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Parameter Estimation for Groundwater Models under Uncertain Irrigation Data

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Abstract

The success of modeling groundwater is strongly influenced by the accuracy of the model parameters that are used to characterize the subsurface system. However, the presence of uncertainty and possibly bias in groundwater model source/sink terms may lead to biased estimates of model parameters and model predictions when the standard regression-based inverse modeling techniques are used. This study first quantifies the levels of bias in groundwater model parameters and predictions due to the presence of errors in irrigation data. Then, a new inverse modeling technique called input uncertainty weighted least-squares (IUWLS) is presented for unbiased estimation of the parameters when pumping and other source/sink data are uncertain. The approach uses the concept of generalized least-squares method with the weight of the objective function depending on the level of pumping uncertainty and iteratively adjusted during the parameter optimization process. We have conducted both analytical and numerical experiments, using irrigation pumping data from the Republican River Basin in Nebraska, to evaluate the performance of ordinary least-squares (OLS) and IUWLS calibration methods under different levels of uncertainty of irrigation data and calibration conditions. The result from the OLS method shows the presence of statistically significant ($p < 0.05$) bias in estimated parameters and model predictions that persist despite calibrating the models to different calibration data and sample sizes. However, by directly accounting for the irrigation pumping uncertainties during the calibration procedures, the proposed IUWLS is able to minimize the bias effectively without adding significant computational burden to the calibration processes.

Introduction

In addition to accurate representation of subsurface geology and boundary conditions, groundwater models require quantitative data on model source/sink (including recharge, evapotranspiration, and irrigation) and parameters (including aquifer transmissivity and storage coefficient). However, in most real-world groundwater modeling applications, data on source/sink and parameters are not readily available through direct measurements. Instead, the source/sink data are derived from extrapolations of few direct and/or indirect measurements, while the parameters are commonly estimated using inverse modeling or calibrations methods. A variety of approaches,

which are typically derived from crop-soil-water dynamics and remote sensing images, are presently available for estimating groundwater recharge (Healy and Scanlon 2010) and evapotranspiration (Jensen et al. 1990). However, these estimates often have considerable uncertainty resulting from natural variations in recharge and evapotranspiration and associated variables, vegetation cover, topography, climatic conditions, soil types, and geology, as well as differences between measurement and model scales (Rorabaugh 1964; Scanlon et al. 2002; Timlin et al. 2003; Allen et al. 2011).

Irrigation water withdrawals, on the other hand, represent point data that can be directly measured and readily used for model construction. However, in most groundwater model applications, irrigation records are limited and might not be reported accurately. In the United States, a majority of the states do not require farmers and other major water users to report groundwater withdrawal (Levin and Zarriello 2013). In some cases, complete records, including geographical locations and amount of withdrawal, may not be available because of legal and privacy issues. As a result, the irrigation withdrawal databases compiled by federal and state agencies contain mostly estimated values based on: (1) crop water demand plus irrigation acreage and application methods (Kenny et al. 2009), (2) electric power consumption along

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with irrigated acreage and pump capacity obtained during permit applications (Vincent 2003). Such estimates, however, can have considerable discrepancies from the actual pumping rates as demonstrated by Fanning et al. (2001) who have found as much as 40% discrepancy between the pump capacities on the permit and the actual pumping rates measured in 32 counties in the state of Georgia, USA. Large irrigation pumping uncertainty was also noted in the Death Valley, Nevada, USA, groundwater model (Belcher and Sweetkind 2010). Pumping data may also be available as a lumped sum, e.g., by county from the USGS National Water Use Information Program database, which may not match the spatial resolution for groundwater modeling. In addition, irrigation further complicates the estimation of recharge because it may simultaneously remove water from recharge sources and create new sources of diffuse recharge in the form of return flows (Garatuza-Payán et al. 1998), which can constitute a substantial amount of recharge in many irrigated farms, especially in arid or semiarid regions where natural recharge rates are low (Faunt 2009).

Despite these recognitions, uncertainty in irrigation data is often neglected in standard groundwater model calibrations and applications. Instead, the error in model prediction is mostly attributed to parameter and model structural errors. Assuming implicitly that the structural errors, including errors related to hydrogeological conceptualization and numerical representations, are white noise with no distinctive correlation and trend, the ordinary least-squares (OLS) method estimates model parameters such as aquifer transmissivity and storativity are estimated by minimizing the fitting errors between the model predictions and the corresponding observed values, such as groundwater heads and contaminant concentrations. However, the presence of systematic and random errors in the irrigation data might violate these assumptions, leading to biased estimates of parameters to compensate for these errors (Wang and Cai 2007a, 2007b; Rojas et al. 2008). This is because parameter estimation methods, which use the fitting errors between computed and observed values as objective functions, lack a mechanism to differentiate among the different sources of errors in the model and thus may result in parameter values that are adjusted not only for errors originating from parameterizations but also from other sources. This could potentially result in biased model predictions when the calibrated model is applied to different modeling conditions than those used for calibration (Demissie et al. 2009). Earlier studies by York (1966) and Carroll et al. (1995) demonstrated the presence of bias in the standard least-squares method when independent variables, such as pumping rates, are uncertain for linear and nonlinear regression models, respectively.

The traditional approach for dealing with source/sink (including irrigation) uncertainty is to include them along with model parameters during calibrations (Cooley 1979; Tiedeman et al. 1997; Sanford 2002). However, the temporal and spatial variability of the source/sink

as well as their likely correlation with hydrogeological parameters cause such approaches to have the potential to suffer from over-parameterization, non-uniqueness, and higher computational demand. Other commonly applied approaches often involve first estimating or calibrating the model parameters using the standard least-squares method and then applying the model to incorporate the source/sink uncertainty using an ensemble of Monte Carlo simulations (Thorsen et al. 2001; Starn and Bagtzoglou 2011), First order second moment (FOSM) estimates of confidence/prediction intervals (Dettinger and Wilson 1981; Townley and Wilson 1985; Kunstmann et al. 2002), and other related methods (e.g., Baalousha and Köngeter 2006). In these approaches, the prediction uncertainty is conditioned to the estimated parameter values as it uses the calibrated model to propagate the source/sink uncertainty to model output, which in turn may lead to an inaccurate estimate of the associated uncertainty in model predictions if the estimated parameters are biased (Kavetski et al. 2002; Huard and Mailhot 2006). The use of different measurements and data sizes for calibration fittings does not necessarily yield better calibration and uncertainty analysis if other sources of uncertainty are neglected during the calibration (Ajami et al. 2007). Refsgaard et al. (2007) emphasized the importance of properly incorporating uncertainties throughout the different stages of model development rather than just adding the components after the completion of the modeling work and calibration. Gupta et al. (2003) also highlighted the importance of accounting all sources of model uncertainty and calibrating against multiple measurements to improve model calibration.

This study uses the intrinsic linear relationship between groundwater pumping and head in a confined aquifer to develop a new and robust calibration approach for estimating the model parameters while explicitly taking pumping uncertainty into account. Specifically, the objectives of this paper are first to demonstrate the presence of bias in the OLS error parameter estimation when irrigation pumping are uncertain, and then to present an alternative inverse modeling technique called input uncertainty weighted least-squares (IUWLS), which explicitly accounts for the uncertainty in pumping rates during the calibration procedures with less computation burden than required by the commonly applied Bayesian and Monte Carlo based approaches. The approach does not estimate the pumping rates directly, and thereby avoids the aforementioned calibration challenges. Instead, we assume that the mean pumping rates and associated uncertainties are known in most cases. The uncertainties can then be used to adjust the weights in the calibration objective function and improve the calibration results. The issue of bias and the potential applicability of the proposed method are examined—analytically and numerically—using typical cases of irrigation pumping from an aquifer that is hydraulically connected to a river and using several hypothetical calibration conditions, which include different levels of pumping uncertainty, calibration data types, and sample sizes. The performance

Figure 1. Schematic of IUWLS, which adds the variance and weight computations shown within the broken line box to the standard generalized least-squares method. The variance propagation can be conducted based on analytical or Monte Carlo method depending on whether the relationships between model response and pumping rates are linear or nonlinear, respectively.

of the calibrated models for prediction is tested based on independent data of drawdown and stream depletion that are not used for calibrations.

The presented IUWLS approach is directly applicable to flow problems related to groundwater pumping from confined aquifer and its associated impact on groundwater head and stream connected to the aquifer. Under these conditions, both groundwater head and stream depletion are linearly related to pumping rates, thus allowing for propagating directly the pumping uncertainty to groundwater head or stream depletion. However, when the governing flow equation contains terms such as $h \frac{\partial h}{\partial x}$, $\left(\frac{\partial h}{\partial x}\right)^2$, or h^2 , as in the case of Boussinesq (1904) and Neuman (1972) equations for unconfined flow, the groundwater head response (h) is a nonlinear function of the pumping rates, and thus might require a numerical approach, such as the Monte Carlo method, which draws random values of pumping rates to estimate the variance in h resulting from pumping variance or uncertainty. However, depending on the size and complexity of the groundwater model, this could be computationally cumbersome. Alternatively, the unconfined flow can be approximated by confined flow if the change in saturated thickness is small (Sheets et al. 2014). This assumption is often applicable in practice, and the USGS has developed appropriate analytical solutions and approaches for linear systems (e.g., Barlow and Leake 2012). Once the variance is propagated from pumping to groundwater head, the remaining steps of the IUWLS (Figure 1) can be applied to estimate the aquifer parameters.

Methodology

Bias in Estimated Groundwater Model Parameters

The presence of bias in groundwater model calibration due to uncertain pumping rates is demonstrated using the classical Thiem (1906) equation that calculates groundwater drawdown caused by a constant rate of pumping in an infinite, confined, and homogenous aquifer using:

$$s = \frac{Q}{2\pi T} \ln\left(\frac{r}{R}\right) \quad (1)$$

where s is groundwater level drawdown at a radial distance r away from a pumping well, R is radius of influence or radial distance from the pumping well where the drawdown $s=0$ for a given constant pumping rate Q and aquifer transmissivity T . In standard groundwater model calibration, T is the only unknown variable in the equation and it can be estimated based on N observations of drawdown $\tilde{s}_i$ ($i = 1, 2, \dots, N$). The least-square estimate of T (or $\hat{T}$) requires minimizing the error objective function Φ :

$$\Phi = \min_T \left[\sum_{i=1}^N w_i (\tilde{s}_i - \hat{s}_i(\hat{T}))^2 \right] \quad (2)$$

which has a solution of (see Appendix S1 for the derivations):

$$\hat{T} = \frac{\hat{Q}^2}{2\pi \tilde{Q}} \frac{\sum_{i=1}^N w_i \ln(r_i/R)^2}{\sum_{i=1}^N w_i \tilde{s}_i \ln(r_i/R)} \quad (3)$$

where $\tilde{Q} = Q + \delta$, $\tilde{s}_i = s_i + \epsilon_i = \frac{Q}{2\pi T} \ln(r_i/R) + \epsilon_i$, Q is the true but unknown pumping rate, $\tilde{Q}$ is the estimated pumping rate with δ measurement or estimation error, s is the true but unknown drawdown, $\tilde{s}$ is the measured drawdown with ϵ measurement error, w is the objective function weight and depends on the drawdown measurement errors. In most practical applications, because of the indirect estimation of pumping rates as well as the presence of natural and instrument errors, the true values of pumping rate Q and drawdown s are not available for model construction. Assuming that the pumping and drawdown measurement errors are independent and uncorrelated, as well as $E(Y/X) \approx E(Y)/E(X)$ when sample size N is large (van Kempen and van Vliet 2000), the expected value of the estimated parameter $\hat{T}$ from Equation 3 is:

$$E(\hat{T}) = \frac{E(\tilde{Q}^2)}{2\pi E(\tilde{Q})} \frac{\sum_{i=1}^N w_i \ln(r_i/R)^2}{\sum_{i=1}^N w_i \left[\left(\frac{Q}{2\pi T} \ln(r_i/R) + \epsilon \right) \ln(r_i/R) \right]} \quad (4)$$

Note that the $\tilde{s}_i$ in Equation 3 is expressed in terms of the true discharge Q , transmissivity T , and measurement error ϵ in Equation 4. Considering that the drawdown

measurement $\tilde{s}$ is unbiased (i.e., $E(\epsilon)=0$), the above expected value can be simplified as:

$$E(\hat{T}) = \frac{E(\tilde{Q}^2)}{E(\tilde{Q})^2} T = \frac{(\text{Var}(\tilde{Q}) + E(\tilde{Q})^2) T}{E(\tilde{Q})^2} \quad (5)$$

If the pumping rates are known/measured accurately (i.e., $\text{Var}(\tilde{Q}) = 0$ and $E(\tilde{Q}) = Q$) and the drawdown measurements are unbiased (i.e., $E(\tilde{s}) = s$) but possibly uncertain, the expected value of $E(\hat{T}) = T$ which is unbiased estimate of the true transmissivity T . However, if the pumping rates are uncertain with variance $\text{Var}(\tilde{Q})$, then the expected value $E(\hat{T})$ becomes:

$$E(\hat{T}) = T \left[1 + \frac{\text{Var}(\tilde{Q})}{E(\tilde{Q})^2} \right] \quad (6)$$

This analytical result shows that the estimated transmissivity is positively biased, with the magnitude of the bias depending on the level of pumping uncertainty and the mean pumping rate (i.e., square of coefficient of variations of pumping). Consistent with the finding by Huard and Mailhot (2006) and Carroll et al. (1995) for regression models, the bias in Equation 6 does not depend on the calibration sample size, implying that calibrating the model using a large number of drawdown data may not minimize the bias caused by model input uncertainty when the standard least-squares calibration method is used. In general, using more data for calibration leads to better calibrations as long as parameters are the main sources of fitting errors between model results and observed values. However, as shown in Equation 6, this may not be necessarily the case if there are considerable uncertainties in the pumping data and are not accounted during the calibration. The estimate also remains biased even if we have done the calibration for multiple times using a large ensemble of random realizations of pumping drawn from a normal distribution of pumping rates, $N(\tilde{Q}, \sigma^2)$. In addition, even if it is a standard practice to estimate the transmissivity parameter using groundwater pumping and drawdown data during low pumping season and when the system is relatively stationary, the above result also indicates the potential bias in estimating the aquifer transmissivity under such low pumping conditions.

Input Uncertainty Weighted Least-Squares (IUWLS)

In order to address the bias in the OLS estimate of groundwater model parameters caused by pumping uncertainty, we propose a new parameter estimation method, known as IUWLS, which uses the general concept of the weighted least squares calibration method. It involves first computing the variance of the groundwater head or flux resulting from the variance of the pumping data, which is then combined with the variance of the head or flux measurements by assuming that the uncertainties in the pumping data and head or flux measurements are normally distributed and uncorrelated. This approach is different from the traditional OLS method, which

considers the weight as the inverse of the variance or uncertainty of calibration data alone. The combined variance is then used to determine the weight w of the least squares objective function given in Equation 2:

$$w_i = (\text{Var}(\tilde{s}_i) + \text{Var}(\hat{s}_i | \text{Var}(\tilde{Q})))^{-1} \quad (7)$$

where $\text{Var}(\tilde{s}_i)$ is the variance due to measurement errors of the calibration data (e.g., drawdown measurements for the Thiem equation) and $\text{Var}(\hat{s}_i | \text{Var}(\tilde{Q}))$ is the estimated variance of model output (e.g., drawdown) resulting from pumping data uncertainty. For confined saturated flow condition, the model outputs, such as groundwater head (or drawdown) and flux, are linearly related to the source/sink terms, such as groundwater pumping, recharge, and evapotranspiration (Hill and Tiedeman 2007). This allows estimating the $\text{Var}(\hat{s}_i | \text{Var}(\tilde{Q}))$ analytically if the pumping uncertainty or variance $\text{Var}(\tilde{Q})$ is known. In the case of nonlinear problem, such as unconfined and unsaturated flow, numerical approaches based on Monte Carlo method can be applied to estimate the variance on model outputs resulted from pumping uncertainty. The weight will decrease proportionally as the pumping uncertainty increases, leading to smaller value of the weighted least-squared error objective function. This can be interpreted as part of the fitting errors between modeled and observed values being attributed to pumping errors, instead of being exclusively attributed to parameter errors as in the case of the standard (OLS) calibration. Thus, the IUWLS allows constraining the calibration processes to a portion of fitting errors resulting from parameter errors and avoiding an over-fitting of the observed datasets. Unlike the standard weighted least-squares method where the weight w is predefined and fixed, the weight in the IUWLS is a function of parameters and is adjusted iteratively throughout the calibration process. The schematic of the procedure is shown in Figure 1.

Case Studies

Steady State Groundwater Pumping

For the steady-state pumping condition (Equation 1), first we estimate the variance of the drawdown resulting from pumping uncertainty using:

$$\text{Var}(\hat{s}_i | \text{Var}(\tilde{Q})) = \left(\frac{\ln(r_i/R)}{2\pi\hat{T}} \right)^2 \text{Var}(\tilde{Q}) \quad (8)$$

Normally, R (or radius of influence of pumping) varies with the pumping rate and the aquifer transmissivity, but in this case we have considered the potential variation in R because of pumping uncertainty to be relatively small in deriving Equation 8. Then, assuming that the uncertainties of pumping and drawdown measurements are independent, the resulting weight of the objective function becomes:

$$w_i = \left(\text{Var}(\tilde{s}_i) + \left(\frac{\ln(r_i/R)}{2\pi\hat{T}} \right)^2 \text{Var}(\tilde{Q}) \right)^{-1} \quad (9)$$

The weight depends on the parameter $\hat{T}$, whose actual value is not known, and thus the initial estimate is used to calculate the weight which will then be adjusted as the parameter value changes during the iterative calibration process. If we substitute the weight (Equation 9) and $\tilde{s}_i$ (Equation 1) into the objective function (Equation 1) and minimize it with respect to $\hat{T}$, the result is (see Appendix S2 for the derivation):

$$\hat{T} = \frac{\tilde{Q} \sum_{i=1}^N \tilde{s}_i \ln(r_i/R)}{2\pi \sum_{i=1}^N \tilde{s}_i^2} = \frac{\tilde{Q}}{Q} T \quad (10)$$

where Q is the true pumping rate and T is the true transmissivity. The above estimate is unbiased (i.e., $E(\hat{T}) = T$) as long as the drawdown measurements have no uncertainty. Otherwise, the full form of the weight in Equation 9 has to be used in the objective function to obtain an unbiased $\hat{T}$ estimate when the drawdown measurements are also uncertain. This is illustrated using a steady-state groundwater numerical problem (Figure 2), which consists of a single pumping well, five locations of drawdown measurements for calibration, and one location for drawdown prediction. The true transmissivity is considered to be 1500 ft²/day (139.35 m²/day). The numerical experiment was conducted for different levels of pumping uncertainty by varying the coefficient of variation of pumping from 0 to 1, and considering a 0.1 coefficient of variation for the drawdown measurements. For each level of uncertainty, we have drawn 2000 Latin-hypercube realizations of pumping rates from a normal distribution $N(\tilde{Q}, \sigma^2)$, and the corresponding $\hat{T}$ values are estimated using the OLS and IUWLS methods that are developed based on the MATLAB[®] optimization toolbox. Figure 3 compares the results from the OLS, IUWLS, and the analytical solution (Equation 6) as a function of pumping uncertainty. The results show that the value

of $\hat{T}$ estimated with the traditional OLS method is up to twice as large as the true value, which in return leads to underestimating the drawdown prediction by half when the coefficient of variation of pumping is 1. This result is not a surprise given $s \propto 1/T$. The IUWLS method, on the other hand, effectively reduces the bias in parameter and drawdown estimations.

Multiple Wells with Cyclic Pumping and Spatially Correlated Pumping Errors

Here we extend the analysis to groundwater drawdown and stream depletion problems caused by multiple and cyclic pumping wells. This case study is developed based upon parameters and irrigation data derived from the Republican River Compact Administration (RRCA) MODFLOW model, which has been used to evaluate impacts of large-scale irrigation pumping on groundwater levels and stream depletion in support of a surface water sharing compact agreed by the three basin states (Nebraska, Kansas, and Colorado) overlying the High Plains aquifer (Vincent 2003). The MODFLOW model uses estimates of irrigation pumping based on a combination of reported water use data, irrigated acreage, crop water demand, electrical energy use, and pumping power requirements obtained at the time of well registration (Vincent 2003). The available RRCA data also report annual water meter readings from a subset of more than 10,000 irrigation wells within the Nebraskan portion of the Republican River Basin. Meter readings are required as part of litigation associated with compliance with the interstate Republican River Compact. However, in order to provide consistent pumping estimates across the entire basin, and because each cell of the MODFLOW model (1 mile² [2.69e+6 m²]) may include multiple wells, the RRCA model smooths the individual well pumping data and thus introduces errors between the estimated and the measured well pumping data. The availability of metered pumping data, which is unusual for agricultural groundwater use, makes the RRCA data suitable for examining the modeling error related to irrigation data and for testing the performance of OLS and IWLSE calibration methods.

There are more than 25,000 irrigation wells in the Republican River Basin, each pumping on average from 3.5 × 10³ feet³ (1 × 10³ m³) to 106 × 10⁶ feet³ (3 × 10⁶ m³) of groundwater annually. The model irrigation type is center-pivot irrigation on quarter sections of land (i.e., a quarter-mile [402 m] long pivot on 160 acres [0.65 m²] of land). This configuration gives an average spacing between wells of about 0.5 mile (800 m) if center pivots are densely packed on quarter sections. Over large portions of the Republican River Basin, adjacent units of land have center pivots so that dense packing of pumping wells on a regularly spaced grid pattern is found. For this study, the analysis focuses on a representative array of equally spaced wells on a 3 × 3 grid adjacent to a river (Figure 4a). The average distance between the wells, average pumping rate, and spatial error covariance are determined based on 339 sets of similar nine well-field configurations that can be

Figure 2. Model setup for the steady-state pumping case study, showing the locations of pumping well, calibration wells, and prediction well.

Figure 3. OLS and IUWLS estimate of transmissivity (a) and the corresponding predictions of drawdown (b) at the prediction well for a single well steady state pumping case study. The dots represent the calibration and prediction results from the 2000 realizations.

extracted from the geospatial database of irrigation wells in the region (<http://www.republicanrivercompact.org/>). The distance from the river to the closest wells is assigned to be 2.5 miles (4000 m), based on a proposal by Kansas for the minimum distance from the Republican River and its tributaries to allow pumping in the region and to meet the compact requirements (Perkins and Larson 2007).

In order to estimate the pumping errors and covariance, two pumping rates for each set of nine wells are compared. First, the nine wells are assumed to pump at the same rate, given by averaging the annual pumping volumes from the wells in the selected dataset. This assumption corresponds to the RRCA MODFLOW methodology and how groundwater pumping estimates are generally determined. Second, the available metered pumping data at each well are considered to be actual or true pumping rates. For both pumping rates, the annual amount is uniformly distributed to the irrigation months in the region (June to September), and five years of seasonal pumping are considered for the test case (Figure 4b). Spatial analysis of the difference between estimated and metered pumping rates can then be used to determine a 9×9 spatial covariance matrix of the pumping errors. Figure 5 shows the histogram and semivariogram of the pumping errors. The semivariogram indicates the potential presence of spatial correlation in the pumping errors among wells located within the correlation length of 9.94 mile (16 km). In addition, given the spacing among the nine wells in each configuration, the semivariogram is used to determine the above covariance matrix. Finally, the effective transmissivity and storativity ($T = 1600 \text{ ft}^2/\text{day}$ [$147 \text{ m}^2/\text{day}$], $S = 3.5\text{e-}3$) for our case study were estimated from the RRCA groundwater model and used as true but unknown parameters.

Considering that the aquifer is confined, the impact of the above pumping conditions on drawdown was simulated using the transient Theis (1935) equation, with the principle of superposition developed by Earlougher (1977) and Kaweck (1993) to represent the multiple

wells, cyclic pumping and recovery phases, as well as the effect of the nearby river. For seasonally uniform pumping, the resulting drawdown $\tilde{s}$ at a given monitoring well location and at any arbitrary time t can be estimated using:

$$\begin{aligned} \tilde{s}_t &= \sum_{c=1}^{N_{ct}} \sum_{w=1}^{N_w} \frac{\tilde{Q}_{cw}}{4\pi T} \\ &\times \left(W(u_{cw}) - W(u'_{cw}) + W(u_{ci}) - W(u'_{ci}) \right) \\ \text{where: } u_{cw} &= \frac{r_w^2 S}{4T\tau_c}; \quad u'_{cw} = \frac{r_w^2 S}{4T\tau'_c}; \\ u_{ci} &= \frac{r_i^2 S}{4T\tau_c}; \quad u'_{ci} = \frac{r_i^2 S}{4T\tau'_c} \end{aligned} \quad (11)$$

The summations represent the temporal and spatial superposition, c is the number of cycles (or seasons) since the start of pumping, N_{ct} is number of pumping seasons up to time t , $\tilde{Q}_{cw}$ is the seasonal pumping rate at well w and season c , N_w is total number of pumping wells which in this case is 9, $W(\cdot)$ is the well function approximated by a fifth-order polynomial (Abramowitz and Stegun 1972), the first and third $W(\cdot)$ terms in Equation 11 represent the well functions for pumping wells w and image wells i , respectively, during all the pumping phases up to time t while the second and fourth $W(\cdot)$ terms represent the well functions for pumping and image wells during the recovery phases up to time t , τ_c and τ'_c are the times corresponding to the beginning and end of pumping for each season c prior to t , r_w and r_i is a radial distance from pumping well w and image well i , respectively, to the point where drawdown is measured, and T and S are the transmissivity and storativity of the aquifer. The resulting drawdowns at calibration and prediction points are presented in Figure 4c, with respective data points indicating the drawdown measurements used for calibration and validation. Data sampled during non-irrigation and irrigation

Figure 4. The transient case study setup containing nine irrigation wells (a) pumping seasonally (b), one drawdown measurement well sampled non-irrigation season for calibration and a drawdown prediction well sampled during irrigation season (c), and a stream depletion prediction point sampled during the entire seasons (d). The lines in (b) and (c) represent the true but known drawdown and stream depletion, respectively, while the markers represent the samples used for calibration and prediction.

seasons from different monitoring wells were used for the calibration and validation datasets, respectively. The effect of the river boundary condition is represented by adding one image well for every real well. A similar approach (i.e., the method of images, Fitts 2002) can be applied if there are other boundaries. If we have recharge, we can use numerical models and the variance from pumping and/or recharge can be propagated to model response analytically or numerically.

Figure 5. Histogram (a) and semivariogram (b) of the pumping errors between metered and estimated pumping data used for the RRCA model.

Following a similar procedure as in the previous case study, implementation of IUWLS requires first relating the pumping and drawdown uncertainties using:

$$\text{Var}(\tilde{s}_t | \text{Var}(\tilde{Q})) = \text{Var}\left(\sum_{c=1}^{N_{ct}} \sum_{w=1}^{N_w} \left(\frac{W(v_{cw})}{4\pi\hat{T}}\right) \tilde{Q}_{cw}\right)$$

Where: $W(v_{cw}) = W(u_{cw}) - W(u'_{cw})$

$$+ W(u_{ci}) - W(u'_{ci}) \quad (12)$$

Assuming that the pumping uncertainty is correlated spatially but is independent temporally, the variance can be simplified as:

$$\begin{aligned} \text{Var}(\tilde{s}_t | \text{Var}(\tilde{Q})) &= \sum_{i=1}^{N_{ct}} \text{Var}\left(\sum_{w=1}^{N_w} \left(\frac{W(v_{cw})}{4\pi\hat{T}}\right) \tilde{Q}_{cw}\right) \\ &= \sum_{c=1}^{N_{ct}} \sum_{j,i=1}^{N_w} \left(\frac{W(v_{ci})}{4\pi\hat{T}}\right) \left(\frac{W(v_{cj})}{4\pi\hat{T}}\right) \text{Cov}(\tilde{Q}_{ci}, \tilde{Q}_{cj}) \end{aligned} \quad (13)$$

where i and j are pumping well locations at distances r_i and r_j from a drawdown measurement point (Figure 4a), and $\text{Cov}(\tilde{Q}_{ci}, \tilde{Q}_{cj})$ is the spatial covariance of pumping error derived from the error semivariogram shown in Figure 5b. In order to test the performance of the OLS and IUWLS calibrations under different levels of uncertainty, instead of using the above covariance directly, we first calculate the corresponding correlation coefficient, which is then used with average pumping rates and coefficient of variation (CV) ranging from 0 to 1 to recalculate the error covariance associated with the selected CV. This covariance is then used in Equation 13 to determine the associated drawdown modeling error that is combined with the variance of drawdown measurement errors (assumed to be 10% of the measurement value) using a similar equation as Equation 9 to determine the weight of the objective function in the IUWLS method. For each level of uncertainty (or CV value) considered, the model is calibrated using OLS and IUWLS methods and 2000 random realizations of pumping rates drawn using a built-in MATLAB® function “lhsnorm” for Latin hypercube sampling from a normal distribution of pumping rates, $N(\bar{Q}, \text{Cov}(\tilde{Q}))$.

The calibrated model performance was evaluated for prediction of drawdown at a well not used for calibration and for prediction of stream depletion (Figure 4c and 4d). The stream depletion resulting from cycling groundwater pumping is calculated by superposition of the Glover and Balmer (1954) equation (Wallace et al. 1990; Hunt 1999), which estimates the rate and volume of stream depletion caused by a constant and steady groundwater pumping. The resulting stream depletion rate $\tilde{q}$ at time t is given as:

$$\tilde{q}_t = \sum_{c=1}^{N_{ct}} \sum_{w=1}^{N_w} \tilde{Q}_{cw} \times \left[\left(1 - \text{erf} \left(t_a / 4\tau_{cw} \right)^{1/2} \right) - \left(1 - \text{erf} \left(t_a / 4\tau'_{cw} \right)^{1/2} \right) \right] \quad (14)$$

where $t_a = r_w S / T$ is response time of aquifer to reach a new equilibrium after a pumping stress $\tilde{Q}_{cw}$ is first applied at a well located at a distance r_w away from the stream, τ_{cw} and τ'_{cw} are time elapsed after the pumping stress $\tilde{Q}_{cw}$ begins and stops, respectively.

Two calibration scenarios are considered: (1) estimating both transmissivity T and storativity S based on drawdown measurements collected during the non-irrigation seasons; (2) estimating T based on stream depletion data collected during the non-irrigation seasons. For case (2), the weight for the IUWLS objective function is determined based on the variance relationship between pumping error and prediction of stream depletion derived from Equation 14, plus the variance of the stream depletion measurement error, which is assumed in this case to be 10% of the depletion rate.

Results and Discussions

Figure 6 shows the normalized estimate of storativity vs. transmissivity for different levels of pumping uncertainty. In each case, the model is calibrated using the OLS and IUWLS methods, and 2000 random realizations of pumping drawn from the corresponding pumping distribution. Overall, the estimation bias from the OLS increases as the uncertainty in irrigation pumping increases. The proposed IUWLS significantly decreased these biases by up to 80–90%. For pumping coefficient of variation less than 0.5, the estimated storativity and transmissivity using OLS show minor bias as the normalized values of both parameters from the 2000 estimates clustered around 1. However, for higher coefficient of variation (CV = 1), the OLS estimates of the storativity and transmissivity can be more than 3 and 1.5 times that of the actual values, respectively. The IUWLS decreased these biases, with the estimates being about 1.5 and 1.1 times that of the actual values of storativity and transmissivity, respectively. The results also show that the storativity estimates from OLS is always higher than the actual value, while the transmissivity estimate can be lower or higher than the actual value depending on the pumping realizations. When the bias in the storativity is higher, the OLS tend to underestimate the transmissivity and vice versa. This correlation

Figure 6. Storativity and transmissivity estimates of OLS and IUWLS calibrations for different levels of pumping uncertainty normalized by their actual values, which is 0.0035 for storativity and 1600 ft²/day (148.6 m²/day) for transmissivity.

between the storativity and transmissivity biases is apparent in Figure 6, and is consistent to our expectation based on the negative correlation of the parameters values in the drawdown model (Equation 11). The spreads in the estimated parameters may indicate the non-uniqueness of the estimated values considering the calibration results have met the objective function criteria for all the realizations and level of pumping uncertainties. As the uncertainty in pumping increased, the potential for non-unique parameters estimation using OLS method also increased. The relatively narrower spreads of the IUWLS parameters estimations indicate that the approach helps to reduce the non-uniqueness issue.

The associated impacts on predicting drawdown and stream depletion are illustrated in Figure 7, which shows the normalized root mean square errors of the stream depletion and drawdown prediction at the non-calibration monitoring well location shown in Figure 4a. Overall, the impact of pumping uncertainty on the OLS parameter estimations and model outputs are minor for a pumping CV less than 0.5, and increase as the CV increases. Relative to the drawdown estimate, the impacts on stream depletion prediction are greater, with the root mean square errors exceeding 50% of the observed average stream depletion when the CV is greater than 0.7, while the drawdown errors are mostly about 30% of the actual drawdown levels. For higher pumping uncertainty, CV = 1.0, the error in the model predictions can be as high as 150% and 80% of the actual values

for stream depletion and drawdown, respectively, for some of the pumping realizations used. Both stream depletion and groundwater drawdown are linearly related to the pumping rate (Equations 11 and 14), making them equally sensitive to the uncertainty in the pumping rate. However, compared to the drawdown, the flux or the stream depletion is known to be more sensitive to the transmissivity and storativity errors. This sensitivity may be the main reason for the relatively higher impacts on stream depletion. On the other hand, the proposed IUWLS effectively reduced these prediction errors, resulting in roughly 10% or less error even when the CV of pumping is 1.0.

For Case 2, which uses stream depletion to calibrate the transmissivity while fixing the storativity to its true value of 3.5×10^{-3} , the transmissivity value estimated by the OLS method is less than the true transmissivity when there is uncertainty in pumping input data, with an underestimation of up to 25% when the CV is 1.0, which results in about 20% biases in both stream depletion and drawdown prediction. Compared to Case 1, the prediction biases, particularly those of the stream depletion are relatively small, which may partly attributed to the fact that only transmissivity is considered as unknown in this case. Despite trying different weighting methods, the higher correlation between storativity and transmissivity makes it difficult to estimate simultaneously their optimal values when stream depletion data are used for calibration. Similar to the previous case, the IUWLS is effective again in reducing these biases.

Finally, we have looked at the spatial distributions of drawdown errors (estimated minus actual drawdown) from the OLS and IUWLS results when CV of pumping is 0 and 1. We have discretized the study area using 50 ft (15.2 m) grids and computed drawdown for each grid using the radial distances between pumping wells and centers of the grids. When there is no pumping uncertainty, the OLS for Cases 1 and 2 provides accurate predictions of the drawdown throughout the modeling region, with the prediction error being randomly distributed and negligible. However, when the CV of pumping is 1 (Figure 8), the model in Case 1 under predicts the actual drawdown, especially near to the stream. Conversely, for Case 2, the model over predicts the drawdown when parameters from OLS are used. The prediction error in this case is large around the pumping wells and smaller close to the stream, with some neighboring regions showing relatively small bias and indicating the possibility that the bias may not be detected if the prediction wells are located in those less sensitive areas. In light of these observations for possible compensation of errors between Cases 1 and 2 calibration scenarios, future calibration efforts using both stream and drawdown measurements under different levels of pumping uncertainty may provide additional insight on the effectiveness of the OLS to address the potential parameter and prediction biases caused by input data uncertainty. Compared to the OLS results, the IUWLS method effectively reduced the error distributions for both Case 1 and Case 2 by an order of magnitude.

Figure 7. Predictions of drawdown and stream depletion for Case 1, normalized by their average values, which is 11.0 ft (3.35 m) and 94,662 ft³/day (8794 m³/day), respectively.

Figure 8. Drawdown error maps for Case 1 (a) and Case 2 (b) derived based on estimated model parameters by OLS and IUWLS, respectively, with uncertain pumping.

Conclusions

Most commonly, groundwater model parameters are estimated based on least squares error nonlinear regression techniques that assume model source/sink terms such as pumping rates are known. We used a hypothetical calibration scenario and real-world data to demonstrate that failure to account for pumping uncertainty during the calibration process can lead to biased estimates of the groundwater model parameters and to potentially erroneous predictions of the impacts of irrigation pumping on groundwater and stream flow. The bias remains despite calibrating the model several times using random realizations of pumping rates as model input and against different calibration datasets of different sizes. The bias in the model prediction may also be undetected or undermined depending on the locations the monitoring wells used for the model validation.

We have presented an alternative and effective calibration method, namely input uncertainty weighted least-squares (IUWLS), which allows simultaneous accounting of both model source/sink and parameter uncertainties and reduces the observed bias in model parameters and predictions. For saturated and confined flow, the approach uses the advantage of the linear relationship between source/sink and state variables of groundwater models to transform easily the forcing uncertainty to model outputs, which is then combined with the output measurement errors in order to determine the weights for the generalized least squares errors method. For nonlinear groundwater flow, the numerical approach is required to propagate the variance of source/sink to variance on model outputs. The resulting weights are a function of parameters and vary

during the calibration iterations. Although the presented case studies are limited to irrigation, the proposed method can be applied to incorporate recharge and evapotranspiration uncertainty in the groundwater model calibration. Further work is needed to implement the IUWLS in three-dimensional finite difference groundwater models such as MODFLOW and evaluate its performance when the probability distributions of source/sink and calibration data uncertainties are different than normal. The IUWLS needs to be tested for a more nonlinear system to understand advantages and limitations in a wider modeling context. Moreover, the errors in typical irrigation data are not well known and require further study to better characterize them in the IUWLS and other related parameter estimation and uncertainty analyzes methods. Calibrated hydrologic models are increasingly being used to estimate impacts of groundwater pumping on stream flow in order to adjudicate interstate water agreements. Thus, decisions based on calibrations have real economic consequences for water users, and so it is important to understand exactly how uncertainty may bias model calibration.

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is for descriptive purposes only and does not imply endorsement by the U.S. government.

Supporting Information

Additional Supporting Information may be found in the online version of this article:

Appendix S1. Derivation of the OLS optimal parameters and its expected values.

Appendix S2. Derivation of the IUWLS optimal parameters and its expected values.

References

- Abramowitz, M., and I. Stegun. 1972. *Handbook of Mathematical Functions*. New York: Dover Publications.
- Ajami, N.K., Q. Duan, and S. Sorooshian. 2007. An integrated hydrologic Bayesian multi-model combination framework: Confronting input, parameter and model structural uncertainty in hydrologic prediction. *Water Resources Research* 43, no. 1: W01403.
- Allen, R.G., L.S. Pereira, T.A. Howell, and M.E. Jensen. 2011. Evapotranspiration information reporting: I. Factors governing measurement accuracy. *Agricultural Water Management* 98, no. 6: 899–920.
- Baalousha, H., and J. Köngeter. 2006. Stochastic modeling and risk analysis of groundwater pollution using FORM coupled with automatic differentiation. *Advances in Water Resources* 29, no. 12: 1815–1832.
- Barlow, P.M., and S.A. Leake. 2012. Streamflow depletion by wells—Understanding and managing the effects of groundwater pumping on streamflow. U.S. Geological Survey Circular 1376. Reston, Virginia: U.S. Geological Survey.
- Belcher, W.R., and D.S. Sweetkind, eds. 2010. Death Valley regional groundwater flow system, Nevada and California—Hydrogeologic framework and transient groundwater flow model. U.S. Geological Survey Professional Paper 1711. Washington, DC: U.S. Geological Survey.
- Boussinesq, J. 1904. Recherches théoriques sur l'écoulement des nappes d'eau infiltrées dans le sol et sur le débit des sources. *Journal de Mathématiques Pures et Appliquées* 10, no. 5–78: 363–394.
- Carroll, R.J., D. Ruppert, and L.A. Stefanski. 1995. *Measurement Error in Nonlinear Models*. New York: Chapman & Hall.
- Cooley, R.L. 1979. A method of estimating parameters and assessing reliability for models of steady-state ground-water flow, 2. Application of statistical analysis. *Water Resources Research* 15, no. 3: 603–617.
- Demissie, Y., A. Valocchi, B. Minsker, and B. Bailey. 2009. Integrating a calibrated groundwater flow model with error-correcting data-driven models to improve predictions. *Journal of Hydrology* 364, no. 3/4: 257–271.
- Dettinger, M.D., and J.L. Wilson. 1981. First order analysis of uncertainty in numerical models of groundwater flow, 1. Mathematical development. *Water Resources Research* 17, no. 1: 149–161.
- Earlougher, R.C. 1977. *Advances in Well Test Analysis*. Henry L. Doherty Series, 5, Society of Petroleum Engineers of AIME. New York.
- Fanning, J.L., G.E. Schwarz, and W.C. Lewis. 2001. A field and statistical modeling study to estimate irrigation water use at benchmark farms study sites in southwestern Georgia, 1995–96. U.S. Geological Survey Water-Resources Investigations Report 00-4292. Atlanta, Georgia: U.S. Geological Survey.
- Faunt, C.C., ed. 2009. Ground water availability and flow in California's Central Valley. U.S. Geological Survey Professional Paper 1766. Reston, Virginia: U.S. Geological Survey.
- Fitts, C. 2002. *Groundwater Science*. New York: Academic Press.
- Garatuza-Payán, J., W.J. Shuttleworth, D. Encinas, D.D. McNeil, J.B. Stewart, H. DeBruin, and C. Watts. 1998. Measurement and modeling evaporation for irrigated crops in Northwest Mexico. *Hydrological Processes* 12, no. 9: 1397–1418.
- Glover, R.E., and G.G. Balmer. 1954. River depletion resulting from pumping a well near a river. *Transactions, American Geophysical Union* 35, no. 3: 468–470.
- Gupta, H.V., L. Bastidas, J.A. Vrugt, and S. Sorooshian. 2003. Multiple criteria global optimization for watershed model calibration. In *Calibration of Watershed Models, Water Science and Application*, Vol. 6, ed. Q. Duan, H.V. Gupta, S. Sorooshian, A.N. Rousseau, and R. Turcotte, 125–132. Washington, DC: American Geophysical Union.
- Healy, R.W., and B.R. Scanlon. 2010. *Estimating Groundwater Recharge*. Cambridge, UK: Cambridge University Press.
- Hill, M.C., and C.R. Tiedeman. 2007. *Effective Groundwater Model Calibration, with Analysis of Data, Sensitivities, Predictions, and Uncertainty*. New York: John Wiley & Sons Inc.
- Huard, D., and A. Mailhot. 2006. A Bayesian perspective on input uncertainty in model calibration: Application to hydrological model “abc”. *Water Resources Research* 42, no. 7: W07416.
- Hunt, B. 1999. Unsteady stream depletion from ground water pumping. *Ground Water* 37, no. 1: 98–102.
- Jensen, M.E., R.D. Burman, and R.G. Allen. 1990. Evapotranspiration and irrigation water requirements. ASCE Manuals and Reports on Engineering Practice No. 70, New York.
- Kavetski, D., S.W. Franks, and G. Kuczera. 2002. Confronting input uncertainty in environmental modelling. In *Calibration of Watershed Models, Water Science and Application*, Vol. 6, ed. Q. Duan, H.V. Gupta, S. Sorooshian, A.N. Rousseau, and R. Turcotte, 49–68. Washington, DC: American Geophysical Union.
- Kawecki, M.W. 1993. Recovery analysis from pumping tests with stepped discharge. *Ground Water* 31, no. 4: 585–592.
- van Kempen, G., and L. van Vliet. 2000. Background estimation in nonlinear image restoration. *Journal of Optical Society of America A* 17, no. 3: 425–433.
- Kenny, J.F., N.L. Barber, S.S. Hutson, K.S. Linsey, J.K. Lovelace, and M.A. Maupin. 2009. Estimated use of water in the United States in 2005. U.S. Geological Survey Circular 1344. Washington, DC: U.S. Geological Survey.
- Kunstmann, H., W. Kinzelbach, and T. Siegfried. 2002. Conditional first-order second-moment method and its application to the quantification of uncertainty in groundwater modeling. *Water Resources Research* 38, no. 4: 1035.
- Levin, S.B., and P.J. Zarriello. 2013. Estimating irrigation water use in the humid eastern United States. U.S. Geological Survey Scientific Investigations Report 2013-5066. Reston, Virginia: U.S. Geological Survey.
- Neuman, S.P. 1972. Theory of flow in unconfined aquifers considering delayed response of the water table. *Water Resources Research* 8, no. 4: 1031–1045.
- Perkins, S.P., and S.P. Larson. 2007. Future impacts of pumping on ground water consumptive use. No. 126, Original, In the Supreme Court of the United States.
- Refsgaard, J.C., J.P. van der Sluijs, A.L. Højberg, and P.A. Vanrolleghem. 2007. Uncertainty in the environmental modelling process—A framework and guidance. *Environmental Modelling & Software* 22, 11: 1543–1556.

- Rojas, R., L. Feyen, and A. Dassargues. 2008. Conceptual model uncertainty in groundwater modelling: Combining generalized likelihood uncertainty estimation and Bayesian model averaging. *Water Resources Research* 44, no. 12: W12418.
- Rorabaugh, M.I. 1964. Estimating changes in bank storage and groundwater contribution to streamflow. *International Association of Hydrological Sciences* 63: 432–441.
- Sanford, W.E. 2002. Recharge and groundwater models: An overview. *Hydrogeology Journal* 10, no. 1: 110–120.
- Scanlon, B.R., R.W. Healy, and P.G. Cook. 2002. Choosing appropriate techniques for quantifying ground-water recharge. *Hydrogeology Journal* 10, no. 1: 18–39.
- Sheets, R.A., M.C. Hill, H.M. Haitjema, A.M. Provost, and J.P. Masterson. 2014. Simulation of water-table aquifers using specified saturated thickness. *Ground Water*. DOI:10.1111/gwat.12164.
- Starn, J.J., and A.C. Bagtzoglou. 2011. Programs for calibration-based Monte Carlo simulation of recharge areas. *Ground Water* 50, no. 3: 472–476.
- Theis, C.V. 1935. The relation between the lowering of the piezometric surface and the rate and duration of discharge of a well using groundwater storage. *Transactions of the American Geophysical Union* 16: 519–524.
- Thiem, G. 1906. *Hydrologische Methoden*. Leipzig, Germany: Gebhardt.
- Thorsen, M., J.C. Refsgaard, S. Hansen, E. Pebesma, J.B. Jensen, and S. Kleeschulte. 2001. Assessment of uncertainty in simulation of nitrate leaching to aquifers at catchment scale. *Journal of Hydrology* 242, no. 3–4: 210–227.
- Tiedeman, C.R., D.J. Goode, and P.A. Hsieh. 1997. Numerical simulation of ground-water flow through glacial deposits and crystalline bedrock in the Mirror Lake area, Grafton County, New Hampshire. U.S. Geological Survey Professional Paper 1572. Denver, Colorado: U.S. Geological Survey.
- Timlin, D., J. Starr, R. Cady, and T. Nicholson. 2003. Comparing ground-water recharge estimates using advanced monitoring techniques and models. NUREG/CR-6836. Washington, DC: U.S. Nuclear Regulatory Commission.
- Townley, L.R., and J.L. Wilson. 1985. Computationally efficient algorithms for parameter estimation and uncertainty propagation in numerical models of groundwater flow. *Water Resources Research* 21, no. 12: 1851–1860.
- Vincent, M. 2003. Final report for the special master with certificate of adoption of RRCA groundwater model. State of Kansas v. State of Nebraska and State of Colorado, in the Supreme Court of the United States. No. 126, Original.
- Wallace, R.B., Y. Darama, and M.D. Annable. 1990. Stream depletion by cyclic pumping of wells. *Water Resources Research* 26, no. 6: 1263–1270.
- Wang, D., and X. Cai. 2007a. Optimal estimation of irrigation schedule—An example of quantifying human interferences to hydrologic processes. *Advances in Water Resources* 30, no. 8: 1844–1857.
- Wang, D., and X. Cai. 2007b. Dealing with unknown and biased errors in hydrologic modeling—A comparison of Kalman and H-infinite filters. *World Environmental and Water Resources Congress 2007*: 1–10. DOI:10.1061/40927(243)418.
- York, D. 1966. Least-squares fitting of a straight line. *Canadian Journal of Physics* 44, no. 5: 1079–1086.

Supporting Information

Appendix A: Derivation of the OLS optimal parameters and its expected values

Least-squares fitting objective function:

$$\begin{aligned}\Phi &= \sum_{i=1}^N w_i \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi \hat{T}} \right)^2 \\ \frac{\partial \Phi}{\partial \hat{T}} &= \sum_{i=1}^N \left[w_i \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi \hat{T}} \right) \frac{\tilde{Q} \ln(r_i/R)}{2\pi \hat{T}^2} \right] = 0 \\ &= \frac{1}{2\pi \hat{T}^2} \sum_{i=1}^N \left[w_i \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi \hat{T}} \right) \tilde{Q} \ln(r_i/R) \right] = 0 \\ &= \tilde{Q} \sum_{i=1}^N w_i \tilde{s}_i \ln(r_i/R) - \frac{\tilde{Q}^2}{2\pi \hat{T}} \sum_{i=1}^N w_i \ln(r_i/R)^2 = 0 \\ \hat{T} &= \frac{\tilde{Q}^2 \sum_{i=1}^N w_i \ln(r_i/R)^2}{2\pi \tilde{Q} \sum_{i=1}^N w_i \tilde{s}_i \ln(r_i/R)}\end{aligned}$$

Substitute $\tilde{s}_i$ and assume it is unbiased:

$$\hat{T} = \frac{\tilde{Q}^2 \sum_{i=1}^N w_i \ln(r_i/R)^2}{2\pi \tilde{Q} \sum_{i=1}^N w_i \frac{Q \ln(r_i/R)^2}{2\pi T}} = \frac{\tilde{Q}^2}{\tilde{Q} Q} T$$

The expected value is:

$$E(\hat{T}) = \frac{E(\tilde{Q}^2)}{E(\tilde{Q} Q)} T = \left(\frac{\text{Var}(\tilde{Q}) + E(\tilde{Q})^2}{E(\tilde{Q})^2} \right) T = \left(\frac{\text{Var}(\tilde{Q})}{E(\tilde{Q})^2} + 1 \right) T$$

Appendix B: Derivation of the IUWLS optimal and expected values

Weighted objective function, with the weight including the pumping uncertainty:

$$\begin{aligned}\Phi &= \sum_{i=1}^N \frac{(2\pi\hat{T})^2}{\ln(r_i/R)^2 \text{Var}(\tilde{Q})} \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right)^2 \\ \frac{\partial \Phi}{\partial \hat{T}} &= \sum_{i=1}^N \left[\frac{8\pi^2 \hat{T}}{\ln(r_i/R)^2 \text{Var}(\tilde{Q})} \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right)^2 + \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) \frac{4\pi\tilde{Q}}{\ln(r_i/R) \text{Var}(\tilde{Q})} \right] \\ &= \sum_{i=1}^N \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) \left[\frac{8\pi^2 \hat{T}}{\ln(r_i/R)^2 \text{Var}(\tilde{Q})} \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) + \frac{4\pi\tilde{Q}}{\ln(r_i/R) \text{Var}(\tilde{Q})} \right] \\ &= \sum_{i=1}^N \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) \left[\frac{8\pi^2 \hat{T} \tilde{s}_i}{\ln(r_i/R)^2 \text{Var}(\tilde{Q})} - \frac{4\pi\tilde{Q}}{\ln(r_i/R) \text{Var}(\tilde{Q})} + \frac{4\pi\tilde{Q}}{\ln(r_i/R) \text{Var}(\tilde{Q})} \right]\end{aligned}$$

To maximize the objective function, the derivation is set to zero

$$\begin{aligned}&= \frac{8\pi^2 \hat{T}}{\text{Var}(\tilde{Q})} \sum_{i=1}^N \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) \left[\frac{\tilde{s}_i}{\ln(r_i/R)} \right] = 0 \\ &= \sum_{i=1}^N \left(\tilde{s}_i - \frac{\tilde{Q} \ln(r_i/R)}{2\pi\hat{T}} \right) \left[\frac{\tilde{s}_i}{\ln(r_i/R)} \right] = 0 \\ &= \sum_{i=1}^N \frac{\tilde{s}_i^2}{\ln(r_i/R)} - \sum_{i=1}^N \frac{\tilde{s}_i \tilde{Q}}{2\pi\hat{T}} = 0\end{aligned}$$

Substitute $\tilde{s}_i$ and assume it is unbiased.

$$\hat{T} = \frac{\tilde{Q} \sum_{i=1}^N \tilde{s}_i \ln(r_i/R)}{2\pi \sum_{i=1}^N \tilde{s}_i^2} = \frac{\tilde{Q} \sum_{i=1}^N \frac{Q}{2\pi\hat{T}} \ln(r_i/R)^2}{2\pi \sum_{i=1}^N \left(\frac{Q}{2\pi\hat{T}} \ln(r_i/R) \right)^2} = \frac{\tilde{Q}}{Q} T$$

25

$$E(\hat{T}) = \frac{E(\tilde{Q})}{E(Q)} T = T$$

26

27

28

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