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Research papers

Towards reliable uncertainty quantification for hydrologic predictions, part II: Characterizing impacts of uncertain factors through an iterative factorial data assimilation framework

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ABSTRACT

In this study, an iterative factorial data assimilation (IFDA) framework is developed to holistically characterize the individual and interactive effects of various uncertain factors on hydrological predictions. The IFDA framework is flexible and is able to reveal the impacts from different numbers of uncertain factors. An iterative factorial analysis (IFA) approach is proposed in IFDA to diminish the biased variance estimation in traditional multilevel factorial designs and provide more reliable impact characterization for the considered factors. The proposed IFDA framework is applied to quantitatively reveal the individual and interactive effects of hydrological models, data assimilation (DA) methods, and uncertainties in inputs, streamflow observations and sample sizes on the deterministic and probabilistic predictions from data assimilation. The results indicate that the hydrological models, DA methods and their interactions would have the most dominant effects on hydrological predictions. This implies that different hydrological models or DA methods would produce significantly distinguishable results. When the hydrological model and DA method have been specified, uncertainties in streamflow observations would more likely have a visible effect on the accuracy of resulting predictions. Moreover, the inherent randomness, mainly caused by the Monte Carlo sampling procedures in data assimilation, would also have noticeable effects on the DA performances, especially when the hydrological model and DA method have been pre-identified. These results suggest that enhancement of hydrological models and data assimilation methods would be the most efficient pathway to generate reliable hydrological predictions.

1. Introduction

In a hydrologic prediction context, model simulations or predictions are subject to various uncertainties stemming from model inputs (i.e., forcing data), model structures, and model parameters (Liu et al., 2012). Sequential data assimilation (SDA) techniques are widely used for explicitly dealing with various uncertainties and for optimally merging observations into uncertain model predictions (Moradkhani et al., 2005a; Vrugt et al., 2005; Clark et al., 2008; Xie and Zhang, 2013). In SDA, the state variables and parameters in a hydrologic model can be continuously updated when new measurements are available, which can provide probabilistic quantifications for model parameters, states as well as the resulting predictions. The ensemble Kalman filter (EnKF) and particle filter (PF) are two of the most widely used sequential data assimilation schemes. The approaches of EnKF, PF and their variants have been widely used in hydrologic data assimilation (e.g. Moradkhani et al., 2005a; b; Parrish et al. 2012; Pathiraja et al. 2016a, b; Fan et al., 2015; 2017a; b).

For a data assimilation (DA) scheme, its performance is generally influenced by a number of factors such as the hydrological model and data assimilation algorithm to be employed, uncertainty reflections in inputs and outputs (e.g., streamflow observations), as well as other factors. A number of studies have been proposed in the past decades to improve hydrological data assimilation through various aspects. For instance, advanced data assimilation approaches, based on the benchmark methods of EnKF and PF, have been proposed in order to alleviate the shortcomings in EnKF and PF. Some of these approaches include the normal-score ensemble Kalman filter (NS-EnKF) method (Xu and

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Gomez-Hernandez, 2016), partitioned update Ensemble Kalman filter (PU_EnKF) method (Xie and Zhang, 2013), particle Markov chain Monte Carlo (PMCMC) method (Moradkhani et al., 2012; Vrugt et al., 2013), implicit particle filter method (Chorin and Tu, 2009; Rafiee et al., 2013), Copula-based particle filter (CopPF) method (Fan et al., 2017a) and also integrated data assimilation methods (Shen and Tang, 2015; Fan et al., 2017b). The results indicate that those advanced data assimilation approaches are able to provide better predictions than traditional EnKF and PF methods in some cases. In addition to the improvement of data assimilation methods, there are also studies to address other impact factors in data assimilation. For example, Xue and Zhang (2014) proposed a multimodel data assimilation method by embedding the EnKF into the Bayesian model averaging framework to account for the uncertainty stemming from the model itself. Ocio et al. (2017) addressed the role of rating curve uncertainty in real-time flood forecasting through data assimilation, in which they has demonstrated that a standard flow measurement error can still represent a reasonable trade-off between complexity and realism when the rating curve is well-defined. A state-dependent model uncertainty estimation method (named SDMU) was proposed by Pathiraja et al. (2018) to characterize model uncertainty in data assimilation studies, in which an objective data-driven approach is adopted to estimate the transition uncertainty in model simulations. Moreover, Liu et al. (2012) has argued that the “optimality” of data assimilation depends critically on the reliability of error estimates for the inputs and the model itself, as well as the proper consideration of interdependencies and interactions among uncertain model components and/or observations. Nevertheless, the extensive test conducted by Thiboult and Anctil (2015) suggests that the updated state variables and the hyper-parameters for reflecting uncertainties in forcing data and outputs should be carefully specified for the optimal implementation of EnKF, but there is no single and universal optimal EnKF implementation for any model.

Amounts of research works, from improvement of DA methods to better quantification for uncertainties in forcing data and outputs, have been proposed in order to enhance the predictability of hydrological data assimilation. However, the performance of a data assimilation scheme is not only influenced by the individual effects from the hydrological model, DA approaches, and uncertainties in forcing data (i.e. inputs) and outputs (e.g., streamflow observations), but also shaped by the interactive effects among these factors. Wang et al. (2017) proposed a robust data assimilation system (RDAS) to adopt a multi-factorial design to examine the individual and interactive effects of uncertainties in inputs, outputs and sample sizes on the performances of EnKF. The results indicated the pairwise interaction between perturbed precipitation and streamflow observations would have the most significant impact on the performance of the EnKF system. However, such a conclusion is obtained for EnKF whilst the impacts from hydrological models and different DA methods are not considered. The results in our companion paper (Fan et al., 2022) have shown that, for the same uncertainty settings in inputs, outputs (i.e., streamflow observations) and sample size, noticeable differences in prediction accuracies can be observed in the results from different DA methods over different hydrological models. Wang et al., (2022) developed a disaggregated multilevel factorial hydrological data assimilation model to investigate the impacts of EnKF and its variants. Lyu and Fan (2021) characterized the impacts of inputs and streamflow observations on different DA methods through the multilevel factorial analysis. Nevertheless, the impact from hydrological models is still overlooked. Moreover, the applicability of the multi-factorial design adopted in previous studies (e.g., Wang et al., 2017; Lyu and Fan, 2021; Huang and Fan, 2021) is restricted by its biased variance estimator, which would lead to underestimations for the variance especially in small sample sizes (Bosshard et al., 2013; Fan et al., 2020; 2021; Di et al., 2021). The iterative factorial analysis (IFA) approach, developed by Fan et al. (2020; 2021), is able to diminish the biased variance estimation in traditional multilevel factorial designs through a subsampling decomposition procedure for those factors with multiple levels. But the IFA approach has only been applied to investigate the impacts of uncertain factors on multivariate risk inferences for compound extremes such as flood peaks and volumes. The applicability of IFA in characterizing the impacts of uncertain factors on hydrological data assimilation has not been demonstrated.

Consequently, this research is to propose an iterative factorial data assimilation (IFDA) framework to reveal both the individual and interactive effects of hydrological models, DA approaches, uncertainties in inputs, streamflow observations and sample sizes on the performances of hydrological data assimilation schemes. As an extension of our companion study, the data assimilation with different uncertainty scenarios will be introduced into IFA method to formulate the IFDA framework. Compared with previous studies (e.g., Wang et al., 2017), the innovations of this study include: (i) a flexible framework is developed to explicitly quantify the effects for uncertain factors on the performances of data assimilation, in which the “flexibility” indicates IFDA is able to analyze different numbers of factors with different levels; (ii) the IFA method in the IFDA framework can generate more reliable quantification for the effects of uncertain factors on both deterministic and probabilistic predictions from data assimilation. This research can also demonstrate the extensive application potentials of the IFA method developed by Fan et al. (2020; 2021) for different hydrological problems. The applicability of IFDA framework will be demonstrated at the River Ouse in UK. The obtained results can help reveal the dominant impact factors for hydrological data assimilation and further identify the most efficient pathway to enhance the predictability of data assimilation.

2. Methodology

2.1. Uncertainties in hydrological data assimilation

Sequential data assimilation approaches have been widely employed for real-time streamflow forecasting. Consider a generic hydrological model consisting of functions for state transition (i.e. $g(.)$) and observational operator (i.e. $h(.)$) as follows:

$$x_t = g(x_{t-1}, u_t, \theta_t) + \omega_t \tag{1}$$

$$y_t = h(x_t \theta_t) + v_t \tag{2}$$

Extensive uncertainties exist in the data assimilation process for the above modelling system. These uncertainties may be embedded in various components such as model structural uncertainty (i.e., $g(.)$ and $h(.)$ in Equations (1) and (2)), uncertainties in the forcing data (i.e., $\boldsymbol{u}$ in Equation (1)), different data assimilation methods and uncertainty in streamflow to be assimilated. These uncertainties may pose significant impacts on the resulting hydrological predictions.

(1) Model structural uncertainty

A hydrological model is developed through a series of mathematical equations to represent the water processes in a catchment. There are uncertainties in the development of hydrological models since the proposed equations are generally simplified representations of real processes. Different model developers would employ different equations or mechanisms to describe different components in the rainfall-runoff process of a catchment. A typical example is that there are two major categories of hydrologic models, physical-based distributed models and lumped conceptual models. The physical-based distributed models divide a catchment into grid cells at fine resolution and assimilate different terrain data and precipitation to different cells (Chen et al., 2016). In comparison, the lumped conceptual models would use the same value of parameters for the whole watershed, ignore the spatial variability, and provide catchment runoff results in a spatially averaged way (Tran et al., 2018; Jaiswal et al., 2020; Hu et al., 2021). Furthermore, there are also extensive uncertainties even for the same category of hydrological models. For instance, the Hymod proposed by Moor (2007) employs three identical quick-flow tanks to route surface flow, while the IHACRES model proposed by Jakeman et al. (1990) uses a linear module consisting of two parallel linear stores to translate effective rainfall into streamflow. Therefore, the Hymod and IHACRES, as described in our companion paper (Fan et al., 2022), applied different mechanisms to model the rainfall-runoff process. This implies that for the same dataset at one catchment, different models would produce distinguishable predictions due to the structural uncertainty in hydrological models.

(2) Data assimilation methods

Sequential data assimilation (SDA) approaches have been widely used to quantify uncertainties for parameters and state variables for a hydrological model and provide probabilistic predictions. Similar to the hydrologic model development, different SDA approaches are distinguishable among each other. For instance, the traditional particle filter (PF) method (Moradkhani et al., 2005b) generally employs a stochastic perturbation technique to evolve model parameters to the next step. Improving upon the PF method, the particle Markov chain Monte Carlo (PMCMC) (Moradkhani et al., 2012) use the Metropolis acceptance ratio mechanism to determine the acceptance of the proposed parameter candidate generated by the stochastic perturbation algorithm. Moreover, the particle copula Metropolis-Hastings (PCMH) method developed in the companion paper (Fan et al., 2022) adopts a mixed evolution algorithm, consisting of a copula sampling and stochastic perturbation schemes, to generate the proposed parameter candidates and then uses the Metropolis acceptance ratio mechanism to determine their acceptance. Also, as demonstrated in the companion paper (Fan et al., 2022), different SDA approaches may have different performances on uncertainty quantification for hydrologic models and thus produce different streamflow predictions.

(3) Uncertainties in forcing data

In hydrological prediction, uncertainties embedded in the forcing data (i.e. $\boldsymbol{u}_t$ in Equation (1)), resulting from sampling and measurement errors are one of the major uncertain sources under consideration. Some approaches have been proposed to reflect uncertainties in the forcing data, and the stochastic perturbation method has been widely adopted in hydrological data assimilation (e.g. Clark et al., 2008; Liu et al., 2012; Fan et al., 2015; Leach et al., 2018). A generic formulation for the stochastic perturbation approach can be formulated as follows:

$$u_t^i = u_t + \xi_t^i \tag{3}$$

where u_t^i is the randomized forcing data at time t for sample member i, u_t is the original forcing data, and ξ_t^i is the noise added to the forcing data to generate the ith sample member (Leach et al., 2018). For different forcing data, different noise distributions would be employed to generateξ_t^i. In general, the Gaussian distributed noise is recommended for the forcing data such as temperature and potential evapotranspiration, which is formulated as (Moradkhani et al., 2005a; Fan et al., 2017a, b; Leach et al., 2018):

$$\xi_t^i \sim \tilde{\mathrm{N}}\left(0, \sum_t^u\right), \ \sum_t^u = \gamma u_t \tag{4}$$

where γ is the proportional factor. For the precipitation which is recognized as the most influential uncertain model input, the lognormal distributed noise is recommended by some studies expressed as follows (e.g. Leisenring and Moradkhani, 2012; DeChant and Moradkhani, 2012; Leach et al., 2018):

$$\xi_t^i \sim \log N\left(0, \sum_t^u\right), \ \sum_t^u = \gamma u_t \tag{5}$$

(4) Uncertainties in streamflow observations

In additional to the uncertainties existing in the forcing data, the random errors, in observations is also one of the major uncertain sources need to be well reflected. Errors in streamflow observations arise from several sources such as errors in river stage measurement, and errors in the rating curve used to transform stage to discharge (McMillan et al., 2013). Some approaches have been proposed to reflect observational uncertainties (e.g. McMillan et al., 2013; Ocio et al., 2017; Pathiraja et al., 2018). The Gaussian random error is the most common one and has been adopted in a number of hydrological data assimilation studies (e.g. Rakovec et al., 2012; DeChant and Moradkhani, 2012; Leach et al., 2018; Liu et al., 2019), which can be formulated as follows:

$$Q_t^i = Q_t + v_t^i, \ v_t^i \sim \tilde{\mathrm{N}}(0, \ \eta Q_t) \tag{6}$$

where η is the proportional factor for the streamflow.

2.2. Iterative factorial analysis

The hydrological predictions for one catchment would be greatly influenced by various uncertain factors such as the hydrologic models to be used, the parameter estimation approaches, random errors in forcing data and streamflow observations. Consequently, it is of great importance to characterize both the individual and interactive effects of those uncertain factors on the resulting hydrologic predictions. To address this challenge, an iterative factorial analysis (IFA) approach would be proposed to reveal the dominant factors on hydrological predictions.

The proposed IFA approach improves upon traditional factorial analysis (FA) method, in which a subsampling procedure would be adopted for those multi-level factors and generate a series of two-level experimental designs. The main and interactive effects of the chosen factors are obtained through averaging the main and interactive effects of all the two-level experimental designs. Such a process will be illustrated through a generic example with three factors. Consider a hydrologic prediction system and its predictability is assumed to be influenced by factors A, B, and C as follows:

$$Y = F(A, B, C) \tag{7}$$

Here A, B, and C are factors to be considered, which can be either numeric (e.g. proportional factors in forcing data or streamflow) or non-numeric (e.g. hydrologic models or data assimilation approaches). $F(.)$ is the generic hydrologic prediction system. Y is the index to evaluate the predictability of the system such as root-mean-square error (RMSE), and Nash-Sutcliffe efficiency (NSE) coefficient and continuous ranked probability score (CRPS).

If each factor has M levels, a subsampling procedure would be adopted in IFA to decompose the M levels into a total number of $\begin{pmatrix} M \\ 2 \end{pmatrix}$ two-level pairs, expressed as a $2 \times \begin{pmatrix} M \\ 2 \end{pmatrix}$ matrix as follows:

$$g_A(h_A, j_A) = \begin{pmatrix} A_1 & A_1 & \cdots & A_1 & A_2 & A_2 & \cdots & A_{M-2} & A_{M-2} & A_{M-1} \\ A_2 & A_3 & \cdots & A_M & A_3 & A_4 & \cdots & A_{M-1} & A_M & A_M \end{pmatrix} \tag{8a}$$

$$g_B(h_B, j_B) = \begin{pmatrix} B_1 & B_1 & \cdots & B_1 & B_2 & B_2 & \cdots & B_{M-2} & B_{M-2} & B_{M-1} \\ B_2 & B_3 & \cdots & B_M & B_3 & B_4 & \cdots & B_{M-1} & B_M & B_M \end{pmatrix} \tag{8b}$$

$$g_C(h_C, j_C) = \begin{pmatrix} C_1 & C_1 & \cdots & C_1 & C_2 & C_2 & \cdots & C_{M-2} & C_{M-2} & C_{M-1} \\ C_2 & C_3 & \cdots & C_M & C_3 & C_4 & \cdots & C_{M-1} & C_M & C_M \end{pmatrix} \tag{8c}$$

Here $g(h, j)$ indicates the matrix generated from the subsampling of a multi-level factor in which the column index $j = 1{:}\begin{pmatrix} M \\ 2 \end{pmatrix}$ represents one two-level pair and $h = 1{:}2$ shows the two corresponding levels. For instance, if the factor of DA is assigned with three levels with each level representing a DA algorithm (e.g., PF, PMCMC, PCMH), these three levels would be decomposed through the subsampling procedure to formulate a $2 \times \binom{3}{2}$ matrix as: $\begin{pmatrix} PF & PF & PMCMC \\ PMCMC & PCMH & PCMH \end{pmatrix}$. Moreover, the factors A, B and C can have different levels which also lead to decomposed two-level pair matrices similar to Equations (8a)–(8c). The subsampling procedure in Equations (8a)–(8c) would result in $\binom{M}{2} \times \binom{M}{2} \times \binom{M}{2}$ iterations in IFA with each iteration consisting of a two-level factorial design. One iteration in IFA is to conduct one two-level factorial design formulated by one column from the decomposed matrices for A, B and C.

In the proposed IFA approach, each iteration from the subsampling procedure will lead to a two-level factorial design. According to the ANOVA theory (Montgomery, 2000), the total variability of Model (1), denoted as the total sum of the squares (SST), can be decomposed as follows:

$$SS_T^{(i)} = SS_A^{(i)} + SS_B^{(i)} + SS_C^{(i)} + SS_I^{(i)} \tag{9a}$$

$$SS_I^{(i)} = SS_{AB}^{(i)} + SS_{AC}^{(i)} + SS_{BC}^{(i)} + SS_{ABC}^{(i)} + SS_E^{(i)} \tag{9b}$$

where, i denotes the ith iteration. SS_A, SS_B and SS_C denote the main effects of factors A, B, and C, respectively. SS_{AB}, SS_{AC}, SS_{BC}, and SS_{ABC} present the interactive effects among those three factors, and SS_E shows the effect of errors. The values of SS_T, SS_A, SS_B, SS_C, SS_{AB}, SS_{AC}, SS_{BC}, SS_{ABC} and SS_E in the ith iteration can be obtained as follows (Fan et al., 2020; 2021):

$$SS_T^{(i)} = \sum_{h_C=1}^{2}\sum_{h_A=1}^{2}\sum_{h_B=1}^{2}\sum_{l=1}^{n} Y^2_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l} - \frac{Y^2_{g_C(o j_C) g_A(o j_A) g_B(o j_B).}}{8n} \tag{10a}$$

$$SS_C^{(i)} = \frac{1}{4n}\sum_{h_C=1}^{2} Y^2_{g_C(h_C j_C) g_A(o j_A) g_B(o j_B).} - \frac{Y^2_{g_C(o j_C) g_A(o j_A) g_B(o j_B).}}{8n} \tag{10b}$$

$$SS_A^{(i)} = \frac{1}{4n}\sum_{h_A=1}^{2} Y^2_{g_A(h_C, o) g_A(h_A j_A) g_B(o j_B).} - \frac{Y^2_{g_C(o j_C) g_A(o j_A) g_B(o j_B).}}{8n} \tag{10c}$$

$$SS_B^{(i)} = \frac{1}{4n}\sum_{h_B=1}^{2} Y^2_{g_C(h_C, o) g_A(o j_A) g_B(h_B j_B).} - \frac{Y^2_{g_C(o j_C) g_A(o j_A) g_B(o j_B).}}{8n} \tag{10d}$$

$$SS_E^{(i)} = \sum_{h_C=1}^{2}\sum_{h_A=1}^{2}\sum_{h_B=1}^{2}\sum_{l=1}^{n} Y^2_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l} - \frac{1}{n}\sum_{h_C=1}^{2}\sum_{h_A=1}^{2} \times \sum_{h_B=1}^{2} Y^2_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B).} \tag{10e}$$

$$SS_I^{(i)} = SS_T^{(i)} - SS_C^{(i)} - SS_A^{(i)} - SS_B^{(i)} - SS_E^{(i)} \tag{10f}$$

where

$$Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B).} = \sum_{l=1}^{n} Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l}$$

$$Y_{g_C(h_C j_C) g_A(o j_A) g_B(o j_B).} = \sum_{h_A=1}^{2}\sum_{h_B=1}^{2}\sum_{l=1}^{n} Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l}$$

$$Y_{g_C(o j_C) g_A(h_A j_A) g_B(o j_B).} = \sum_{h_C=1}^{2}\sum_{h_B=1}^{2}\sum_{l=1}^{n} Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l}$$

$$Y_{g_C(o j_C) g_A(o j_A) g_B(h_B j_B).} = \sum_{h_C=1}^{2}\sum_{h_A=1}^{2}\sum_{l=1}^{n} Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l}$$

$$Y_{g_C(o j_C) g_A(o j_A) g_B(o j_B).} = \sum_{h_B=1}^{2}\sum_{h_C=1}^{2}\sum_{h_A=1}^{2}\sum_{l=1}^{n} Y_{g_C(h_C j_C) g_A(h_A j_A) g_B(h_B j_B) l}$$

Based on Equations (10a)–(10f), the individuation and interactive contributions for factors A, B and C can be obtained as:

$$\eta_A^{(i)} = SS_A^{(i)} \Big/ SS_T^{(i)} \tag{11a}$$

$$\eta_B^{(i)} = SS_B^{(i)} \Big/ SS_T^{(i)} \tag{11b}$$

$$\eta_C^{(i)} = SS_C^{(i)} \Big/ SS_T^{(i)} \tag{11c}$$

$$\eta_E^{(i)} = SS_E^{(i)} \Big/ SS_T^{(i)} \tag{11d}$$

$$\eta_I^{(i)} = 1 - \eta_A^{(i)} - \eta_B^{(i)} - \eta_C^{(i)} - \eta_E^{(i)} \tag{11e}$$

By averaging the contributions of the studied factors over all iterations, both the individual and interactive contributions can be generated as follows:

$$\eta_A = \frac{1}{N}\sum_{i=1}^{N}\eta_A^{(i)} \tag{12a}$$

$$\eta_B = \frac{1}{N}\sum_{i=1}^{N}\eta_B^{(i)} \tag{12b}$$

$$\eta_C = \frac{1}{N}\sum_{i=1}^{N}\eta_C^{(i)} \tag{12c}$$

$$\eta_E = \frac{1}{N}\sum_{i=1}^{N}\eta_E^{(i)} \tag{12d}$$

$$\eta_I = \frac{1}{N}\sum_{i=1}^{N}\eta_I^{(i)} \tag{12e}$$

where N indicates the total iteration in IFA and $N = \binom{M}{2} \times \binom{M}{2} \times \binom{M}{2}$ since three factors with M levels are under consideration.

2.3. Iterative factorial data assimilation framework

The hydrological predictions are generally influenced by a number of uncertain factors. Particularly in hydrological data assimilation, the resulting predictions would be subject to hydrological models and the DA approaches to be used, uncertainties in forcing data and outputs (e.g., streamflow observations), and other relevant factors such as sample sizes. Different factors may have different impacts on the accuracy of hydrological predictions. In order to comprehensively investigate both the individual and interactive effects of uncertain factors on hydrological data assimilation, those uncertain factors would be integrated into the proposed IFA approach, which lead to an interactive factorial data assimilation (IFDA) framework.

Fig. 1 presents the framework of the IFDA framework. In IFDA, uncertainties in inputs, hydrological models, streamflow observations, DA approaches, and sample sizes are set to have different levels. These levels can be numerical (e.g. uncertainties in inputs and streamflow observations) and non-numerical (e.g. hydrological models and DA approaches). The detailed procedures of IFDA are described as follows:

Step 1: Select the uncertain factors under consideration.

Step 2: For one factor with multiple levels (i.e., multiple choices), decompose the multiple levels of the factor into two level pairs through Equations (8). For instance, if three hydrological models (assumed as M1, M2 and M3) are considered in IFDA, the factor of hydrological models would have three levels. Such a three-level factor can be

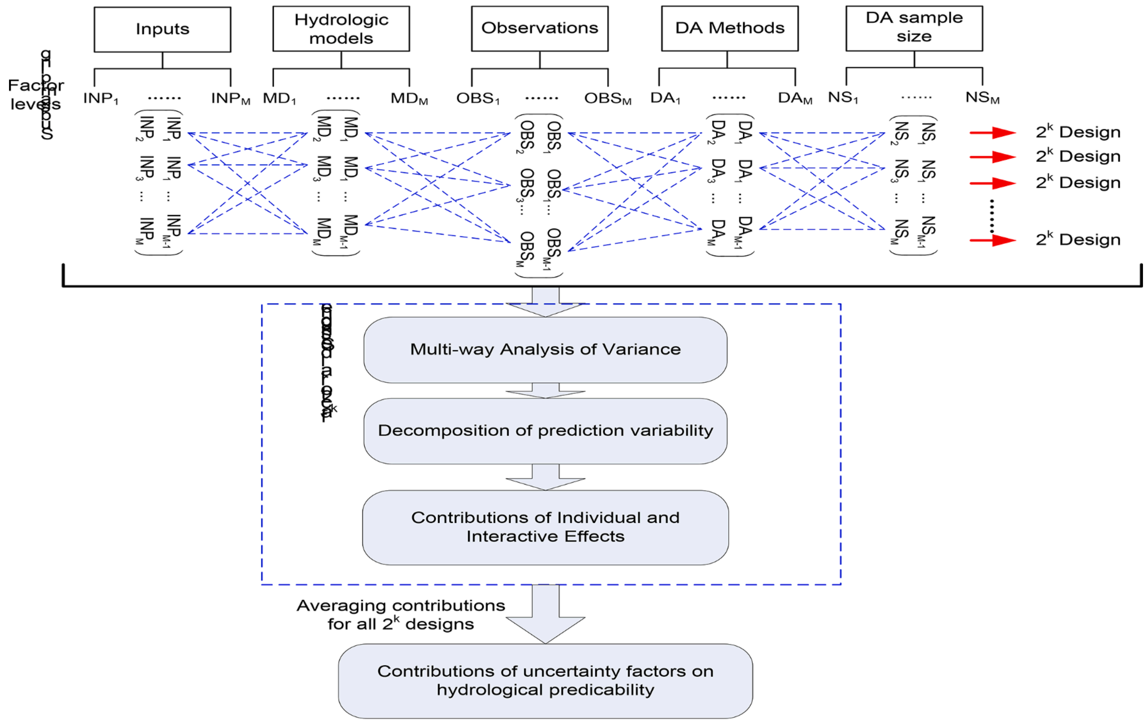

Fig. 1. Framework of the IFDA framework.

decomposed into three 2-level pairs as: $\begin{pmatrix} M1 & M1 & M2 \\ M2 & M3 & M3 \end{pmatrix}$. Similar decomposition matrices can be formulated for other factors under consideration.

Step 3: For each column in the decomposition matrices for all factors, formulate the 2^k (k is the factors under consideration) factorial design matrix, in which each row indicates a data assimilation experiment with specified hydrological model, DA approach, sample size, and uncertainty representations in forcings and streamflow observations.

Step 4: Run all data assimilation experiments listed in the 2^k factorial design matrix. Moreover, each experiment will be run 10 times (i.e., replicates) in order to reflect the inherent uncertainty in the Monte Carlo-based data assimilation experiment.

Step 5: Generate the total variability (i.e., SS_T) for the evaluation indices (i.e., Y in Equation (7)) of the data assimilation experiment as well as its decomposition components based on Equations (9) and (10).

Step 6: Obtain the single and interactive effects of the uncertain factors on the predictability within the 2^k factorial design based on Equations (11).

Step 7: Repeat Steps 3 – 6 for all the combinations of the columns in the decomposition matrices, and generate the associated individual and interactive effects for the uncertain factors for the generated 2^k factorial designs.

Step 8: Generate the overall single and interactive contributions for the studied factors to the predictive variabilities in hydrological prediction system through averaging the corresponding results from all the 2^k factorial designs as expressed in Equations (12).

3. Case study

3.1. Experiment setup

The proposed IFDA framework will be applied for River Ouse in UK to explore the major factors on the accuracy and uncertainty of hydrological predictions. As a companion paper, the IFDA framework will be applied to reveal the major impact factors on hydrological data assimilation based on some results from our first paper (Fan et al., 2022). In detail, three levels would be considered to reflect the model structural uncertainty, in which each level represent one hydrological model and thus three models (i.e., Hymod, GR4J and IHACRES) would be adopted in IFDA. Similarly, the impact from data assimilation method would be reflected through considering different DA algorithms in the IFDA framework. In this study, the factor of DA method would also be assigned with three levels consisting of three different DA algorithms. The particle filter (PF) method and its two variants (i.e., particle Markov chain Monte Carlo (PMCMC) and particle copula Metropolis Hastings (PCMH)) would be included in the IFDA framework. Since the precipitation and potential evapotranspiration are used in all the three hydrological models, the stochastic perturbation approach with different proportional factors (i.e. Equations (3) - (5)) will be adopted to reflect the impacts of inputs uncertainties on the hydrological predictions. Similarly, the Gaussian perturbation method (i.e. Equation (6)) with different proportional factor values would be employed to reflect the impact of uncertainty in streamflow observations on the resulting hydrological predictions. Moreover, the PF, PMCMC and PCMH methods are all based on Monte Carlo simulation, and the sample sizes will be another factor under consideration in the IFDA framework. Table 1 summarizes all the factors and their levels in the IFDA framework.

The proposed IFDA framework is a flexible framework which can be expanded or shrunken based on the factors to be addressed. For instance, if the proportional factors in model inputs and streamflow observations are merely under consideration, the IFDA framework can characterize the impacts of uncertainties in model inputs and streamflow

Table 1
Uncertainty factors in the IFDA framework.

Factors	Name	Level 1	Level 2	Level 3
A	Hydrological model	Hymod	GR4J	IHACRES
B	Data assimilation method	PF	PMCMC	PCMH
C	Proportional factor in potential evapotranspiration (PET)	0.15	0.25	0.35
D	Proportional factor in precipitation	0.15	0.25	0.35
E	Proportional factor in streamflow	0.15	0.25	0.35
F	Sample size	50	100	200

observations on the performance of a specific data assimilation method on a specific hydrologic model. Moreover, the IFDA can also be employed to reveal whether a DA method would produce a noticeable impact on the predictability of a hydrologic model when the sample size, DA methods, and uncertainties in inputs and streamflow observations are involved in IFDA.

3.2. Experiment responses

In the IFDA framework, the response, denoted as Y in Equation (7) would be some criteria to evaluate the performances of the chosen hydrologic prediction system subject to specific hydrological model, DA method, as well as uncertainty settings in inputs, streamflow observations and sample size. As an extension for our companion study in Fan et al. (2022), the root-mean-square error (RMSE), and Nash-Sutcliffe efficiency (NSE) coefficient and continuous ranked probability score (CRPS) will be used as the responses in the proposed IFDA framework, which can be expressed as:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(Q_{obs,i} - Q_{sim,i}\right)^2} \tag{13}$$

$$NSE = 1 - \frac{\sum_{i=1}^{N}\left(Q_{obs,i} - Q_{sim,i}\right)^2}{\sum_{i=1}^{N}\left(Q_{obsi} - \overline{Q_{obs}}\right)^2} \tag{14}$$

$$CRPS = \int_{-\infty}^{+\infty}\left[F^f(x) - F^o(x)\right]^2 dx \tag{15}$$

where N is the total number of streamflow measurements (or predictions), Q_{obs} and Q_{sim} are streamflow observations and model predictions, respectively, and $\overline{Q_{obs}}$ is the mean value of observations. F^o and F^f are cumulative distribution functions for observations and model predictions, respectively. In this study, the mean prediction at each time step (i.e., Q_{sim} in Equations (13) and (14)) would be adopted to calculate NSE and RMSE. In comparison, the ensemble predictions in each time step would be used to calculate F^f and the perturbed observations are employed to generate the value of F^o.

4. Results analysis

The proposed IFDA framework is employed to characterize both the individual and interactive effects of various uncertain factors on the accuracy of hydrological predictions. In detail, there are six factors in total to be examined in the IFDA framework, as presented in Table 1, with each factor having 3 levels. For the factor of hydrological model, each level represents a specific hydrological model (i.e., Hymod, GR4J or IHACRES) whilst each level for the factor of data assimilation method represents a specific DA algorithm (i.e., PF, PMCMC or PCMH). The six factors with 3 different levels will lead to 729 (i.e. 3^6) combinations of hydrologic data assimilation schemes. Each data assimilation scheme will consist of a specific hydrological model (i.e. Hymod, GR4J, or IHACRES), DA approach (i.e. PF, PMCMC, or PCMH), sample size (i.e. 50, 100, or 200), and proportional factor value respectively for precipitation (i.e., γ in Equation (5)), potential evapotranspiration (i.e., γ in Equation (4)), and streamflow observations (i.e., η in Equation (6)). Moreover, 10 runs will be performed for each data assimilation scheme, which means that a specified DA scheme would be repeated for 10 times. The purpose for repeating is to reveal the inherent uncertainty in those Monte Carlo based data assimilation approaches. Consequently, we would have a total number of 7290 runs in the IFDA framework. The computational burden is relatively high in this case since 10 replicates are used. However, the total number of runs in IFA is the same as the traditional multi-level factorial analysis (MFA) method, and thus IFA would not increase computational requirement compared with the MFA method. Nevertheless, this computation requirement would be still less than some other global sensitivity analysis methods such as Sobol's method as demonstrated in Wang et al. (2020). Moreover, the replicates can be reduced to mitigate the computation requirement in IFA (e.g., 1458 runs are required if 2 replicates are adopted). In addition, one of the most significant merits of IFA is that it can deal with both discrete and continuous factors and get comparable results with some benchmark methods like Sobol's method (Wang et al., 2020).

Fig. 2 presents the performance variation for different data assimilation schemes in the proposed IFDA framework. It indicates that for different data assimilation schemes with different hydrological models, data assimilation techniques, as well as uncertainties in inputs and outputs, their performances would generally vary significantly in terms of both deterministic and probabilistic predictions. As for the 7290 runs within the IFDA framework, they will lead to mean values for NSE, RMSE and CRPS respectively being 0.69, 34.06, 17.63. Nevertheless, the 90% variation intervals bounded by the 5% and 95% quantiles for NSE, RMSE and CRPS would be [0.45, 0.84], [25.24, 45.05], and [9.93, 28.80], presenting significant changes for different data assimilation schemes. These changes may be subject to several factors such as the choice of hydrological models and data assimilation techniques, uncertainties in inputs and streamflow observations, and also the inherent randomness in the Monte Carlo based data assimilation methods in IFDA framework. Consequently, it is desired to further characterize the dominant factors that influence the performances of different data assimilation schemes.

4.1. Impacts of uncertainties in inputs, observations and sample sizes

The impacts of uncertainties in inputs, observations and sample sizes for different sequential data assimilation techniques over different hydrological models are firstly characterized through the proposed IFDA framework. In detail, the proportional factors are set to be 0.15, 0.25, and 0.35 for the potential evapotranspiration (i.e. C), precipitation (i.e. D), and streamflow observations (i.e. E) to reflect their uncertainties. Three sample scenarios (i.e. F) of 50, 100, and 200 are adopted to reflect the uncertainty in sample size in data assimilation process. Since PF, PMCMC and PCMH employed in IFDA are random in nature, 10 replicates would be performed for each DA scheme with specific uncertainty setting for inputs, streamflow observation, and sample size.

Fig. 3 exhibits the contributions of the factors C, D, E and F to the variations of deterministic predictions from different DA approaches on different hydrologic models. It is apparent that the uncertainties in inputs, streamflow observations and sample sizes pose different impacts on the deterministic predictability of different DA approaches on different hydrological models. In detail, for the PF approach, the inherent uncertainty (denoted as *Residual* in Fig. 3) would have the dominant effect on its predictability on Hymod and IHACRES, whilst the uncertainty in streamflow observation will have a major effect on the deterministic predictability from PF on GR4J. This suggest that more accurate quantification for inputs and streamflow observations, and larger sample sizes may hardly lead to better performances for PF on Hymod and IHACRES. Nevertheless, the performance of PF on GR4J can be enhanced through better uncertainty reflection in streamflow observations. For the PMCMC approach, it can be observed that its performances for deterministic predictions are mainly subject to its inherent randomness, which can have contributions of 82.5%, 60.8% and 85.2% respectively to the variations of NSE for Hymod, GR4J and IHACRES. However, uncertainties in streamflow observation and sample sizes would have apparent impacts (15.8% and 14.5% respectively) on the predictability of PMCMC on the GR4J model. Compared with PMCMC and PF, the performances of PCMH would be less impacted by its inherent uncertainties. For instance, the uncertainty in streamflow observations poses a most dominant impact on the predictions of PCMH on Hymod and GR4J. Even for IHACRES, the sample size (i.e. F) also has a visible impact (7.98%) on the performance of PCMH. The contributions of these four factors to variations of RMSE show a similar pattern

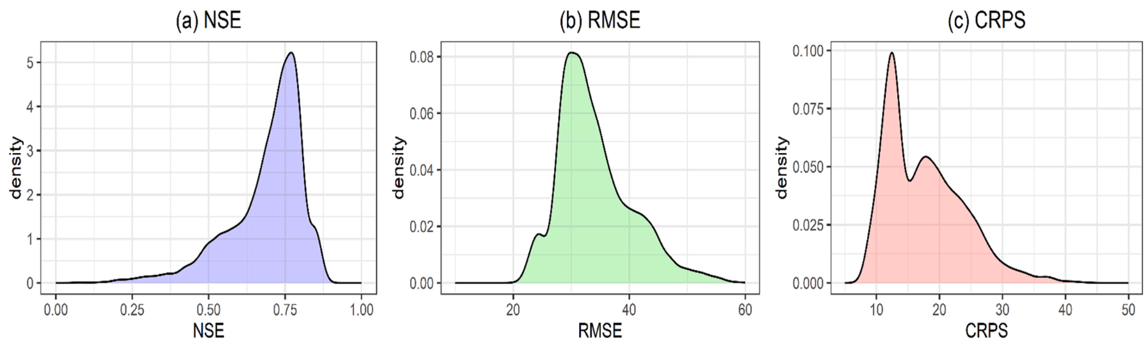

Fig. 2. Performance variation for different data assimilation schemes within the IFDA framework.

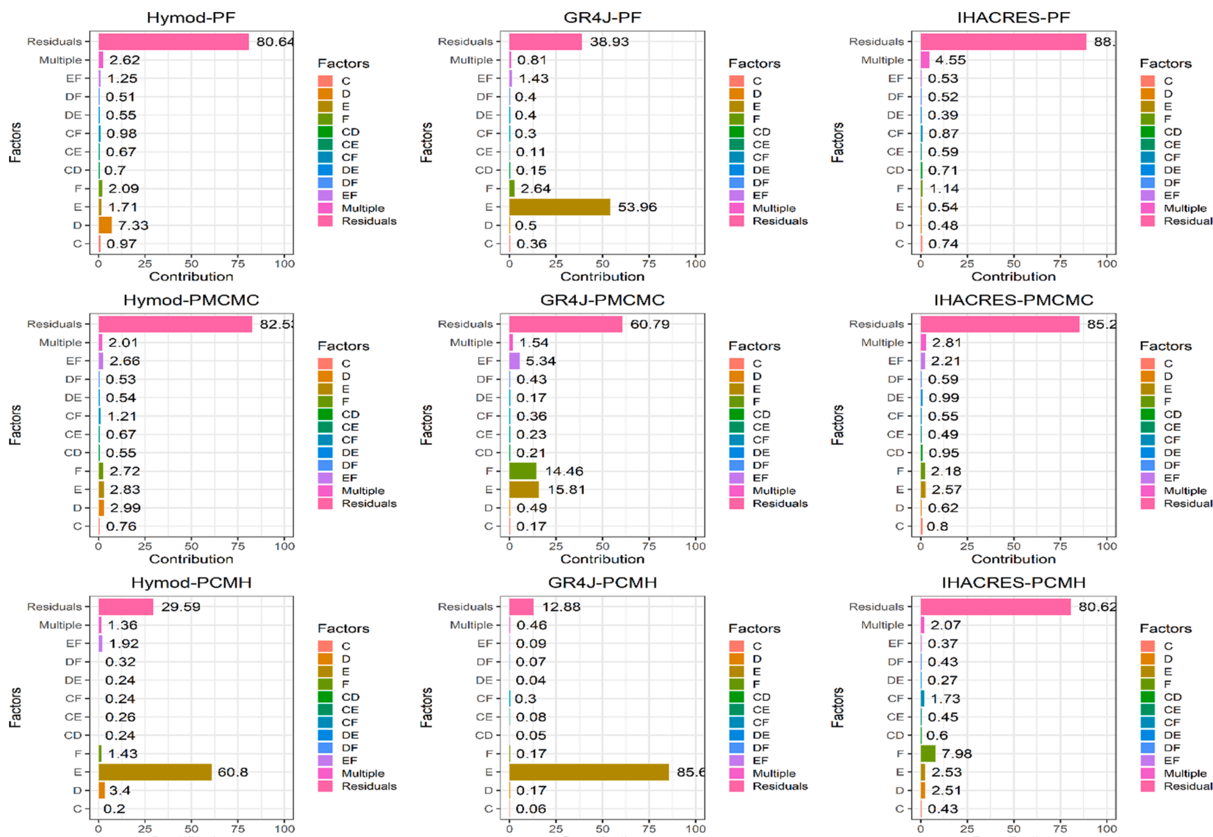

Fig. 3. The contributions of uncertainties in potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by NSE) for different data assimilation approaches on different hydrologic models. Here *Multiple* indicates the sum of all multiple interactions (e.g., *CDE* + *CDF* +…) and *Residual* represents the effect from the randomness of the DA method.

with the results to the NSE fluctuations, which is presented in Figure S1.

In addition to the deterministic predictions, the probabilistic predictions from different DA approaches on different models may also be influenced by uncertainties in inputs (i.e. C, D), streamflow observations (i.e. E) and sample sizes (i.e. F). Fig. 4 presents the contributions of those four factors to the variations of CRPS for different DA approaches on different hydrological models. It indicates that the impacts of those four uncertainty factors on the probabilistic predictions would have some similar features with their impacts on deterministic predictions. The inherent randomness of PF, PMCMC and PCMH would have a most dominant effect on the probabilistic predictions from IHACRES, with a contribution of 78% for PCMH and more than 80% for PF and PMCMC. For the Hymod, even though the inherent randomness would also have noticeable effects on all the three DA approaches, uncertainties in precipitation (i.e. D), streamflow observations (i.e. E) and sample size (i.e. F) would pose more impacts as the DA approach changes from PF to PCMH. The impacts of these three factors (i.e. D, E, F) on probabilistic predictions of Hymod are different from their impacts on the deterministic results, especially for the PCMH approach, where the factors of D and F would have large effects (i.e. 18.8% and 7.7%) on the probabilistic predictions, whilst the factor E has a much less effect (i.e. 15.4%). For the GR4J model, uncertainty in streamflow observations would have a major effect on the probabilistic predictions from PF and PCMH, with its contribution to PCMH as high as 86.6%. Moreover, this factor, as well as the sample size would also have visible effects on the PMCMC approach, with their contributions being 33.7% and 17.6% respectively. Such an impact pattern is similar with the results for deterministic predictions of GR4J.

For the uncertainties in inputs (i.e. C, D), streamflow observations (i. e. E) and sample size (i.e. F), their impacts on data assimilation would be

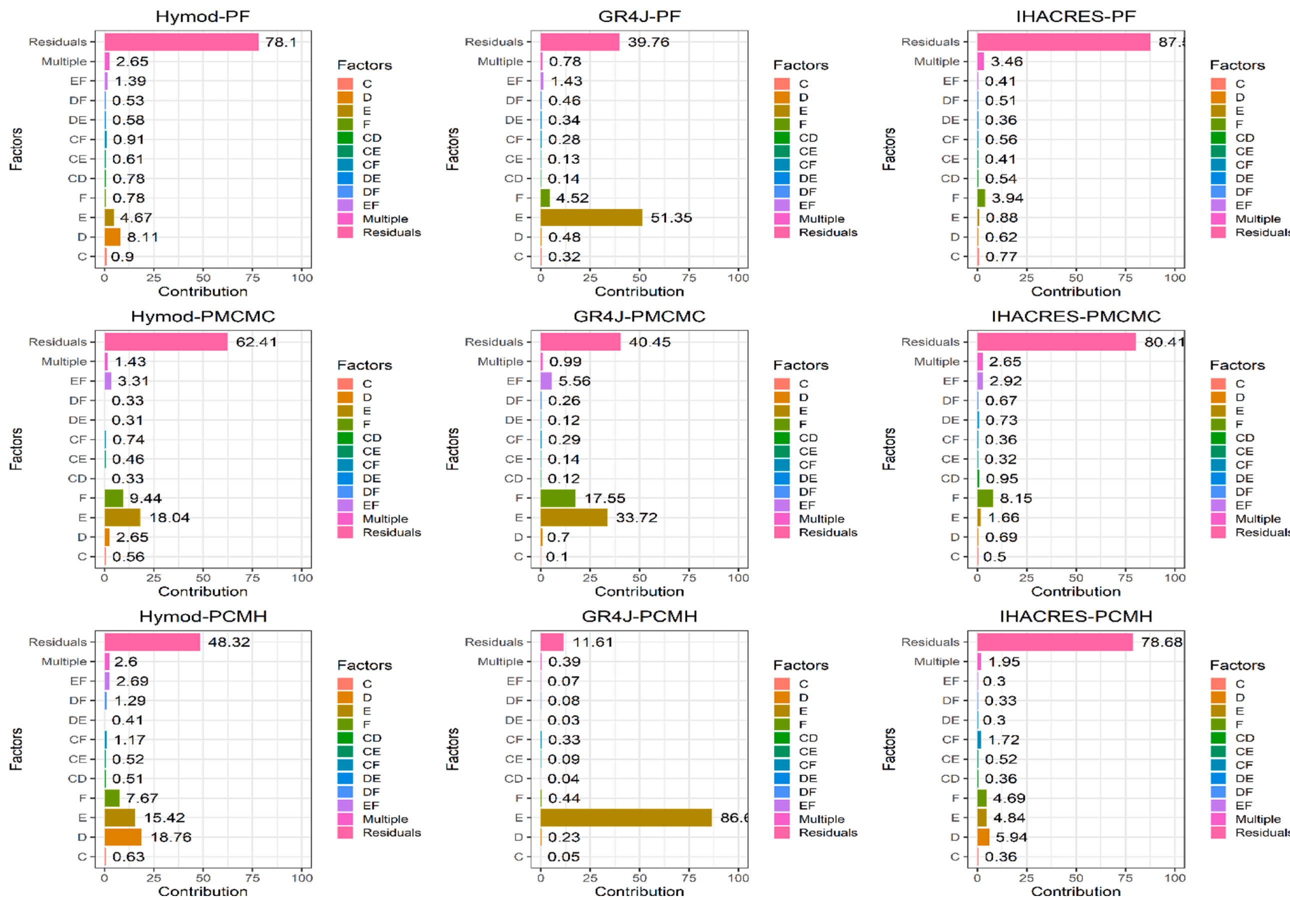

Fig. 4. The contributions of uncertainties in potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by CRPS) for different data assimilation approaches on different hydrologic models. Here *Multiple* indicates the sum of all multiple interactions (e.g., *CDE* + *CDF* + …) and *Residual* represents the effect from the randomness of the DA method.

different for different DA approaches on different hydrological models. However, we can generally conclude that, regardless of the inherent randomness of the DA approaches, the uncertainty in streamflow observations seems to more likely pose a significant impact on the data assimilation process. Moreover, for DA approaches, the PCMH approach would be less influenced by its inherent randomness. This is because the contributions of PCMH randomness over the three hydrological models, as shown in Fig. 4, are always less than the corresponding contributions for the other two DA methods. This indicates that the PCMH is more robust than PF and PMCMC, which has been elaborated in our companion paper. The performance of PCMH is more easily enhanced through better quantification for uncertainties in inputs, streamflow observations and sample size.

4.2. *Impacts of uncertainties in DA approaches, inputs, observations and sample sizes*

In general, different data assimilation approaches would generate different prediction results even for the same uncertainty settings in inputs, streamflow observations and sample size, which has been demonstrated in a number of studies. However, it is not well elaborated how much the DA method can contribute to the improvement of the hydrological data assimilation process. In current study, different DA approaches (i.e. B) including PF, PMCMC and PCMH, as well as uncertainties in inputs (i.e. C, D), streamflow observations (i.e. E) and sample size (i.e. F) are integrated within the proposed IFDA framework to explore their contributions to variations in both deterministic and probabilistic predictions from hydrological data assimilation process.

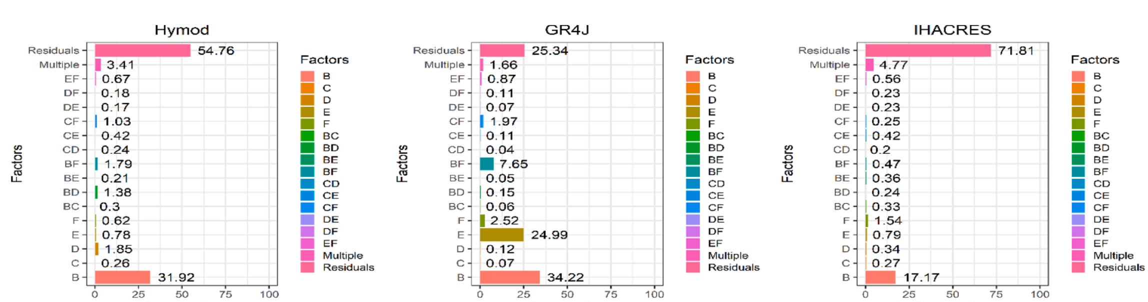

Fig. 5. The contributions of uncertainties in DA methods (*B*), potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by NSE) for different hydrologic models. Here *Multiple* indicates the sum of all multiple interactions (e.g., *BCD* + *BCE* + …) and *Residual* represents the effect from the randomness of the DA method.

Fig. 5 presents the impacts of B, C, D, E, and F on the variations of deterministic predictions from different hydrological models. The randomness of the DA approaches would pose remarkable, or even dominant impacts on the performances of the three hydrological models. However, it is noticeable that factor B (i.e. DA approaches) would also have significant impacts on the deterministic predictions from all the three hydrological models, with its contributions being 31.9%, 33.2% and 17.2% respectively for Hymod, GR4J, and IHACRES. For the factors of C, D, E and F, their impacts in such a circumstance are significantly different from their contributions when the factor of DA methods is not involved. The uncertainty in streamflow observation would have a visible effect on the GR4J model with its contribution less than the contribution of factor B. Moreover, the interaction of DA methods (B) and sample size (F) also has an explicit effect on the performance of GR4J model. For the deterministic predictions evaluated by RMSE, the impacts of B, C, D, E and F, as presented in Figure S2, show similar features with their impacts on the variation of NSE. In spite of the inherent randomness, the DA approaches would pose the most significant impacts on the performances of all the three hydrological models, larger than other individual or interactive effects.

For the probabilistic predictions evaluated by CRPS, those five factors would have similar impacts on the Hymod and GR4J with their corresponding effects on the deterministic prediction. Nevertheless, as presented in Fig. 6, the DA methods (i.e. B) would contribute more to the probabilistic predictions than the deterministic predictions. The factor of DA methods would make a contribution of 44% and 37.3% to the variation of CRPS from Hymod and GR4J, respectively, higher than its contribution to NSE (in Fig. 5) and RMSE (in Figure S2) variations. However, the probabilistic predictions from IHACRES seem to be dominated by the inherent randomness of the DA approaches, with only a small visible effect from the sample size (i.e. F). In fact, the mean CRPS values from PCMH, PF and PMCMC on the IHACRES model, over all uncertainty combinations (810 runs for each DA approach) for inputs, streamflow observations and sample size, are 21.5, 23.2 and 23.0, presenting an indistinguishable difference among each other.

When the impact of the DA approaches is under consideration, the results from the IFDA framework indicate that the DA approach would generally have more contributions to both the deterministic and probabilistic predictions than other factors. Such an effect is remarkably obvious for the Hymod and GR4J models. These results suggest the significance of developing advanced data assimilation approaches, which can very probably lead to better predictions for the hydrological data assimilation process. Moreover, uncertainty in streamflow observations would be another factor to be considered, which can have significant effects on predictions from some hydrological models.

4.3. *Impacts of uncertainties in hydrological models, DA approaches, inputs, observations and sample sizes*

The predictions from hydrological data assimilation are generally affected by various factors, such as the hydrological model and DA technique to be adopted, uncertainties in inputs, streamflow observations, and sample sizes. Moreover, the inherence randomness in some Monte Carlo based DA methods may also have significant effects on the resulting predictions. All these factors are integrated into the proposed IFDA framework to quantitatively reveal their individual and interactive effects on the predictions from hydrological data assimilation.

Fig. 7 presents the individual and interactive effects of all the six factors (i.e. A ~ F) on the deterministic predictions from hydrological data assimilation. The results indicate that, even though the inherent randomness (i.e. *Residuals* in Fig. 7) has the most significant effect on the deterministic predictions, the hydrological models (i.e. A), DA methods (i.e. B) and their interactions also make noticeable contributions to the deterministic predictability of the hydrological data assimilation schemes. As presented in Fig. 7, the contributions of A, B, and AB would be 14.8%, 16.4% and 9.5%, respectively, which are much higher than the individual and interactive effects from other factors. For the predictions evaluated by RMSE, the effects of all the six factors, as shown in Figure S3, are quite similar with their effects on the NSE variation since both NSE and RMSE reflect the accuracy of deterministic predictions. In comparison, for the probabilistic predictions, the individual and interactive effects of factors A ~ F are different from their impacts on the deterministic predictions (here the mean predictions are adopted) evaluated by NSE and RMSE. As presented in Fig. 8, the hydrological model (i.e. A) would have a much higher effect (31.3%) on the variation of CRPS than its effect (14.8%) on the NSE variation. Conversely, the impact of the DA methods (i.e. B) and its interaction with hydrological models would have less effects (13.2% for B and 8.5% for AB) on the probabilistic predictions. Moreover, the inherent randomness of the DA scheme would pose less effect on the probabilistic predictions than the deterministic predictions.

When uncertainties in hydrological models, DA methods, inputs, streamflow observations and sample sizes in a data assimilation process are under consideration, the results indicate that the hydrological models and DA approaches would have more significant effects than other factors on the resulting predictions. This would conclude an implication that we would be able to expect better predictions in data assimilation through choosing an appropriate hydrological model and advanced DA method. Moreover, the inherent randomness in the data assimilation process also has noticeable effects on both deterministic and probabilistic predictions. The robustness of the DA approach would be another factor to be addressed to enhance the predictability of the hydrological data assimilation process.

5. Discussion

5.1. *Impact variations for DA methods and hydrological models*

In the proposed IFDA framework, a number of two-level factorial designs would be generated based on those uncertain factors with

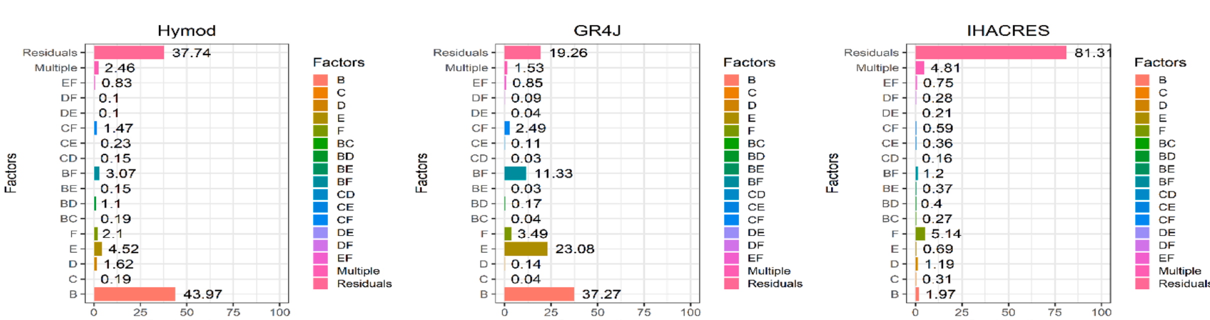

Fig. 6. The contributions of uncertainties in DA methods (*B*), potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by CRPS) for different hydrologic models. Here *Multiple* indicates the sum of all multiple interactions (e.g., *BCD* + *BCE* + …) and *Residual* represents the effect from the randomness of the DA method.

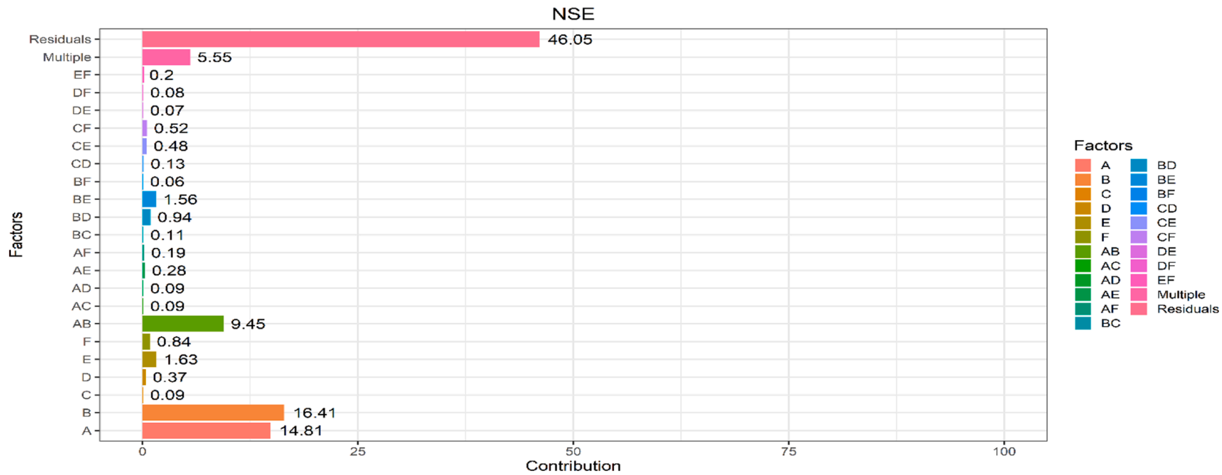

Fig. 7. The contributions of uncertainties in hydrological models (*A*), DA methods (*B*), potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by NSE) for different hydrologic data assimilation schemes. Here *Multiple* indicates the sum of all multiple interactions (e.g., *ABC* + *ABCD* + *ABCE* + …) and *Residual* represents the effect from the randomness of the DA method.

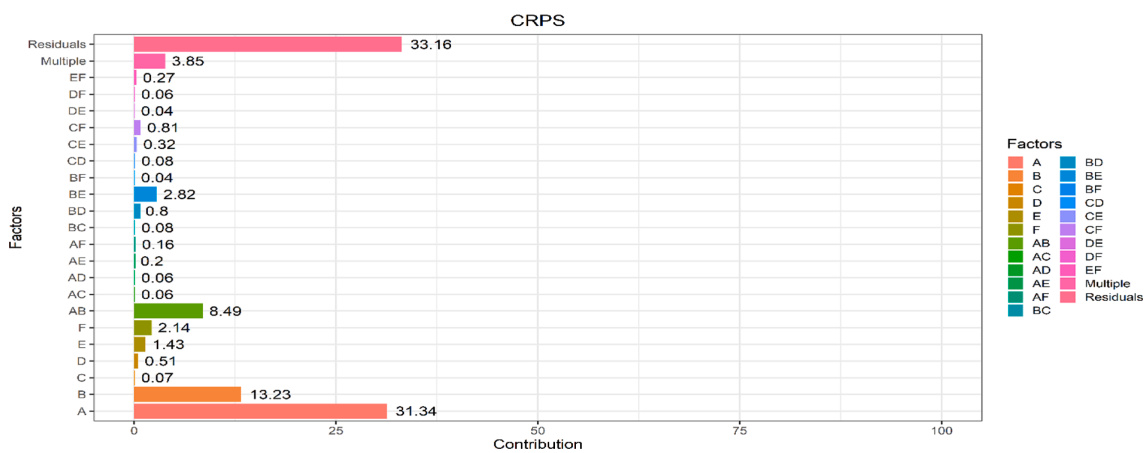

Fig. 8. The contributions of uncertainties in hydrological models (*A*), DA methods (*B*), potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances (evaluated by CRPS) for different hydrologic data assimilation schemes. Here *Multiple* indicates the sum of all multiple interactions (e.g., ABC + *ABCD* + *ABCE* + …….) and *Residual* represents the effect from the randomness of the DA method.

multiple levels. For different two-level factorial designs, the factor levels for a specific factor (e.g. hydrological models, DA methods) may be different, which would further lead to different impact characterizations for this factor. Fig. 9 presents the contribution variations of hydrologic models and DA methods for different hydrologic data assimilation schemes obtained by the two-level factorial designs within the IFDA framework. It can be observed that, when different levels are applied to one factor, the resulting impact on the data assimilation would vary significantly. As presented in Fig. 9, the contribution of hydrologic model to deterministic prediction remarkably ranges within [0, 0.5], with most values located within [0, 0.25]. Similarly, the DA approach would have an effect, significantly ranging within [0, 0.5], on hydrological data assimilation. Compared with hydrological model, a large part of the contributions of DA method are located within [0.25, 0.5], which lead to a higher average contribution of DA method (i.e. 16.4% in Fig. 7) than that for hydrological model (i.e. 14.8% in Fig. 7). Moreover, for the probabilistic predictions, the contributions of hydrological model and DA method would also vary significantly for different levels under consideration, as shown in Fig. 9. However, the contribution variations of these two factors for probabilistic predictions are not consistent with the variations for deterministic predictions. Most contributions of hydrological model are larger than 0.25, which also leads to a higher contribution in average than that for DA methods.

5.2. Comparison with traditional multi-level factorial analysis

In the proposed IFDA framework, six factors with each one having three levels are addressed to reveal their impacts on the predictability of hydrological data assimilation. Their individual and interactive effects can also be characterized by a three-level (i.e. 3^6) factorial design. Figures S4–S7 shows the main effects and their interactions of these six factors on both deterministic (evaluated by NSE) and probabilistic (evaluated by CRPS) predictions. Significant effects can be observed for hydrological model, DA approach and their interactions on both deterministic and probabilistic predictions, which have also been characterized by the developed IFDA framework. Nevertheless, for the detailed contributions for each factor and their interactions, the values from the three-level factorial design are visibly different from those obtained by the IFDA framework. As presented in Fig. 10, the three-level factorial design would provide an overestimation for the contribution of hydrological models and underestimations for the main effects of other factors. It is noticed that the contribution characterizations from three-level factorial design may also lead to a different rank for these factors. It is concluded from the three-level factorial design that the hydrological models would have the most significant effect on the deterministic predictions while, based on the proposed IFDA framework, the contribution (16.4%) of DA methods is apparently higher than the

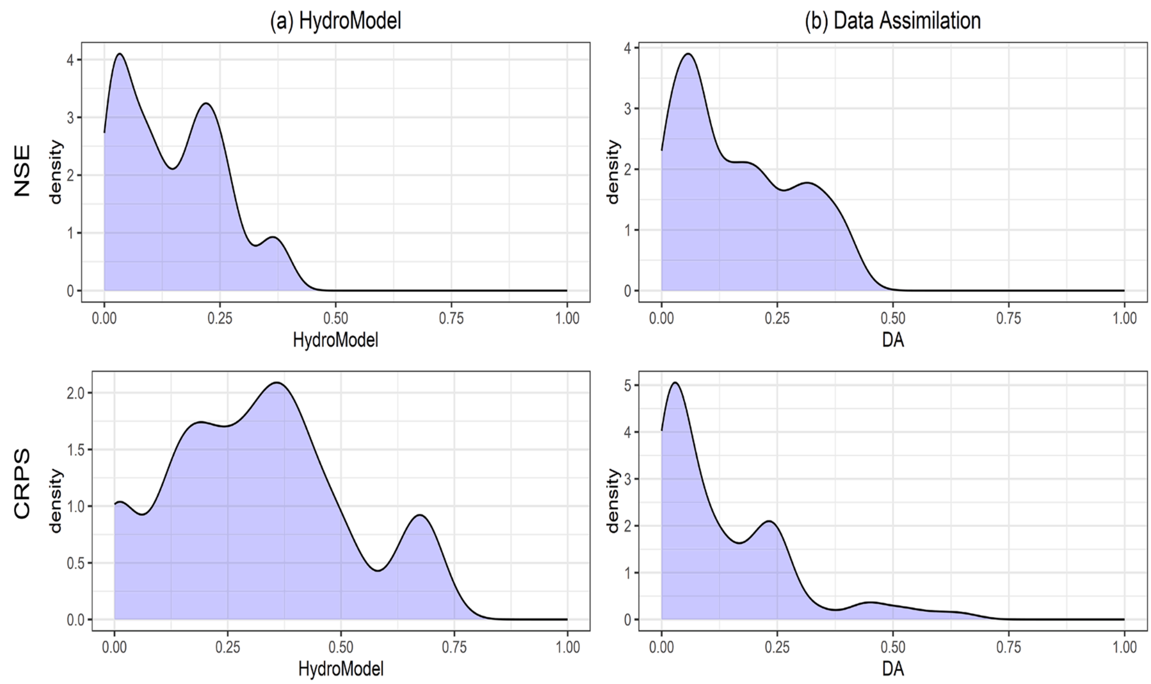

Fig. 9. The contribution variations of hydrologic models and DA methods for different hydrologic data assimilation schemes.

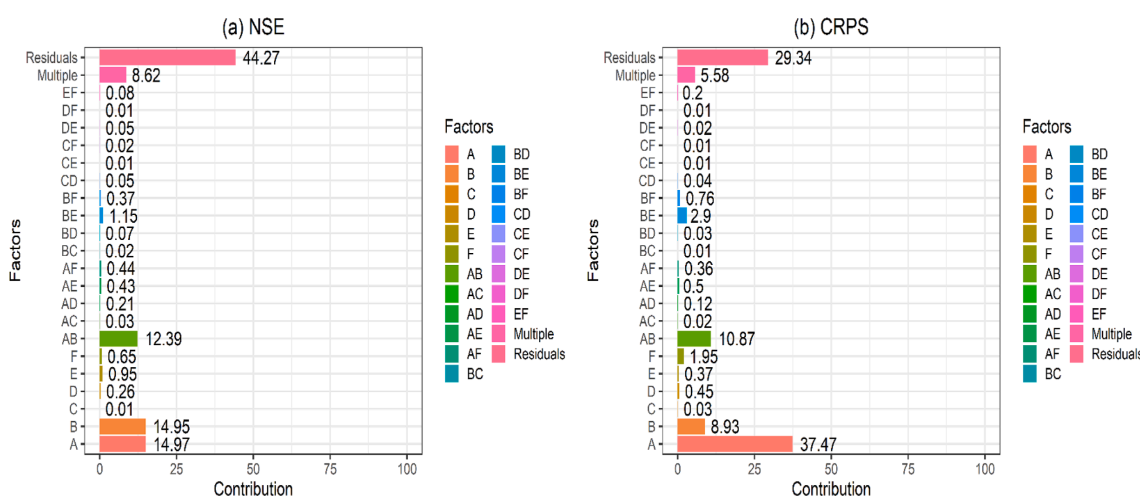

Fig. 10. The contributions of uncertainties in hydrological models (*A*), DA methods (*B*), potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances for different hydrologic data assimilation schemes from the three-level factorial design. *Multiple* indicates the sum of all multiple interactions and *Residual* represents the effect from the randomness of the DA method.

contribution (14.8%) of hydrological models. Moreover, the three-level factorial design also provides an overestimation for the interactive effect of hydrological models and DA approaches. These discrepancies may due to the biased estimations for the total sum of the squares and its components, as presented in Equations (9) and (10).

5.3. Impacts of uncertain factors for data assimilation with calibrated models

The above analyses for factor contributions to the predictability of hydrological data assimilation are based on the results from the dual state-parameter estimation framework in which both model parameters and state variables are quantified simultaneously. However, another possible pathway for hydrological data assimilation is to quantify the uncertainty in state variables with calibrated model parameters. In this case, the model parameters would be calibrated before starting the data assimilation process and thus probabilistic uncertainties would be obtained only for the state variables and predictions. Consequently, the impacts of uncertain factors may have different patterns with those in the dual state-parameter estimation framework.

Nevertheless, the proposed IFDA framework can also be applied to reveal the impacts of different factors on hydrological data assimilation with calibrated models. In such a case, the 10-year dataset at the River Ouse in UK described in our companion paper (Fan et al., 2022) has been splitted into two parts with the first 5-year data for parameter calibration and the latter 5-year data for data assimilation. Since the model parameters are not estimated in data assimilation and thus only the PF method is needed for this issue.

Fig. 11 presents the individual and interactive effects of uncertainties inputs (i.e., C for potential evapotranspiration, D for precipitation), observations (i.e., E) and sample sizes (i.e., F) on both deterministic and probabilistic predictions from data assimilation. It is noticeable that,

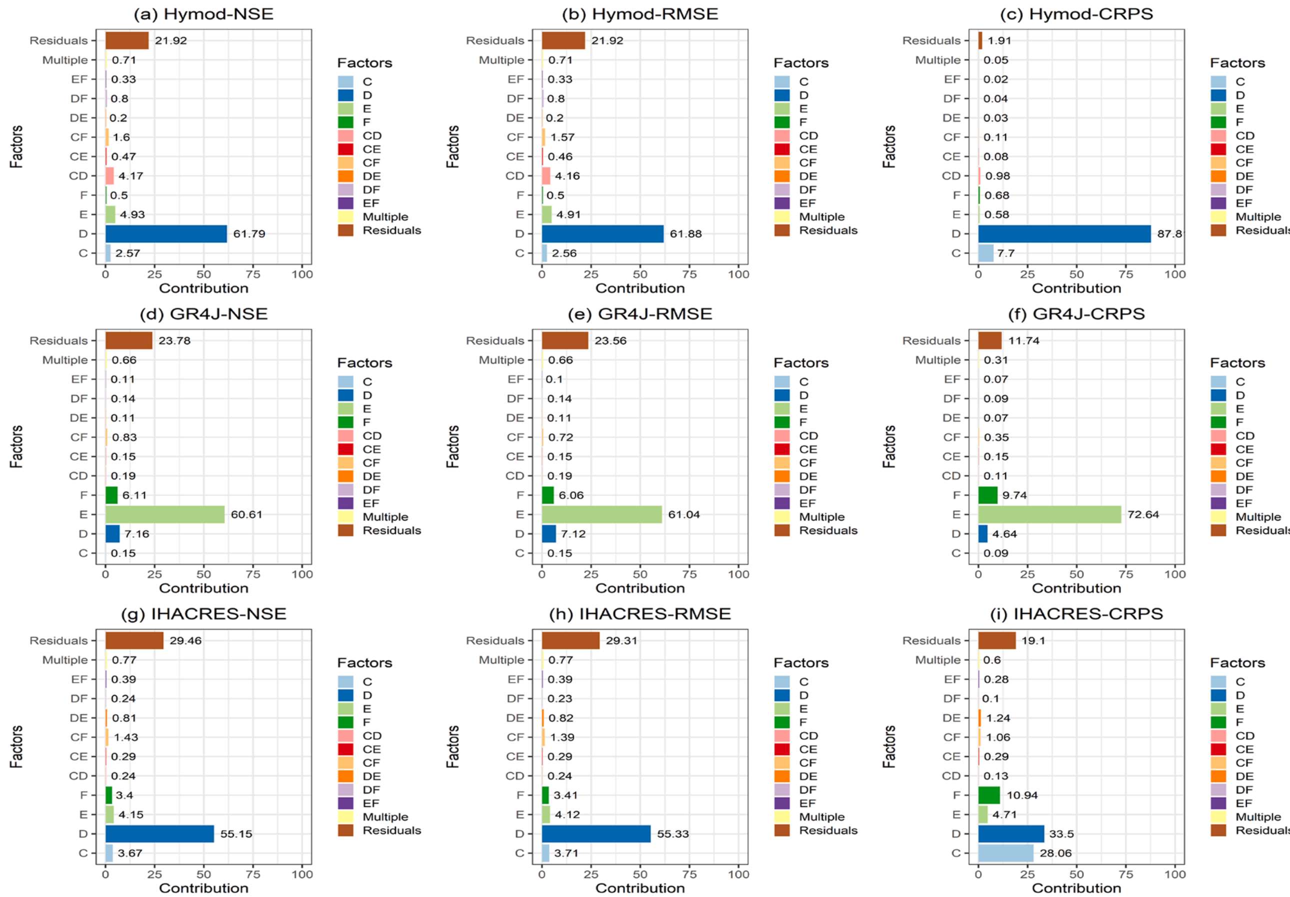

Fig. 11. The contributions of uncertainties in potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*) to the performances of data assimilation through different hydrological models with prior calibrated parameters. *Multiple* indicates the sum of all multiple interactions and *Residual* represents the effect from the randomness of the DA method.

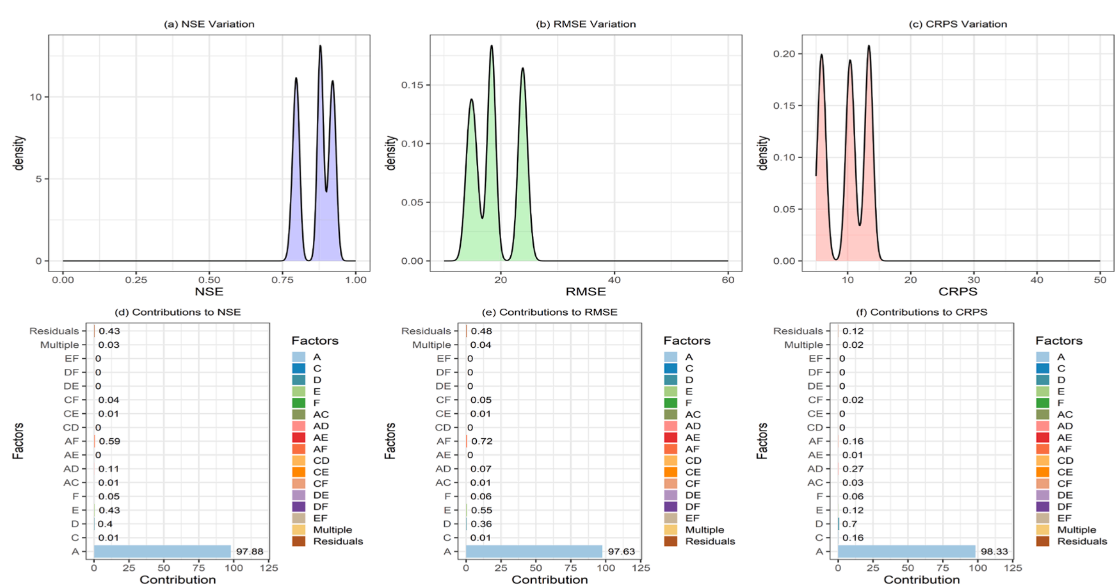

Fig. 12. The performance variations of data assimilation considering different calibrated hydrological models (*A*), uncertainties in potential evapotranspiration (*C*), precipitation (*D*), streamflow observations (*E*) and sample sizes (*F*), as well as their contributions. *Multiple* indicates the sum of all multiple interactions and *Residual* represents the effect from the randomness of the DA method.

compared with the results in dual state-parameter estimation framework presented in Figs. 3 and 4, the inherent randomness in PF (i.e., Residuals in Fig. 11) would be more controllable especially for the probabilistic predictions. For instance, the highest contribution from the inherent randomness of the DA algorithm would be found for IHACRES model in both data assimilation scenarios. But the contributions of the randomness would be around 88% for deterministic predictions (in Fig. 3) and 87% for probabilistic predictions (in Fig. 4) in the dual state-parameter framework, whilst those contributions can be significantly reduced to 29.5% for deterministic predictions (i.e., Fig. 11(g)) and 19.1% for probabilistic predictions (i.e., Fig. 11(i)) if the calibrated IHACRES model is adopted. Compared with the reduced contributions from PF randomness, some factors would have significantly higher impacts on the data assimilation performances for calibrated models. But one specific factor may have different effects when different models are adopted, in which the uncertainty in precipitation would have the highest impact on data assimilation for Hymod and IHACRES and the uncertainty in streamflow observations would have the highest contribution for GR4J. Moreover, another interesting promise concluded from Fig. 11 is that the sample size of PF would not be likely to pose visible impacts on data assimilation for calibrated models. This implies that only a small sample size may be required for data assimilation through calibrated hydrological models, which can significantly reduce computation burden in the data assimilation process.

Fig. 12(a)–(c) present the performance variations for both deterministic and probabilistic predictions considering all the three hydrological models and different uncertain scenarios in inputs and streamflow observations. It is obvious that the histograms of NSE, RMSE and CRPS values show three peaks, implying a dominant factor to influence the data assimilation process. Fig. 12(d)–(f) show the detailed individual and interactive contributions of the uncertain factors to the deterministic and probabilistic predictions of data assimilation. It is concluded that the hydrological model would mainly control the performance of data assimilation process whilst impacts from other uncertainties including the inherent randomness of the DA algorithm seem to be negligible. This indicates that using an appropriate hydrological model with well calibrated parameters would be the most efficient way to improve the data assimilation process.

6. Conclusions

Sequential data assimilation (SDA) techniques have been widely used for uncertainty quantification and reduction in hydrologic prediction. In a data assimilation scheme, its performance is critically influenced by a number of factors such as the hydrological model and data assimilation methods to be used, uncertainty representation in inputs, streamflow observations and also sample sizes. In this study, an interactive factorial data assimilation (IFDA) framework has been developed to characterize both individual and interactive effects of hydrological models, DA approaches, and uncertainties in inputs, streamflow observations and sample sizes on the resulting predictions. In detail, three hydrological models (i.e., Hymod, GR4J, IHACRES), three DA approaches (i.e., PF, PMCMC, PCMH), and three uncertainty settings for inputs, streamflow observations, and sample sizes are under consideration in the IFDA framework. The interactive factorial analysis (IFA) was then proposed to explore the impacts of these factors on deterministic and probabilistic predictions.

The proposed IFDA framework has been applied to the River Ouse in UK. Some key results can be concluded:

i) When uncertainties in inputs, streamflow observations, and sample sizes are under consideration, they would have discrepant effects on different data assimilation methods over different hydrological models. However, uncertainties in streamflow observations, except the inherent randomness in data assimilation, would more likely pose significant impacts on the resulting predictions.
ii) If the choice of data assimilation methods is further considered, these factors also pose different impacts on the predictions from different models. However, the data assimilation methods, regardless of the inherent randomness, would generally have more impacts than other factors on the predictions.
iii) For uncertainties in hydrological models, data assimilation approaches, inputs, streamflow observations and sample sizes, the first two factors (i.e. hydrological models and data assimilation approaches) and their interactions would have much more impacts than uncertainties in other factors on the resulting predictions.
iv) In addition to those uncertain factors, the inherent randomness, mainly caused by the Monte Carlo sampling process, would also have noticeable effects on the resulting predictions. This is particularly obvious if the hydrological model and data assimilation method are not well identified in advance, such as the IHACRES model in this study.
v) Parameter calibration prior to data assimilation can significantly reduce the impact from the inherent randomness. The uncertainty in model structure would be dominant the data assimilation process when calibrated model parameters are adopted, whilst other uncertain factors may show invisible impacts.

As an extension of our companion paper, this study firstly proposed an interactive factorial data assimilation (IFDA) framework to gives a reliable quantification for the individual and interactive impacts of uncertain factors in data assimilation process. Such a framework is flexible and can explore the impacts for different numbers of factors. The obtained results in this study indicate that enhancement of hydrological models and data assimilation methods would be the most efficient pathway to generate reliable hydrological predictions. Moreover, the robustness of a data assimilation method can also enhance the predictability of the hydrological model, which is able to alleviate the effect of the inherent randomness in data assimilation.

7. Data Availability

Daily precipitation and streamflow data for the River Ouse can be accessed from the National River Flow Archive (NRFA) (https://nrfa.ceh.ac.uk/). The potential evapotranspiration can be obtained from NERC Environmental Information Data Centre, deposited by Tanguy et al. (2017) (https://catalogue.ceh.ac.uk/documents/17b9c4f7-1c30-4b6f-b2fe-f7780159939c). The IFDA framework are coded in R and can be available from the authors upon request (yurui.fan@brunel.ac.uk).

CRediT authorship contribution statement

Y.R. Fan: Data curation, Software, Writing – original draft. **J. Shi:** Writing – review & editing. **Q.Y. Duan:** Writing – review & editing. **L. Yu:** Visualization, Writing – original draft.

Declaration of Competing Interest

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

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jhydrol.2022.128136.

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