Science of the Total Environment 497–498 (2014) 578–584

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Assessing uncertainty in pollutant wash-off modelling via model validation

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HIGHLIGHTS

- Assessing uncertainty in water quality modelling is important but rarely undertaken.
- Uncertainty assessment enhances stormwater management decision making.
- Monte Carlo cross validation applied for assessing uncertainty in modelling
- MCCV is likely to result in a more realistic measure of model coefficients than LOO.

ARTICLE INFO

Article history:
Received 7 April 2014
Received in revised form 5 August 2014
Accepted 8 August 2014
Available online 27 August 2014

Editor: Simon Pollard

Keywords:
Model uncertainty
Monte Carlo cross validation
Pollutant wash-off
Stormwater pollutant processes
Stormwater quality

ABSTRACT

Stormwater pollution is linked to stream ecosystem degradation. In predicting stormwater pollution, various types of modelling techniques are adopted. The accuracy of predictions provided by these models depends on the data quality, appropriate estimation of model parameters, and the validation undertaken. It is well understood that available water quality datasets in urban areas span only relatively short time scales unlike water quantity data, which limits the applicability of the developed models in engineering and ecological assessment of urban waterways. This paper presents the application of leave-one-out (LOO) and Monte Carlo cross validation (MCCV) procedures in a Monte Carlo framework for the validation and estimation of uncertainty associated with pollutant wash-off when models are developed using a limited dataset. It was found that the application of MCCV is likely to result in a more realistic measure of model coefficients than LOO. Most importantly, MCCV and LOO were found to be effective in model validation when dealing with a small sample size which hinders detailed model validation and can undermine the effectiveness of stormwater quality management strategies.

1. Introduction

Stormwater pollution is a primary non-point pollution source of concern, and is linked to stream ecosystem degradation (Walsh et al., 2004; Cizek and Hunt, 2013). Estimation of stormwater pollutant loads and/or concentrations is a pre-requisite for effective decision-making for the protection of receiving water environments. Various types of models are used in estimating stormwater pollutant wash-off loadings (Zhang et al., 2010; Kotti et al., 2013; Chen et al., 2014), which are then used to restore and improve the ecology of urban waterways through appropriate management interventions. However, the accuracy of the predictions provided by various models is dependent on the appropriate estimation of model parameters, which has not received appreciable research attention in the past.

The development of stormwater quality models still faces many challenges which can be primarily attributed to the complexities in pollutant processes due to stereotyping of site characteristics and the inadequacy of the datasets available. As reported by Zhang et al. (2007, 2008), stormwater pollution is affected by a range of land use, catchment and rainfall characteristics. The key issues relating to inadequate datasets are their subjectivity to spatial scales, high variability and availability over relatively short time scales (Kanso et al., 2006) unlike in the case of water quantity data (Haddad et al., 2010; van der Sterren et al., 2012). Past research has shown that the heterogeneity of the system characteristics can vary over space and time scales and are typically not known with great accuracy (UNESCO, 2005; Smith et al., 1997). Consequently, water quality modelling outcomes are not highly reliable as these are constraints which inhibit taking due consideration of the variability associated with pollutant processes and natural phenomena (Stewart, 2000). The establishment of more reliable models may be achieved if more comprehensive datasets are used. However, due to

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http://dx.doi.org/10.1016/j.scitotenv.2014.08.027
0048-9697/

the high cost associated with water quality data collection, such datasets are usually scarce.

Consequently, it is well known that all modelling approaches are subject to various forms of uncertainty (Zoppou, 2001; Nix, 1994). The main three sources of uncertainty are: i) data uncertainty — uncertainty associated with model input which is the data used to calibrate the model; ii) parameter uncertainty — uncertainty associated with the model parameters which arises from the method used to estimate those parameters; and iii) model structure uncertainty — uncertainty arising from the incomplete conceptual understanding of the systems under study which can be attributed to the reliance on models that are simplified representations of the true complexities of natural processes (Willems, 2008; Refsgaard et al., 2006, 2007; Freni et al., 2009).

Therefore, uncertainty analysis is an essential requirement for evaluating model reliability (Freni et al., 2009). A range of studies have focused on assessing uncertainty resulting from input data and measurements (for example, Sohrabi et al., 2003; Kanso et al., 2003, 2005; Kuczera et al., 2006; Bertrand-Krajewski, 2007; Haydon and Deletic, 2009; Freni et al., 2009; Wang et al., 2009; Franceschini and Tsai, 2010; Liu et al., 2012a, 2012b; Haddad et al., 2013a). The methodologies for uncertainty analysis discussed in the literature are accepted as standard in the water quality modelling area. The methods range from classical statistical analysis to Bayesian inference techniques. However, these uncertainty analysis methods agree on representing uncertainty by giving a range of values or a probability distribution that are most likely to cover the possible true value of a specific simulated value. Past studies have focused on assessing both, the overall modelling uncertainty and the uncertainty associated with modelling specific pollutant processes such as pollutant build-up and wash-off by using a range of routing methods. This provides only a dimension of understanding of the accuracy of stormwater quality models for replicating pollutant processes.

As the study discussed in the paper has employed statistical methods, a discussion on statistical models is relevant to provide context. Statistical models that have been used for estimating stormwater runoff quantity and quality are generally based on regression models which are considered to be a stochastic modelling approach. Regression models that are commonly used include simple linear, multiple linear, nonlinear semi-log and log–log transforms. Examples of statistical models used in water quality modelling can be found in Driver and Tasker (1988), Egodawatta et al. (2012) and Haddad et al. (2013a). It has been recognised that linear regression under certain conditions is not well suited for modelling water quality data (Jewell and Adrian, 1981; Zoppou, 2001; Haddad et al., 2013a). A fundamental limitation in the statistical relationship developed is often due to the very limited dataset used, the high level of error associated with the dataset and the fact the dataset itself only reflects a specific spatial arrangement (Zoppou, 2001). In the event of a different spatial setup and process, the regression relationships may need to be re-formulated based on the new data.

Some of the limitations in regression approaches discussed above can be overcome through the use of model validation techniques such as leave-one-out (LOO) and Monte Carlo cross validation (MCCV) (Song Xu et al., 2005). In LOO, one data point is left out while building a regression model (or other form of model) and then the model is tested on the previously left out data point. The procedure is repeated until all the data points are independently tested. In the case of MCCV, the technique leaves out a notable part of the sample at a time during model building and validation and repeats the procedure many times. MCCV may be more desirable in uncertainty estimation of water quality models as it evaluates the different models according to their predictive ability using different combinations of validation datasets.

LOO and MCCV presented in this paper were carried out differently to the classical approach commonly used, which is based on determining a suitable model from many candidate models (Haddad et al, 2013b). The aim of LOO and MCCV applied in this study was to assess the uncertainty in water quality models in practical situations through validating different combinations of data, reflecting coefficient estimation uncertainty. LOO and MCCV are able to overcome the limitations of small datasets making the interpretation of uncertainty associated with water-quality models more reliable.

This paper has three primary objectives: (i) demonstration of the application of MCCV method in water quality modelling using regression analysis; (ii) comparison of MCCV with the most commonly used LOO validation technique for assessing the overall uncertainty of the developed regression equation; and (iii) demonstration of the best use of the limited datasets which are commonly encountered in water quality modelling and can hinder the detailed validation of water quality regression models.

2. Materials and methods

2.1. Data collection

This research study used roof wash-off data collected at a number of sites located in South East Queensland, Australia. Egodawatta et al. (2009) have confirmed that the pollutant wash-off process for road and roof surfaces, which are the primary impervious surfaces in an urban catchment are similar and the differences due to surface characteristics can be replicated using different coefficients. Therefore, research outcomes derived for roof surfaces is easily extendable to road surfaces. Furthermore, in an urban catchment, the total roof area can be 2–3 times greater than the total road area (Egodawatta et al., 2012). Also, understanding of pollutant processes on roof surfaces is important as rainwater harvesting is being increasingly considered as an alternative water source particularly in water deficient regions.

The pollutant wash-off samples were collected from model roofs of 3 m^2 area used as test plots. This approach eliminated the possible heterogeneity in pollutant distribution and the practical difficulties of collecting pollutant wash-off samples from actual roof surfaces. The model roofs were mounted on a scissor lift arrangement as shown in Fig. 1. The roofs were raised to the typical roofing height to enable pollutant build-up under natural conditions and then lowered to ground level for wash-off sample collection using a rainfall simulator. Two roofing products, corrugated steel and concrete tiles were used for cladding as these are the most widely used roofing materials in the study region. Further details of wash-off sample collection are presented in Egodawatta et al. (2009).

A specially designed rainfall simulator was used to simulate the rainfall events on the model roof surfaces. The simulator was designed to replicate natural rainfall events as closely as possible in relation to rainfall drop size distribution and kinetic energy of rain drops which are the key rainfall characteristics which influence pollutant wash-off. Details on the design and operation of the rainfall simulator can be found in Herngren et al. (2005). For sample collection, the rainfall simulator was positioned over the lowered model roofs and subjected to predetermined rainfall intensities as shown in Fig. 1. Rainfall intensities of 20, 40, 86 and 115 mm/h were simulated on the roof surfaces. For each simulation, runoff samples were collected for a range of different durations to match design storms of specific Average Recurrent Intervals (ARI). Altogether, 46 runoff samples were collected representing four rainfall intensities for the two types of roof cladding materials, concrete tiles and corrugated steel. The sample collections were conducted on a weekly basis. Egodawatta et al. (2013) have shown that an appreciable amount of pollutant build-up will occur on a roof surface over a 7 day antecedent dry period.

2.2. Laboratory analysis

Samples collected were transported to the laboratory for testing, with sample handling and preservation undertaken according to AS/NZS (1998). Samples were tested for total suspended solids (TSS) as