</sup> iteration was saved (thinning) to reduce the correlation between consecutive values in the chain and the rest discarded. Therefore, 3000 iterations (3 \* (12000 - 2000) / 10) were saved in MCMC sampling. Further, the convergence of the chains was checked using trace plots.

Different types of models were defined and model checking was performed starting with the basic model with minimum number of random effects. Table 1 presents six of them including the model

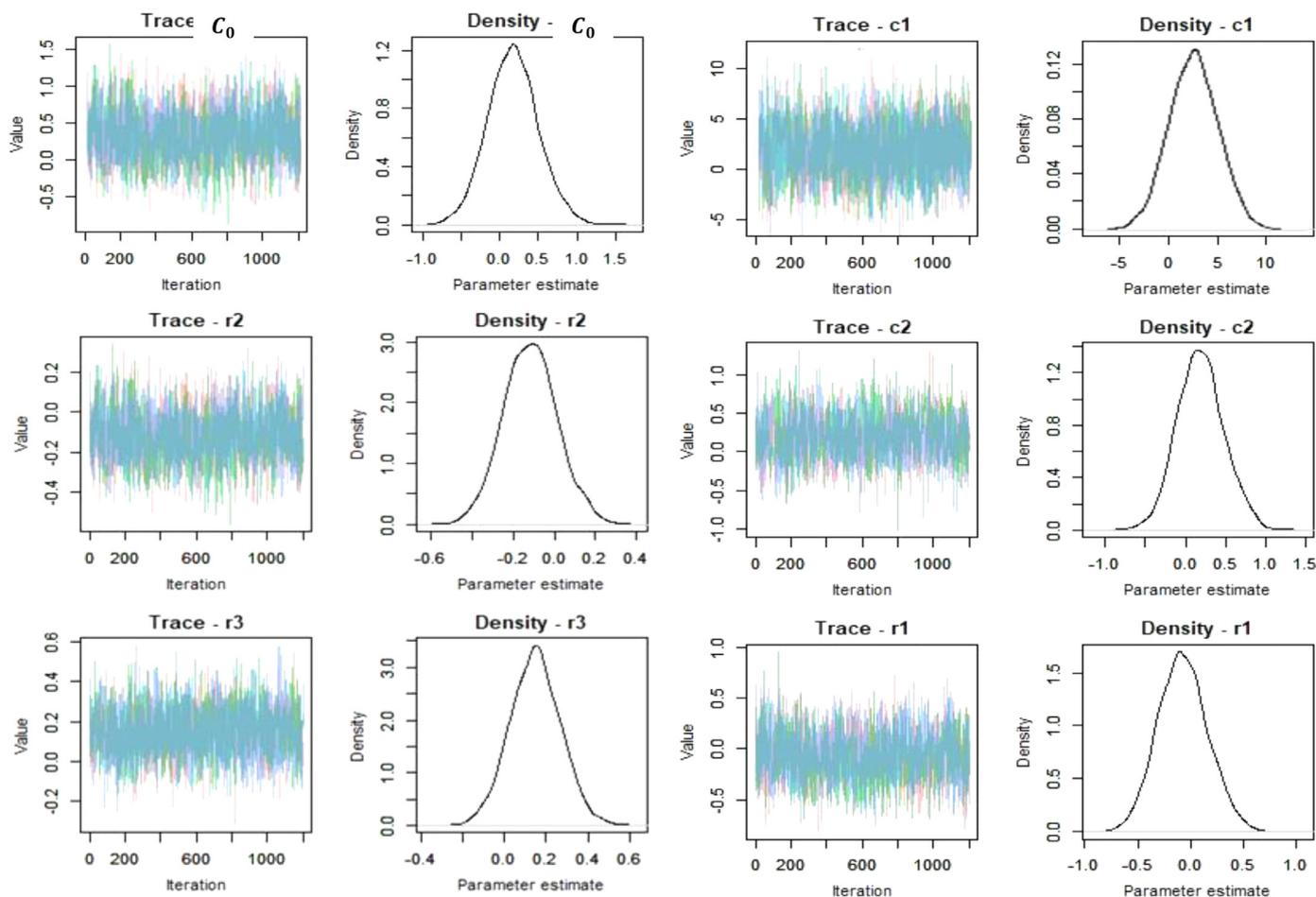


Fig. 3. Trace plots and the corresponding density plots for the estimated posterior distributions of parameters.

shown to be the best to fit the data (Only the definition of the mean value of the distribution is given). In Table 1, parameters have the same meaning as described in Section 2.4.

The models were compiled using “Rjags” package in R statistical software. Accordingly, the fifth model which the equation for the average concentration at time  $t$  of an event  $i$  at  $j^{th}$  catchment is given in Equation 6 was selected as the best among the others. The summary statistics of MCMC simulation for the fifth model is given in Table 2.

$$\mu_{jit} = \log C_0 + u_{oi} + w_{oj} + r_1 AvgI + r_2 D + r_3 ADP + c_1 TC + c_2 EIA - k_j V_i \tag{6}$$

All the six models showed convergence, but with different DIC. It can be identified that some models tend to increase the DIC by adding new parameters, but some others have increased the DIC whenever some parameters are excluded. Therefore, the model that gave the minimum deviance was selected. Accordingly, the model defined by the fifth equation was selected as the best among the others. The summary statistics of MCMC simulation for the fifth model is given in Table 2.

Table 2 shows that  $\hat{R}$  values for each parameter are close to 1 suggesting that the model has converged. Table 2 further gives the posterior predictive intervals for each parameter including their lower and upper 95% credible limits. Fig. 3 demonstrates the trace plots and the density plots for the estimated model parameters, the fixed intercept  $C_0$  and the random intercept parameters  $c_1, c_2, r_1, r_2$  and  $r_3$ . For the rest of the parameters which are the catchment specific slope parameters  $r_j, j = 1 \dots 7$  and the catch-

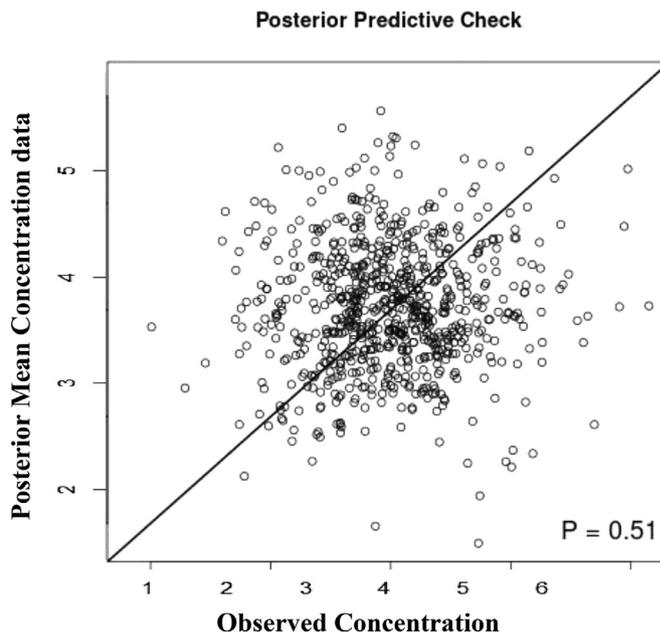
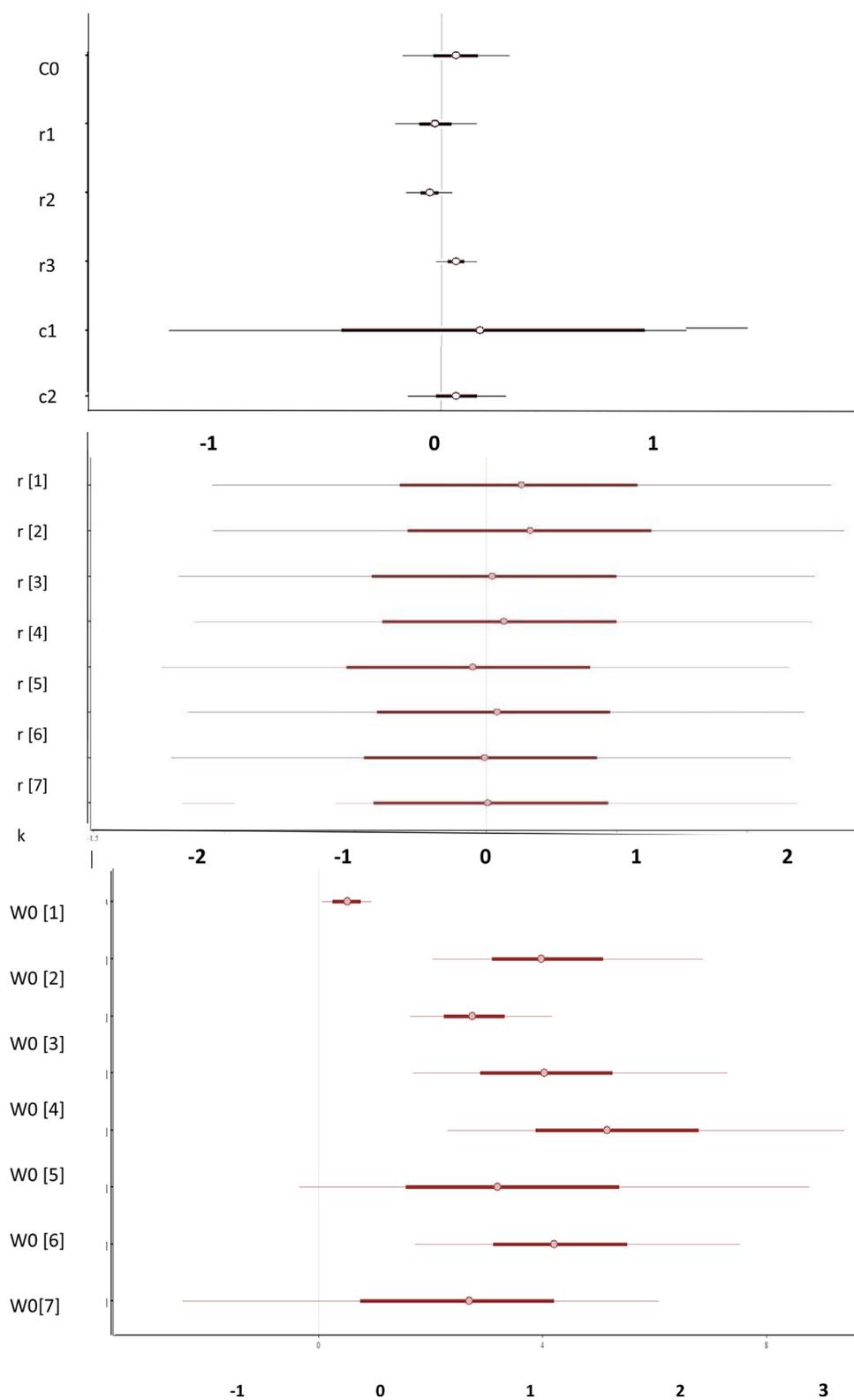


Fig. 4. The plot of posterior predictive check.

ment specific random intercept  $b_j, j = 1 \dots 7$ , the trace plots are shown in Figure S1 in the Supplementary Information.



**Fig. 5.** (a): credible intervals for rainfall and catchment specific random intercept parameters. (b): credible intervals for catchment specific parameters. (c): credible intervals for rainfall and catchment specific random intercept parameters.

In a Bayesian model, the expectation is to obtain stationary distributions for the parameter posterior distributions. Therefore, Markov chain estimations should converge to stationary distributions. In Fig. 3, it can be noted that the three chains have most likely converged and mixed well. The trace plots are not showing any long-term pattern and the average value of the chains are

roughly horizontal. Figure S1 provides similar observations suggesting the chains contain samples from the appropriate distribution. Therefore, it can be concluded that the selected model shows good convergence with minimum DIC.

After the initial diagnostic checking for convergence, it was important to check for model suitability. Accordingly, posterior pre-

dictive checking (ppc) was performed. The reason for ppc is to check whether the observed data look reasonable under the posterior predictive distribution. Accordingly, ppc p-value was estimated by calculating the fraction of predicted values that are more extreme for the test statistic than the observed value for that statistic. This implies that a p-value greater than, say, 0.50 indicates that the model fits the data. (Derpanopoulos, 2016). Fig. 4 shows the ppc plot with a p-value of 0.51. This indicates a good fit of the model to the data.

## 4. Discussion

### 4.1. Results on variable scale

The 95% posterior credible intervals of the model parameters, the fixed intercept parameter  $C_0$  and the random intercept parameters  $c_1$ ,  $c_2$ ,  $r_1$ ,  $r_2$  and  $r_3$ , corresponding to the variables TC, EIA, AvgI, D and ADP are shown in Fig. 5(a). The dot corresponds to the median, while the red line represents the 80% interval, and the thin black line is the 95% interval. The parameters  $c_1$ ,  $c_2$ ,  $r_1$ ,  $r_2$  and  $r_3$  can be interpreted as the contribution coefficients of the corresponding variable to the random intercept. It is clear that  $C_0$ ,  $c_2$ ,  $r_1$ ,  $r_2$  and  $r_3$  do not vary in a wide range means that those variables do not account for much variability in pollutant concentration at a given runoff volume. However,  $c_1$  varies in a wide range. Therefore, the TC of the catchment contributes to a large variability in the resulting pollutant concentration (Here the intercept of the model can change largely depending on the TC) and it suggests that the effect of TC is uncertain.

The model output also shows that ADP provides a positive contribution to the intercept. This is not surprising as a long ADP results in high loads of pollutants on the catchment surfaces at the beginning of a runoff event, which then increases the initial concentration. Similarly, the AvgI and D shows a negative contribution. This implies that high intensity rainfall can quickly wash-off the initial build-up pollutant load and longer duration also makes the initial concentration lower.

Fig. 5(b) shows the credible intervals for catchment specific decay parameters  $r_j$ ,  $j = 1..7$  and the overall population parameter  $k$ . It is evident that based on the catchment, the rate of decay in the concentration varies significantly. Therefore, adding the catchment specific decay parameter can improve the accuracy of prediction of pollutant concentration by accounting for the uncertainty created by the catchment characteristics. Similarly, Fig. 5(c) demonstrates the distribution of the catchment specific random intercept parameter  $w_{0j}$ . It is evident that  $w_{0j}$ ,  $j = 1..7$  vary in a wide positive range, which means that there is high variability in the intercept by catchment related characteristics which cannot be explained by including those variables into the model.

The illustrations provided in Fig. 5 highlight that adding random effects to the basic model for deriving pollutographs can account for much of the variability incurred by the random variability in data. Adding catchment specific parameters further improves the model and thereby result in catchment specific pollutographs. Accordingly, the selected model provides relatively good estimations of model parameters and thereby can be used for modelling the pollutographs with associated uncertainties. It is clear that, if there is a single catchment with known EIA and TC, the resultant pollutograph is catchment specific, but varies depending on the rainfall characteristics. Therefore, this method can be used to generate catchment specific runoff pollutographs with associated uncertainties in rainfall characteristics.

### 4.2. Practical implications of the study

This study modified the existing linear relationship between the natural logarithmic transformed pollutant concentration in the

runoff and the runoff volume given in Equation 2 by incorporating a set of catchment and rainfall variables. Therefore, the outcomes of this approach can be used to reproduce the catchment-based runoff pollutographs rather than deriving separate pollutographs based on runoff events. This model also helps to account for the variability associated with the variability in rainfall characteristics. Therefore, a single catchment specific model can be used to model the variability in runoff concentration with the associated uncertainty incurred by the uncertainty in the rainfall characteristics.

In terms of stormwater quality treatment systems, it is important to design treatment facilities separately for different catchments by considering the specific characteristics of the catchments. In this regard, a catchment specific pollutograph is important to analyse the variability in water quality at different times during the runoff event. Such analysis would then help to identify the most polluted critical runoff volume in the overall runoff hydrograph. The identification of highly concentrated runoff can then be treated to reduce the cost and space required for larger stormwater treatment systems. Therefore, this study provides a robust methodology for producing runoff pollutographs separately for individual catchments by considering their topographical characteristics and thereby assist in formulating urban stormwater quality treatment strategies.

## 5. Conclusions

This study provides a new contribution to the field of stormwater quality modelling. A new and innovative approach (Bayesian hierarchical linear regression) was tested with measured data incorporating the uncertainty in the variables influencing stormwater quality characteristics. This approach overcomes significant limitations where several other model structures such as linear regression models have failed to provide satisfactory results.

Accordingly, Bayesian hierarchical linear regression models were constructed for examining the relationship between catchment and rainfall characteristics with stormwater SS concentration. The data collected over seven urban catchments were used to derive the posterior distributions. Accordingly, catchment specific models were developed incorporating the random effects of variables under consideration.

Catchment characteristics such as the effective impervious area and the time of concentration was shown to impact SS concentration in the runoff. The hierarchical model revealed that the variability in the rainfall characteristics significantly influence the SS concentrations within the same catchment. Furthermore, the antecedent dry period, rainfall duration and the average intensity were found to have relatively high contribution to the variability in runoff pollutant concentration.

The model structure presented in this study was shown to be efficient compared to the traditional regression models as it provides with a level of confidence, a credible interval which a parameter can vary. Therefore, predictions can be more reliable and variations in the prediction can also be determined. Further, this provides a new insight for reproducing pollutographs. The catchment specific model can be used to construct catchment-based water quality treatment measures through the analysis of variability in pollutant concentration during the occurrence of a runoff event.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Acknowledgments

The authors would like to acknowledge the University Grant Commission of Sri Lanka for the scholarship provided to the first author to carry out postgraduate research studies. We are also thankful to the Queensland University of Technology (QUT) for providing the opportunity to undertake this study.

## Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.watres.2021.117076.

## References

- Al Ali, S., Rodriguez, F., Bonhomme, C., Chebbo, G., 2018. Accounting for the spatio-temporal variability of pollutant processes in stormwater tss modeling based on stochastic approaches. *Water* 10 (12), 1773.
- Allenby, G.M., Rossi, P.E., McCulloch, R., 2005. Hierarchical bayes models: A practitioners guide. Grover r, vriens m eds. *SSRN Electronj*.
- Amiri, B.J., Nakane, K., 2009. Modeling the linkage between river water quality and landscape metrics in the chugoku district of japan. *Water resources management* 23 (5), 931–956.
- Bach, Daly, E., McCarthy, D., Deletic, A., 2010. Investigating pollutant variability for the development of a semi-stochastic water quality model of urban stormwater runoff. Proceedings of the 6th Sewer Processes and Networks Conference (SPN6)At: Gold Coast.
- Bilotta, G., Brazier, R., 2008. Understanding the influence of suspended solids on water quality and aquatic biota. *Water Research* 42 (12), 2849–2861.
- Borris, M., Viklander, M., Gustafsson, A.M., Marsalek, J., 2014. Modelling the effects of changes in rainfall event characteristics on tss loads in urban runoff. *Hydrological Processes* 28 (4), 1787–1796.
- Brodie, I.M., Dunn, P.K., 2010. Commonality of rainfall variables influencing suspended solids concentrations in storm runoff from three different urban impervious surfaces. *Journal of Hydrology* 387 (3–4), 202–211.
- Charbeneau, R.J., Barrett, M.E., 1998. Evaluation of methods for estimating stormwater pollutant loads. *Water Environment Research* 70 (7), 1295–1302.
- Cristiano, E., ten Veldhuis, M.-c., van de Giesen, N., 2017. Spatial and temporal variability of rainfall and their effects on hydrological response in urban areas-a review. *Hydrology & Earth System Sciences* 21 (7), 3859–3878.
- Daly, E., Bach, P.M., Deletic, A., 2014. Stormwater pollutant runoff: A stochastic approach. *Advances in Water Resources* 74, 148–155.
- Derpanopoulos, G., 2016. Bayesian model checking & comparison Retrieved from <https://geogederpa.github.io/teaching/modelChecking.html>.
- Fu, B., Merritt, W.S., Croke, B.F., Weber, T.R., Jakeman, A.J., 2019. A review of catchment-scale water quality and erosion models and a synthesis of future prospects. *Environmental Modelling & Software* 114, 75–97.
- Gelman, A., Hill, J., 2007. Data analysis using regression and multilevelhierarchical models, 1. Cambridge University Press, New York, NY, USA.
- Göbel, P., Dierkes, C., Coldewey, W., 2007. Storm water runoff concentration matrix for urban areas. *Journal of contaminant hydrology* 91 (1–2), 26–42.
- Goddard, M., 2003. Introduction to bayesian statistics. University of Melbourne an Victorian Institute of Animal Science, Australia.
- Goonetilleke, A., Egodawatta, P., Kitchen, B., 2009. Evaluation of pollutant build-up and wash-off from selected land uses at the port of brisbane, australia. *Marine pollution bulletin* 58 (2), 213–221.
- Goonetilleke, A., Thomas, E., Ginn, S., Gilbert, D., 2005. Understanding the role of land use in urban stormwater quality management. *Journal of Environmental management* 74 (1), 31–42.
- Gunawardana, C., Goonetilleke, A., Egodawatta, P., Dawes, L., Kokot, S., 2011. Role of solids in heavy metals buildup on urban road surfaces. *Journal of Environmental Engineering* 138 (4), 490–498.
- Guo, D., Lintern, A., Webb, J.A., Ryu, D., Liu, S., Bende-Michl, U., Western, A., 2019. Key factors affecting temporal variability in stream water quality. *Water Resources Research* 55 (1), 112–129.
- Haris, H., Chow, M., Usman, F., Sidek, L., Roseli, Z., Norlida, M., 2016. Urban stormwater management model and tools for designing stormwater management of green infrastructure practices Paper presented at the IOP conference series: earth and environmental science.
- Harms, R.L., Roebroek, A., 2018. Robust and fast markov chain monte carlo sampling of diffusion mri microstructure models. *Frontiers in neuroinformatics* 12, 97.
- Helmreich, B., Hilliges, R., Schriewer, A., Horn, H., 2010. Runoff pollutants of a highly trafficked urban road—correlation analysis and seasonal influences. *Chemosphere* 80 (9), 991–997.
- Hsieh, C.-h., Davis, A.P., 2005. Evaluation and optimization of bioretention media for treatment of urban storm water runoff. *Journal of Environmental Engineering* 131 (11), 1521–1531.
- Jayarathne, A., Wijesiri, B., Egodawatta, P., Ayoko, G.A., Goonetilleke, A., 2019. Role of adsorption behavior on metal build-up in urban road dust. *Journal of Environmental Sciences* 83, 85–95.
- Kang, J.-H., Lee, S.W., Cho, K.H., Ki, S.J., Cha, S.M., Kim, J.H., 2010. Linking land-use type and stream water quality using spatial data of fecal indicator bacteria and heavy metals in the yeongsan river basin. *Water Research* 44 (14), 4143–4157.
- Kim, L.-H., Kayhanian, M., Lau, S.-L., Stenstrom, M.K., 2005. A new modeling approach for estimating first flush metal mass loading. *Water Science and Technology* 51 (3–4), 159–167.
- Liu, A., 2011. Influence of rainfall and catchment characteristics on urban stormwater quality. Queensland University of Technology PhD.
- Liu, A., Gunawardana, C., Gunawardana, J., Egodawatta, P., Ayoko, G.A., Goonetilleke, A., 2016. Taxonomy of factors which influence heavy metal build-up on urban road surfaces. *Journal of hazardous materials* 310, 20–29.
- Liu, Y., Guan, Y., Tam, N.F.Y., Mizuno, T., Tsuno, H., Zhu, W., 2010. Influence of rainfall and basic water quality parameters on the distribution of endocrine-disrupting chemicals in coastal area. *Water, Air, & Soil Pollution* 209 (1), 333–343.
- Memon, S., Paule, M.C., Yoo, S., Umer, R., Lee, B.-Y., Sukhbaatar, C., Lee, C.-H., 2017. Trend of storm water runoff pollutants temporal variability from different land use sites in korea. *Desalin. Water Treat* 63, 433–441.
- Miguntanna, Liu, A., Egodawatta, P., Goonetilleke, A., 2013. Characterising nutrients wash-off for effective urban stormwater treatment design. *Journal of Environmental management* 120, 61–67.
- Nakagawa, S., Schielzeth, H., 2013. A general and simple method for obtaining r2 from generalized linear mixed-effects models. *Methods in ecology and evolution* 4 (2), 133–142.
- Obropta, C.C., Kardos, J.S., 2007. Review of urban stormwater quality models: Deterministic, stochastic, and hybrid approaches 1. *JAWRA Journal of the American Water Resources Association* 43 (6), 1508–1523.
- Pinheiro, J.C., Bates, D.M., 2000. Linear mixed-effects models: Basic concepts and examples. In: Pinheiro, J.C., Bates, D.M. (Eds.), *Mixed-effects models in s and s-plus*. Springer New York, pp. 3–56.
- Pooley, C., Marion, G., 2018. Bayesian model evidence as a practical alternative to deviance information criterion. *Royal Society open science* 5 (3), 171519.
- Qin, H., He, K.-m., Fu, G., 2016. Modeling middle and final flush effects of urban runoff pollution in an urbanizing catchment. *Journal of Hydrology* 534, 638–647.
- Qin, H.-P., Khu, S.-T., Yu, X.-Y., 2010. Spatial variations of storm runoff pollution and their correlation with land-use in a rapidly urbanizing catchment in china. *Science of the Total Environment* 408 (20), 4613–4623.
- Sandoval, S., Vezzano, L., Bertrand-Krajewski, J.-L., 2018. Revisiting conceptual stormwater quality models by reconstructing virtual state variables. *Water Science and Technology* 78 (3), 655–663.
- Sartor, J.D., Boyd, G.B., 1972. Water pollution aspects of street surface contaminants. Office of Research and Monitoring, U. S. Environmental Protection Agency, Washington DC EPA-R2-72-081.
- Sharifi, S., Massoudieh, A., Kayhanian, M., 2011. Stochastic stormwater quality volume-sizing method with first flush emphasis. *Water Environment* (83) 2025–2035.
- Sheng, Y., Sansalone, J., Calomino, F., 2006. Estimation of solids loadings to rainfall-runoff unit operations using a unit pollutograph concept for source area watersheds. *Water Science and Technology* 54 (6–7), 363–369.
- Sorensen, T., Vasishth, S., 2015. Bayesian linear mixed models using stan: A tutorial for psychologists, linguists, and cognitive scientists *arXiv preprint arXiv:1506.06201*.
- Tiefenthaler, L., Schiff, K., Leecaster, M., 2000. Temporal variability patterns of stormwater concentrations in urban stormwater runoff. Southern California coastal water research project annual report 28–44.
- Vogel, R.M., Rudolph, B.E., Hooper, R.P., 2005. Probabilistic behavior of water-quality loads. *Journal of Environmental Engineering* 131 (7), 1081–1089.
- Wan, R., Cai, S., Li, H., Yang, G., Li, Z., Nie, X., 2014. Inferring land use and land cover impact on stream water quality using a bayesian hierarchical modeling approach in the xitaoxi river watershed, china. *Journal of Environmental management* 133, 1–11.
- Williamson, T.N., Crawford, C.G., 2011. Estimation of suspended-sediment concentration from total suspended solids and turbidity data for kentucky, 1978–1995 1. *JAWRA Journal of the American Water Resources Association* 47 (4), 739–749.
- Winter, B., 2013. A very basic tutorial for performing linear mixed effects analyses *arXiv preprint arXiv:1308.5499*.