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Data Uncertainty Estimation Tool for Hydrology and Water Quality (DUET-H/WQ): Estimating Measurement Uncertainty for Monitoring and Modelling Applications

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Abstract: In spite of advanced modelling capabilities, hydrologic and water quality data remain vital for scientific assessment, management, decision-making, and modelling. Although uncertainty in measured data affects all of these applications, measurement uncertainty is typically ignored in monitoring projects. To change this, we published an uncertainty estimation framework for measured discharge and water quality data in 2006. From this framework, the Data Uncertainty Estimation Tool for Hydrology and Water Quality (DUET-H/WQ) was designed as a user-friendly tool to facilitate uncertainty estimation. DUET-H/WQ provides published uncertainty estimates for data collection procedures and then estimates the uncertainty within each procedural category as well as the cumulative uncertainty. The software estimates uncertainty for individual measured values as contributed by measurement and data processing and management. It does not account for uncertainties associated with spatial variability or influences of scale. The broad applicability of DUET-H/WQ was established by its application to data collected in five monitoring projects from a variety of watershed conditions. Results indicated that uncertainty in individual values was typically least for discharge, higher for sediment and dissolved N and P, and higher yet for total N and P. The uncertainty inherent in measured data has numerous economic, societal, and environmental implications; therefore, scientists can no longer ignore measurement uncertainty in data collection and reporting. It is our hope that DUET-H/WQ will contribute to making uncertainty estimation a routine component in hydrologic and water quality monitoring projects.

Measurement uncertainty also has important implications in modelling applications. The impact of uncertainty in model calibration and validation data is commonly discussed, but rarely included, in the evaluation of model accuracy. In order to change this oversight, we recently modified several goodness-of-fit indicators to incorporate measurement uncertainty into model calibration and validation. A similar method is currently being tested that incorporates both measurement and model uncertainty into model goodness-of-fit evaluation.

Keywords: *Data collection; discharge; water quality; model calibration; model validation.*

1. INTRODUCTION

In spite of advanced modeling capabilities, natural resource decision-making relies on measured environmental data, for which an understanding of data uncertainty is important in many aspects (Brown et al., 2005). Specifically for water resources, measured

hydrologic and water quality data remain vital for scientific assessment, management, and modeling (Silberstein, 2006). First, optimal water quality monitoring can only be achieved if measurement uncertainty and alternatives to reduce uncertainty are understood and considered in project design and implementation (Beven, 2006a; Harmel et al., 2006b; Rode and Suhr, 2007). Second, enhanced decision-making and stakeholder understanding can only be fully realized if measurement uncertainty is estimated and adequately communicated to other scientists, modelers, public interest groups, regulators, and elected officials (Collins et al., 2000; Bonta and Cleland, 2003; Reckhow, 2003; Nature, 2005; Beven, 2006a; Pappenberger and Beven, 2006). Similarly, analysis of uncertainty in measured data, which drive model calibration and validation, improves model application and enhances decisions based on modeling results (Reckhow, 1994; Kavetski et al., 2002; Pappenberger and Beven, 2006; Beven, 2006b; Shirmohammadi et al., 2006; Harmel and Smith, 2007).

According to Beven (2006a), the first step in advancing hydrologic and water quality science related to measurement uncertainty is determining realistic methods of representing that uncertainty. The value of uncertainty estimates, as well as the scientific integrity of communicating measurement uncertainty, prompted Harmel et al. (2006a) to make this initial step by developing a framework for quantifying the uncertainty in measured discharge and water quality (chemical constituent) data collected at the field and small watershed scale. That framework was then applied to estimate the cumulative uncertainty for a variety of arbitrary “data quality” scenarios. While several researchers (e.g. Gentry et al., 2007; McCarthy et al., 2008; Keener et al., 2008) have accepted and applied this framework, it can be cumbersome to apply to data sets with multiple values for multiple parameters. Therefore, we developed the Data Uncertainty Estimation Tool for Hydrology and Water Quality (DUET-H/WQ) and applied it to estimate the uncertainty in measured discharge and water quality data collected in several monitoring projects.

2. METHODS

2.1 Development of DUET-H/WQ

DUET-H/WQ (Harmel et al., 2008) was developed to be a user-friendly application of an existing uncertainty estimation framework for discharge and constituent flux measurements. The framework (Harmel et al., 2006a) contains two foundational components: 1) procedural categories within which to classify monitoring methods and 2) an established method for estimating cumulative uncertainty in individual measured values resulting from individual steps within procedural categories.

The first component established four procedural categories: Discharge Measurement, Sample Collection, Sample Preservation/Storage, and Laboratory Analysis. An additional category, Data Processing and Management, was later added to include uncertainty introduced by missing values, assumptions made to estimate missing values, and mistakes in data management and reporting.

The second component presented the Topping (1972) root mean square error (RMSE) propagation calculation and applied it to estimate cumulative or “combined” uncertainty in measured hydrology and water quality data. The RMSE method was selected for the framework because it is simple and has been widely applied to estimate cumulative uncertainty in individual discharge measurements (Cooper, 2002; Sauer and Meyer, 1992), in sediment volume estimates (Allmendinger et al., 2007), and in pesticide analytical methods (Cuadros-Rodriguez et al., 2002). Within the uncertainty estimation framework, the uncertainty from each step with each procedural category is propagated to produce a realistic uncertainty estimate, which is best termed “cumulative probable uncertainty” as represented by the probable error (eq. 1),

$$EP = \sqrt{\sum (E_Q^2 + E_C^2 + E_{PS}^2 + E_A^2 + E_{DPM}^2)} \quad [1]$$

where: EP = the probable error (\pm %), E_Q = uncertainty in discharge measurement (\pm %), E_C = uncertainty in sample collection (\pm %), E_{PS} = uncertainty in sample preservation/storage (\pm %), E_A = uncertainty in laboratory analysis (\pm %), and E_{DPM} = uncertainty in data processing and management (\pm %).

The RMSE calculation for individual measured values assumes that uncertainty is symmetric about the value and thus bi-directional with equal likelihood of over- and under-estimation and that errors for each procedural step are independent (Topping, 1972). Thus in the absence of contrary data, uncertainties for procedural steps are assumed to be independent and the covariance is omitted.

2.2 Application of DUET-H/WQ

The uncertainty estimation framework was initially applied to arbitrary best case, worst case, and typical scenarios in Harmel et al. (2006a). While those results can be used to establish reasonable uncertainty estimates in the absence of project-specific information, it was also important to apply the framework to real-world monitoring data to quantify uncertainty in actual field data. Thus, the DUET-H/WQ software tool based on this framework was applied to measured data from small watersheds in Texas (Riesel, Hamilton, and Austin), Indiana (Waterloo), and Ohio (Centerburg) (Harmel et al., 2008). These sites were selected to represent a wide range of monitoring conditions with respect to hydrologic setting, land use, watershed size, and field and laboratory techniques to demonstrate its broad applicability. For each measured data set, DUET-H/WQ was used to estimate the uncertainty in each step within each procedural category and to estimate the cumulative uncertainty for individual measured values. Specifically, uncertainties were estimated for individual discharge, total suspended solids (TSS), $\text{NO}_3\text{-N}$, $\text{PO}_4\text{-P}$, total N, and total P data.

A Beta version completed in December 2007 was used in the present analyses. This version is available at <ftp.brc.tamus.edu/pub/outgoing/gmitchell/DataUncertaintyEstimationTool/>. It is important to note that the DUET-H/WQ framework basis was developed for discharge, sediment, and nutrient data collection from small watersheds. Therefore, application to basin scale data and/or additional constituents may require appropriate adjustment.

The first step in applying DUET-H/WQ to estimate the uncertainty for individual measured values is to enter the individual data collection steps utilized to collect that data. To accomplish this, the user selects the appropriate techniques used and/or conditions encountered in the appropriate DUET-H/WQ lookup tables for the discharge measurement, sample collection, sample preservation/storage, and laboratory analysis procedural categories (Figs. 1-4). For these procedural categories, a DUET-H/WQ lookup table lists the common techniques utilized and monitoring conditions encountered along with published uncertainty estimates. These tables are based on Harmel et al. (2006a), which provides a detailed description of methodologies and associated uncertainties within each procedural category. Then, the user selects an appropriate uncertainty estimate from published uncertainty data displayed by the software. The user can adjust these uncertainty estimates based on project-specific information and/or professional experience. DUET-H/WQ then calculates the uncertainty introduced by each procedural category (eq. 1). The software then allows the user to input the uncertainty contributed by project-specific data processing and management issues (Fig. 5). Finally, DUET-H/WQ calculates the cumulative uncertainty for individual discharge, concentration, or load values (eq. 1). The user can choose to either apply that same estimated uncertainty to other data collected with the same procedure and under similar conditions or to repeat the uncertainty estimation procedure for other measured values.

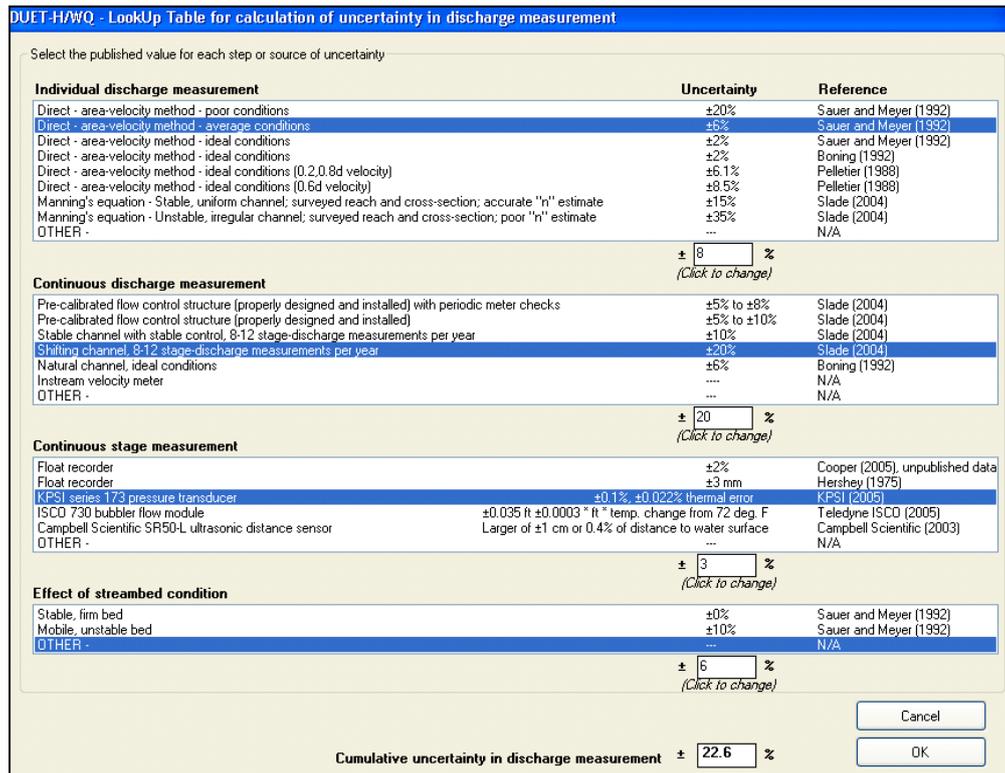


Figure 1. Example DUET-H/WQ Lookup Table for discharge measurement.

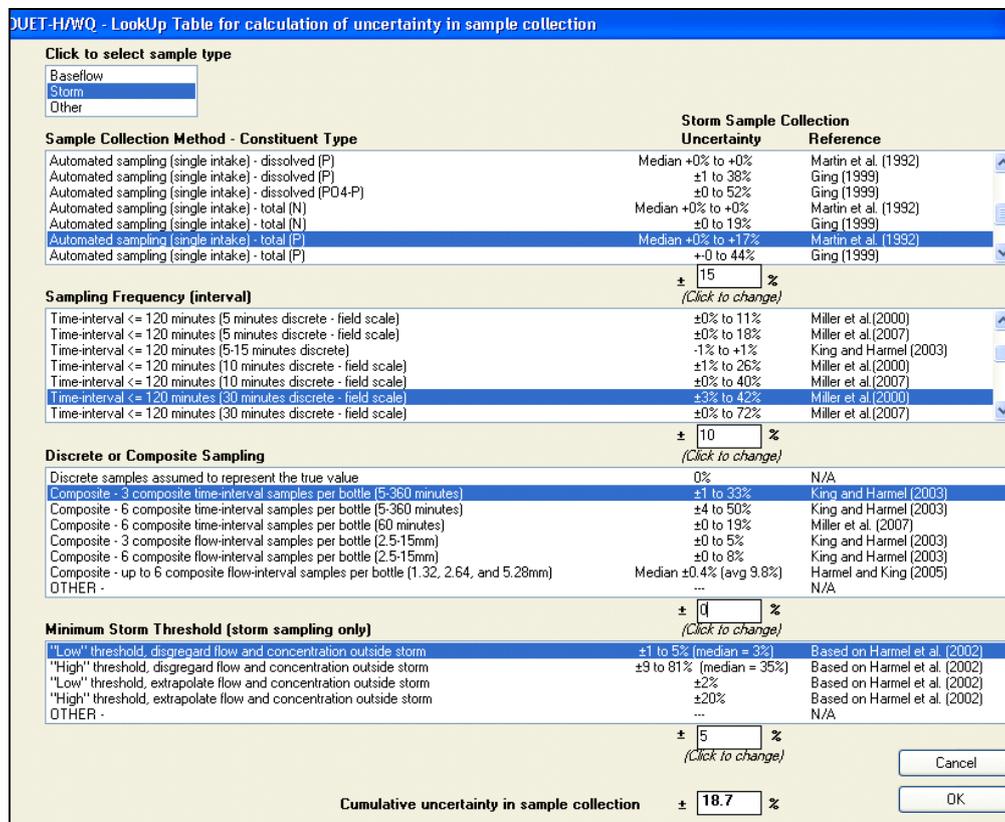


Figure 2. Example DUET-H/WQ Lookup Table for sample collection.

DUET-H/WQ - LookUp Table for calculation of uncertainty

Data on the contribution of individual steps within the sample are not available; therefore, cumulative uncertainty data result.

Click to select constituent

Total N(whole water sample) Total P(whole water sample) OTHER

Duration from sample collection until retrieval

Duration	Uncertainty
< 6 hours	...
< 1 day	...
1 to 3 days	...
> 3 days	...
OTHER -	...

± 10 %

Preservation/storage of sample prior to retrieval

(Click to enter)

Refrigeration	...
Filtration	...
Acidification	...
Unpreserved	...
Dark Environment	...
OTHER -	...

± 0 %

Duration from sample retrieval until analysis

(Click to enter)

< 1 day	...
< 1 week	...
< 1 month	...
1 to 3 months	...
> 3 months	...
OTHER -	...

± 10 %

Preservation/storage of sample prior to retrieval

(Click to enter)

Refrigeration	...
Filtration	...
Acidification	...
Unpreserved	...
Dark Environment	...
OTHER -	...

± 2 %

Cumulative uncertainty in sample preservation and storage ± 14.3 %

Figure 3. Example DUET-H/WQ Lookup Table for sample preservation/storage.

DUET-H/WQ - LookUp Table for calculation of uncertainty

DUET-H/WQ - Published Cumulative Uncertainty Data for Laboratory Analysis

Data on the contribution of individual steps within the sample are not available; therefore, cumulative uncertainty data result.

Click to select constituent

Total N(particulate) Total P(particulate) Total N(whole water sample) Total P(whole water sample) Done

Constituent - Total-P(Whole water sample)	Uncertainty	Reference
micro-Kjeldahl, colorimetric	median bias 0% to 4%	Ludtke et al. (2000)

Quality of Standards

Total P(whole water sample) Uncertainty

Commercial standard(s)	...
Make standard(s) - mass and volume determination	...
Dilute commercial standard(s) - volume determination	...
Other -	...

± 3 %

Pre-analytical processing

(Click to enter)

Digestion	...
Filtration	...
Drying	...
Other -	...

± 10 %

Quality of standard relationship(to determine sample concentration)

(Click to enter)

Concentration within standard range, good fit overall, similar range of concentrations for standards and sample	...
Concentration within standard range, good fit overall, standard concentration range exceeds sample concentration	...
Concentration within standard range, good fit overall, standard concentration range greatly exceeds sample concentration	...
Extrapolate concentration outside range of standards	...
Other -	...

± 10 %

Accuracy of analytical procedure/equipment

(Click to enter)

Ion specific electrode	...
Colorimetric	...
ICP	...
Combustion	...
Mass determination	...
Other -	...

± 5 %

Cumulative uncertainty in laboratory analysis ± 15.3 %

Figure 4. Example DUET-H/WQ Lookup Table for laboratory analysis.

DUET-H/WQ - Load Uncertainty

Click on each button below to estimate load uncertainty.

Select option

Use default load uncertainty

Calculate load uncertainty

(uncertainty ±%)

Calculate Discharge Uncertainty	22.6
Calculate Sample Collection Uncertainty	18.7
Calculate Preservation and Storage Uncertainty	14.3
Calculate Laboratory Analysis Uncertainty	15.3
Enter Data Processing and Management Uncertainty	0
Load Uncertainty	36

Cancel OK

Figure 5. Example DUET-H/WQ summary calculation for load uncertainty.

3. RESULTS AND DISCUSSION

In the five monitoring projects, uncertainties were estimated for measured data from a total of 131 storm events. The uncertainty in discharge measurements for individual storm events ranged from 7-27% with a median of 14% (Fig. 6). For TSS, the load uncertainty ranged from 15-35% with a median of 20%, and the uncertainty in concentrations ranged from 12-26% with a median of 18%. The uncertainty in TSS loads was typically less than other constituents because of limited post-collection transformation, relatively simple analytical procedures, and high concentration values. No equipment malfunction, which would have increased the uncertainty dramatically, occurred related to discharge or TSS data.

It is important to note that the uncertainty associated with measured concentrations is always less than or equal to that of measured loads. This reduction occurs because the discharge measurement procedural category (and its associated steps and uncertainty contribution) is irrelevant in concentration determination. The resulting reduction ranged from 10-37% depending on the relative magnitudes of other sources of uncertainty.

Little difference in uncertainty was evident between dissolved $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ (Fig. 6). The median uncertainty in $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ flux measured for individual events were 22-23% for loads and 17-19% for concentrations. Much higher uncertainty (up to 104%) occasionally occurred due to extreme high flows and missing samples. The reduction in uncertainty created by the irrelevance of discharge measurement in $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ concentrations ranged from 1-35%. The uncertainty in dissolved $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ loads was typically higher than in TSS loads because of post-collection transformation potential, more complex analytical procedures, and lower concentration values, which counteracted reduced difficulty in sample collection for dissolved constituents.

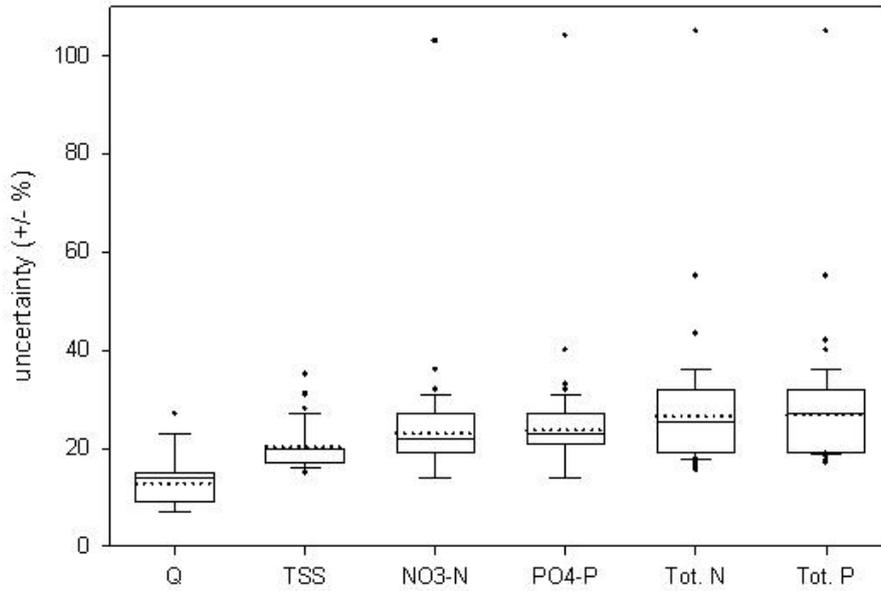


Figure 6. Uncertainty in individual storm discharge and constituent load values.

Similar to dissolved $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$, little difference in uncertainty occurred between total N and total P (Fig. 6). For individual loads, the uncertainty ranged from 15-105% (median = 25-27%) with increased uncertainties again occurring due to extreme high flows and missing samples. The uncertainties for measured concentrations ranged from 14-104% (median = 23-24%), which represents 0-25% uncertainty reduction compared to load uncertainty. The uncertainty in total N and P loads was typically higher than for TSS loads because of more complex analytical procedures. Total N and P load uncertainty was also higher than for dissolved loads because of increased difficulty in collecting representative particulate samples and additional analytical steps when total N and P were determined by summing dissolved and particulate fractions.

4. INCORPORATION OF UNCERTAINTY INTO MODEL EVALUATION

With uncertainty estimates for model calibration and validation data, this uncertainty can be used to enhance model evaluation. A correction factor was recently developed by Harmel and Smith (2007) to modify the error or deviation term (eq. 2) in several common goodness-of-fit indicators (Nash Sutcliffe coefficient of efficiency, E_{NS} ; Index of Agreement, d ; root mean square error, $RMSE$; mean absolute error, MAE). Although this correction factor (eq. 3) better represents model goodness-of-fit in the presence of measurement uncertainty, it does not consider the effect of model (prediction) uncertainty.

$$e_i = O_i - P_i \quad [2]$$

where: e_i = deviation between paired observed (O_i) and predicted (P_i) data.

$$eu2_i = \frac{CF_i}{0.5} \times (O_i - P_i) \quad [3]$$

where: $eu2_i$ = modified deviation considering measurement uncertainty, and CF_i = correction factor based on the probability distribution of each measured value.

In the presence of measurement and model uncertainty, it is more appropriate to evaluate models considering both sources of uncertainty. Thus, correction factors for measurement and prediction uncertainty were developed to enhance goodness-of-fit evaluation by producing realistic estimates of the deviations between measured values and model predictions (eq. 4).

$$eu3_i = \frac{\frac{CF(O_i)}{A} + \frac{CF(P_i)}{B}}{2.0} \times (O_i - P_i) \quad [4]$$

where: $eu3_i$ = modified deviation considering measurement and model uncertainty, $CF(O_i)$ = correction factor based on the probability distribution for each measured value, $CF(P_i)$ = correction factor based on the probability distribution for each predicted value, A = the value of the 1-sided probability of the measurement uncertainty distribution on the side corresponding to the predicted value, and B = the value of the 1-sided probability of the model uncertainty distribution on the side corresponding to the observed value.

These correction factors were developed based on the theory that the deviation between measured and predicted values should be adjusted accordingly to represent their relation to the other's uncertainty distribution (Fig. 7). The degree of overlap between corresponding measurement and predicted probability distribution functions (pdfs) is indicative of the model's predictive ability (Haan et al., 1995). The correction factors are currently being tested for several assumed uncertainty distributions (normal, symmetrical triangular, and uniform) by application to measured and corresponding predicted data sets.

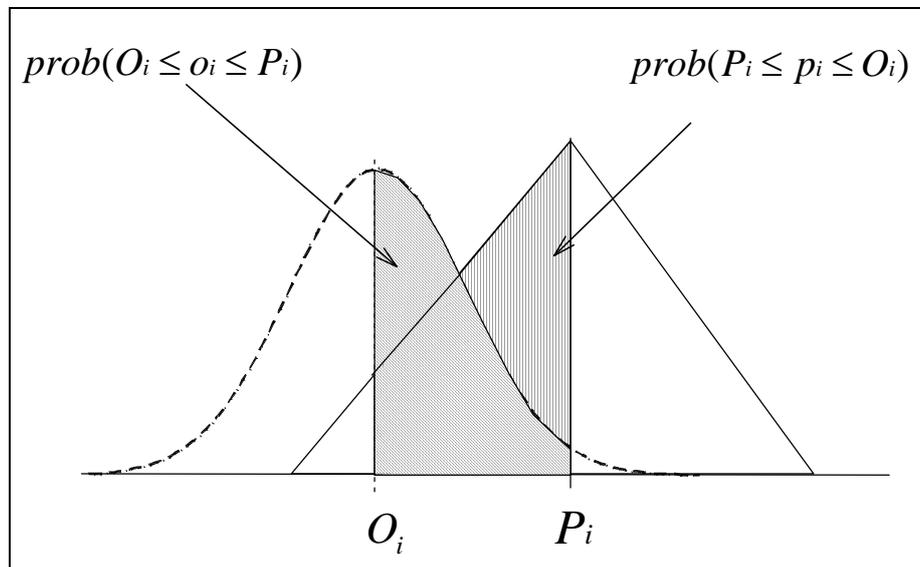


Figure 7. Graphical representation of correction factors that consider both measurement and model uncertainty (for the case $O_i < P_i$).

5. CONCLUSIONS

The multiple benefits of uncertainty estimates corresponding to hydrologic and water quality data (specifically improved monitoring design, enhanced decision-making, and improved model application and understanding) will not be fully realized without a

relatively simple, straight-forward procedure to estimate uncertainty. The Data Uncertainty Estimation Tool for Hydrology and Water Quality (DUET-H/WQ) was developed with these benefits in mind to be a user-friendly tool for data collectors and data users to estimate uncertainty in discharge and water quality data. DUET-H/WQ was designed to estimate the uncertainty contributed by measurement and data processing and management in *individual* values. As such, it does not directly account for influences of spatial variability (number and/or locations of sampling points within watersheds), changes in scale, or differences in sampling strategies (such as intensive storm sampling versus monthly grab sampling). DUET-H/WQ can, however, be used with GIS and modelling tools to address such issues.

Because of the economic, societal, and environmental implications of measurement uncertainty, it is important that uncertainty estimation become a routine procedure in hydrologic and water quality data collection and reporting. It is our hope DUET-H/WQ will contribute to this advancement.

The broad applicability of DUET-H/WQ was recently established by its application to data collected in five monitoring projects from a variety of watershed conditions. This application was important because the initial framework development and evaluation estimated the uncertainty only for arbitrary “data quality” scenarios not actual measured data. When applied to individual measured values the estimated uncertainty typically followed a predictable pattern ($Q < \text{TSS} < \text{dissolved N and P} < \text{total N and P}$).

With estimates of uncertainty for discharge and water quality measurements, which are often used as model calibration and validation data, the effects of measurement uncertainty on model accuracy can now be incorporated into model evaluation. Similarly, a method to incorporate both measurement and model uncertainty into model calibration and validation has been developed and will soon be available once testing is completed.

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