Dear Reviewer,

Thank you very much for your scan and the valuable questions of our manuscript “Improvement of model evaluation by incorporating prediction and measurement uncertainty”. We have carefully considered your comments and detailed responses can be summarized as follows:

Comments: 1) The idea of evaluating the goodness of model fit by comparing the distributions of model predicted values and observed values is appealing. However, in typical setting of a hydrological/water quality modeling problem, the distributions of model predictions are constructed using certain “calibration” process, as already indicated in manuscript. The definition of measure of goodness of fit, which could be used for model evaluation such as the Nash–Sutcliffe model efficiency, should be able to be used to help reduce the parametric uncertainty of the model or, using the terms from GLUE, differentiate between “behavioral” and “non-behavioral” parameter sets. I did not see the CDFA approach proposed in this manuscript can function this way according to the description of the method provided in section 2.1. To put it another way, when there is knowledge of uncertainty or distributions of observed values, it is desirable to incorporate this knowledge into model calibration. However, it seems to me that the proposed CDFA approach does not provide a way to allow that information into model calibration and simply provides an alternative metric to summarize the model calibration results at the post-calibration stage. The utility of the new approach is therefore not significant.

Response: Thank for very much for this suggestion. I agree with your idea that the distributions of model predictions and measurement data should be used for the calibration process. In fact, the objective of this study is indeed to develop a new framework for model evaluation by incorporating prediction and measurement uncertainty. In traditional indicators (such as Nash–Sutcliffe model efficiency), the deviation between the measured and predicted data is expressed by the absolute distance \((O_i - P_i)\) between the paired data points. This method is questionable because it fails to incorporate prediction and measurement uncertainty. In this regard, we have developed an interval-deviation approach (IDA), which demonstrated that H/WQ models should be evaluated against both the nearest and farthest boundaries (the inherent uncertainty intervals). And this work has been published in Chen et al. (2014). However, we have noted that this IDA approach is suitable for incomplete data conditions, but when more data could be collected or when a continuous and random
data distribution could be assumed, these intervals may not always be practical. Thus, we have developed CDFA method.

The idea behind the CDFA was to replace the point-to-point comparison with the deviation between uncertain measured data and predicted data expressed as cumulative distribution functions. In fact, this is a modification of traditional good-of-fit indicators by replacing the calculations of their $O_1 - P_1$ term by using stochastic distances between the paired probability density functions (PDFs). Thus, this CDFA could be used during the calibration and validation process if PDFs could be obtained for both prediction data and measurement data (why we only did it during post-calibration stage would be explained below). This process could be described as below:

1) The prediction and measurement uncertainty are generated or assumed using previous knowledge.

2) The prediction and measurement data intervals are analysed, and the cumulative distribution functions of the prediction uncertainty ($F_o(x)$) and the measurement uncertainty ($F_p(x)$) are calculated.

3) The topological interval (area distance) between the two functions $F_o(x)$ and $F_p(x)$ is quantified.

4) The new $O_1 - P_1$ is quantified, and the modified evaluation indicators are used for model evaluation.

Based on the results obtained from this study, we found that the model performance worsened when a larger error range existed, and the choice of PDF affected the model performance, especially for non-point source (NPS) pollution predictions. These proposed methods could be extended to other goodness-of-fit indicators and other watershed models to provide a substitution for traditional model evaluations within an uncertainty framework. Thus, the authors do believe our method could be a substitute of traditional goodness-of-fit indicators and they could be used for the calibration and validation process.

However, it should be noted that we only compare the results between traditional Nash–Sutcliffe model efficiency and CDFA during certain “post-calibration” process. The reasons could be due to the imperfect knowledge of prediction uncertainty as well as the huge calculation effects. First, the meteorological-, geological-, hydrological-, and ecological processes in catchments are notably complex and are not always well known. Faced with such insufficient knowledge and natural randomness, uncertainty
becomes an inherent part of watershed modeling. On one hand, measurement uncertainty may stem from errors in flow measurements, water quality sample collection, the processes of preservation, storage, transport and laboratory analysis, could be fixed as certain PDFs. In a thorough review (Harmel et al., 2006), all possible errors in the H/WQ measured data were compiled, indicating that appreciable inherent errors exist in the measured data even when following strict quality assurance and quality control (QA/QC) guidelines (Beven et al., 2012). Thus, we could fix certain possible errors or PDFs for each H/WQ measured data and used them during the calibration or validation process. One the other hand, the prediction uncertainty is more complex due to different sources of uncertainty, uncertainty propagation, evaluation methods, uncertainty expression and the control of uncertainty. Beck (1987) reported that residual uncertainty exists even with the best model structure and input data. Thus, we could not set fixed PDFs or error range for prediction data due to insufficient knowledge and natural randomness. That is the main reason why we did not use the CDFA method during the whole calibration process. Second, it should be noted the CDFA is more complex than the traditional indicators so this method would take more running time. Although the increasing techniques expand the calibration process, the execution of CDFA (also for MCA) is computationally expensive and technical complex, especially for large numbers of simulations during the parameter optimization process. In this paper, we have tried the CDFA into the calibration process (only for CN2) but we found the computing time is large.

We agree with your idea that there are a number of concerns surrounding the application of this new algorithm in practice. In fact, we have focused on this issue (using the CDFA for model calibration) recently. First, we have considered different sources of uncertainty and the possible range of model performances in a real application. Second, we have incorporated a more realistic but simpler simulator to decrease the computational complexity while making full use of CDFA’s strengths. Thus, these issues would be solved in the future, and CDFA could be applied effectively for model calibration.

**Comments:** 2) As for the MCA approach, I am afraid I could not find which variables are discrete variables of interest in the case study designed to demonstrate the implementation of MCA approach (section 4.2). All SWAT output variables mentioned in the case studies seem to be continuous.

**Response:** In this study, two methods, the Cumulative Distribution Function
Approach (CDFA) and the Monte Carlo Approach (MCA), were proposed for different situations. For the CDFA, cumulative distribution functions were used to describe uncertain data because they are simple and do not depend on the distributional properties throughout the data sets. The MCA was proposed as a supplement to the CDFA when the uncertain data were discrete or when no specific distributions could be used. A flowchart of the model evaluation within the uncertainty framework is presented in Figure 1.

Previous studies have noted that if prediction uncertainty exists, the predicted data could be expressed as a confidence interval (CI) or a probability density function (PDF) (Franz and Hogue, 2011; Shen et al., 2012). Current research tends to express uncertain data as certain function distributions to express an error term (Zhang et al., 2009), which might lead to a more feasible expression than the traditional indicators. However, prediction uncertainty can be expressed as discrete variables of interest. For example, uncertainty related to rainfall is currently recognized as the major challenge for hydrological modeling science. Many previous studies have investigated uncertainty associated with measurement errors and spatial variability associated with rainfall. A number of researchers have investigated deviations in measured data, such as Sun et al. (2000), Kaventski et al. (2006), Bárdossy and Das (2008), McMillan et al. (2011). This uncertainty originates mainly from inaccuracy in measuring devices, local meteorological effects, and errors in data transmission. This kind of uncertainty could be expressed as confidence interval (CI) or a probability density function (PDF).

However, another important source of uncertainty that can be expressed as discrete variables also existed. For example, even in ideal conditions, where the dense and well-distributed gauges are available, the rain-gauge network cannot fully capture every point over the watershed. It is more common to have only a few stations distributed in space over the watershed. Rainfall at unknown points is thus estimated by means of interpolation techniques. Several techniques—such as the Centroid method, the Thiessen Polygon method, IDW and the Kriging method—have been used in spatial interpolation to produce information on the spatial distribution of rainfall (Mamillapalli, 1998; Chaubey et al., 1999; Bárdossy and Das, 2008; Hamed et al., 2009; Cho et al., 2009; Fu et al., 2011). It is therefore logical to take interpolation methods into account when determining the impacts of spatial rainfall variability on H/NPS predictions in large watershed.

We have investigated variability in spatial rainfall estimates associated with
interpolation methods on modeling in large watershed. In our previous studies, the uncertainty introduced by spatial rainfall variability was determined using a number of different interpolation methods. These comprehensively-used techniques are: 1) the Centroid method; 2) the Thiessen Polygon method; 3) the Inverse Distance Weighted (IDW) method; 4) the Disjunctive Kriging method, and 5) the Co-Kriging method. A semi-distributed model—the Soil and Water Assessment tool (SWAT) was used in a large watershed in the Three Gorges Reservoir Area (TGRA), China. The modeling outputs considered were flow, sediment, and total phosphorus (TP) at the watershed outlet. Results indicated that spatial interpolation techniques resulted in considerable uncertainty of rainfall spatial variability and transferred even larger uncertainty to H/NPS modeling. Similar studies could be also been found in our other previous studies. For example, we have been carried out into the effect of GIS data on water quality modeling and the uncertainty related to the combination of the available GIS maps (Shen et al., 2013). Besides, we have focused on the structural uncertainty caused by the algorithms and equations that are used to describe the phosphorus (P) cycle at the watershed scale. All these kinds of prediction uncertainty relating to limited model structures or model input datasets could result in discrete variables.

Thus, we also considered this kind of the measurement and prediction uncertainties, which might be expressed as discrete data. To incorporate this type of uncertainty, MCA was implemented using the Monte Carlo technique, which has been used in many hydrological uncertainty studies (Sun et al., 2008; Zhang et al., 2016). The Monte Carlo technique is a type of random sampling method that considers combinations of different input components and determines a statistical distribution for the output data (Shen et al., 2013). A key step is sampling variables randomly for discrete data so that the measurement and prediction data can be expressed as certain distributions. Here, \((O_i - P_i)\) was replaced by a stochastic expression of the deviation between pairs of data groups, and these stochastic deviations were then used to calculate the evaluation indicators.

Thank you very much for your wonderful job. Hope that our responses are satisfactory, and look forward to hearing from you. Best regards.

Best wishes,
Zhenyao Shen
Professor
School of Environment, Beijing Normal University, Beijing, China, 100875
Tel: +86-10-5880 0398
E-mail: zyshen@bnu.edu.cn
Reference:
Shen, Z. et al., 2013. Uncertainty in flow and water quality measurement data: A case study in the
