Exploring hydrologic post-processing of ensemble streamflow forecasts based on Affine kernel dressing and Nondominated sorting genetic algorithm II

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Abstract. Forecast uncertainties are unfortunately inevitable when conducting the deterministic analysis of a dynamical system. The cascade of uncertainty originates from different components of the forecasting chain, such as the chaotic nature of the atmosphere, various initial conditions and boundaries, inappropriate conceptual hydrologic modeling, and the inconsistent stationarity assumption in a changing environment. Ensemble forecasting proves to be a powerful tool to represent error growth in the dynamical system and to capture the uncertainties associated with different sources. However, space still exists for improving their predictive skill and credibility through proper hydrologic post-processing. We tested the post-processing skills of Affine kernel dressing (AKD) and Non-dominated sorting genetic algorithm II (NSGA-II). Those two methods are theoretically/technically distinct, yet however share the same feature that both of them relax the parametric assumption of the underlying distribution of the data (i.e., streamflow ensemble forecast). AKD transformed ensemble and the Pareto fronts generated with NSGA-II demonstrated the superiority of post-processed ensemble in efficiently eliminating forecast biases and maintaining a proper dispersion with the increasing forecasting horizon.

Keywords: Hydrologic ensemble prediction systems (H-EPS), Hydrologic post-processing, Affine kernel dressing (AKD), Evolutionary multiobjective optimization, Non-dominated sorting genetic algorithm II (NSGA-II).

1 Introduction

Hydrologic forecasting is crucial for flood warning and mitigation (e.g., Shim and Fontane, 2002; Cheng and Chau, 2004), water supply operation and reservoir management (e.g., Datta and Burges, 1984; Coulibaly et al., 2000; Boucher et al., 2011), navigation, and other related activities. Sufficient risk awareness, enhanced disaster preparedness in the flood mitigation measures, and strengthened early warning systems are crucial in reducing the weather-related event losses. Hydrologic models are typically driven by dynamic meteorological models in order to issue forecasts over a medium range horizon of 2 to 15 days (Cloke and Pappenberger, 2009). This kind of coupled hydrometeorologic forecasting systems are admitted as effective tools to issue longer lead times. Inherent in the coupled hydrometeorologic forecasting systems, some predictive uncertainties are then inevitable given the limits of knowledge and available information (Ajami et al., 2007). In fact, those uncertainties

occur all along the different steps of the hydrometeorological modeling chain (e.g., Liu and Gupta, 2007; Beven and Binley, 2014). These different sources of uncertainty are related to deficiencies in the meteorological forcing, mis-specified hydrologic initial and boundary conditions, inherent hydrologic model structure errors, and biased estimated parameters (e.g., Vrugt and Robinson, 2007; Ajami et al., 2007; Salamon and Feyen, 2010; Thiboult et al., 2016). Among most cases, a single deterministic forecasts turns out to be way more insufficient.

Many substantive theories have been proposed in order to quantify and reduce the different sources of cascading forecast uncertainties and to add good values to flood forecasting and warning. Among them, the superiority of ensemble forecasting systems in quantifying the propagation of predictive uncertainties (over deterministic systems) is now well established (e.g., Cloke and Pappenberger, 2009; Palmer, 2002; Seo et al., 2006; Velázquez et al., 2009; Abaza et al., 2013; Wetterhall et al., 2013; Madadgar et al., 2014). Numerous challenges have been well tackled, for example: (1) meteorological ensemble prediction systems (M-EPSs) (e.g., Palmer, 1993; Houtekamer et al., 1996; Toth and Kalnay, 1997) are refined and operated worldwide by national agencies such as the European Centre for Medium-Range Weather Forecasts (ECMWF), the National Center for Environmental Prediction (NCEP), the Meteorological Service of Canada (MSC), and more; (2) the forecast accuracy is highly improved by adopting higher resolution data collection and assimilation. Sequential data assimilation techniques, such as the particle filter (e.g., Moradkhani et al., 2012; Thirel et al., 2013) and the ensemble Kalman filter (e.g., Evensen , 1994; Reichle et al., 2002; Moradkhani et al, 2005; McMillan et al., 2013) provide an ensemble of possible re-initializations of the initial conditions, expressed in the hydrologic model as state variables, such as soil moisture, groundwater level and so on; (3) forecasting skills of the coupled hydrometeorologic forecasting systems are also improved by tracking predictive errors using the full uncertainty analysis. Multimodel schemes were proposed to increase performance and decipher structural uncertainty (e.g., Duan et al., 2007; Fisher et al., 2008; Weigel et al., 2008; Najafi et al., 2011; Velázquez et al., 2011; Marty et al., 2015; Mockler et al., 2016). Thiboult et al. (2016) compared many H-EPS, accounting for the three main sources of uncertainties located along the hydrometeorological modeling chain. They pointed out that EnKF probabilistic data assimilation provided most of the dispersion for the early forecasting horizons but failed in maintaining its effectiveness with increasing lead times. A multimodel scheme allowed sharper and more reliable ensemble predictions over a longer forecast horizon; (4) statistical hydrologic post-processing component is added in the H-EPS for rectifying biases and dispersion errors (i.e., too narrow/too large) are numerous, as reviewed by Li et al. (2017). It is noteworthy that many hydrologic variables, such as discharge, follow a skewed distribution (i.e., low probability associated to the highest streamflow values), which complicates the task. Usually, in a hydrologic ensemble prediction system (H-EPS) framework (e.g., Schaake et al., 2007; Cloke and Pappenberger, 2009; Velázquez et al., 2009; Boucher et al., 2012; Abaza et al., 2017), the post-processing procedure over the atmospheric input ensemble is often referred as pre-processing, while post-processing aims at improving the hydrologic ensemble forecasting outputs.

However, another challenge still remains: how to improve the human interpretation of probabilistic forecasts and the communication of integrated ensemble forecast products to end-users (e.g., operational hydrologists, water managers, local conservation authorities, stakeholders and other relevant decision makers). Buizza et al. (2007) emphasized that both functional and technical qualities are supposed to be assessed for evaluating the overall forecast value of a hydrometeorologic forecasts.

Ramos et al. (2010) further note that the best way to communicate probabilistic forecast and interpret its usefulness should be in harmony with the goals of the forecasting system and the specific needs of end-users. She also demonstrated the main achievements from two studies obtained from a Member States workshop (Thielen et al., 2005) role-play game and another survey to explore the users' risk perception of forecasting uncertainties and how they dealt with uncertain forecasts for decision-making. The results revealed that there is still space for enhancing the forecasters' knowledge and experience on bridging the communication gap between predictive uncertainties quantification and effective decision-making.

Hence, in practice, which forecast quality impacts a given decision the most? Different end-users share their unique requirements: Crochemore et al. (2017) produced the seasonal streamflow forecasting by conditioning climatology with precipitations indices (SPI3). Forecast reliability, sharpness (i.e., the ensemble spread), overall performance and low-flow event detection were verified to assess the conditioning impact. In some cases, the reliability and sharpness could be improved simultaneously while more often, there was a trade-off between them. Another IMPREX project conduct an optimization for the reservoir-based hydropower production to explore the relationship between the forecast quality and economic values. They found that an over-estimation comes along with more penalization.

The study is a contribution to probe this topic by exploring hydrological post-processing of ensemble streamflow forecasts based on Affine kernel dressing (AKD) and Non-dominated sorting genetic algorithm II (NSGA-II). The mechanisms of these two statistical post-processing methods are completely different. However, they share one similarity from another perspective, which is they can estimate the probability density directly from the data (i.e., ensemble forecast) without assuming any particular underlying distribution. As a more conventional method, Silverman (1986) firstly proposed the kernel density smoothing method to estimate the distribution from the data by centering a kernel function K that determines the shape of a probability distribution (i.e., kernel) fitted around every data point (i.e., ensemble members). The smooth kernel estimate is then the sum of those kernels. As for the choice of bandwidth h of each dressing kernel, Silverman's rule of thumb finds an optimal bandwidth h by assuming that the data is normally distributed. Improvements to the original idea were soon to follow. For instance, the improved Sheather Jones (ISJ) algorithm is more suitable and robust with respect to multimodality (Wand and Jones, 1994). Roulston and Smith (2003) rely on the series of "best forecasts" (i.e., best-member dressing) to compute the kernel bandwidth h. Wang and Bishop (2005) as well as Fortin et al. (2006) further improved the best member method. The later advocated that the more extreme ensemble members are more likely to be the best member of raw under-dispersive forecasts, while the central members tend to be more "precise" for over-dispersive ensemble. They proposed the idea that different predictive weights should be set over each ensemble member, given each member's rank within the ensemble. Instead of standard dressing kernels that act on individual ensemble members, Bröcker and Smith (2008) proposed the AKD method by assuming an affine mapping between ensemble members and observation over the entire ensemble. They approximate the distribution of the observation given the ensemble.

NSGA-II opens up the opportunity of improving the forecast quality in harmony with the forecasting aims and the specific needs of end-users. Given the single-model H-EPSs studied here, the hydrologic ensemble is generated by activating two forecasting tools: the ensemble weather forecasts and the EnKF. Henceforth, enhancing the H-EPS forecasting skill by assigning different credibility to ensemble members becomes preferred than reducing the number of members. Multiple ob-

jective functions (i.e., here, verifying scores) for evaluating the forecasting performances of the H-EPS are selected to guide the optimization process. The expected output is a group of solutions, also known as Pareto fronts, that can give the trade-offs between different objectives. Other post-processing techniques, like the Non-dominated sorting genetic algorithm II (NSGA-II), are now common (e.g., Liong et al., 2001; De Vos and Rientjes, 2007; Confesor and Whittaker, 2007). Such techniques are conceptually linked to the multiobjective parameter calibration of hydrologic models using Pareto approaches. Indeed, formulating a model structure or representing the hydrologic processes using a unique global optimal parameter set proves to be very subjective. Multiple optimal parameter sets exist with satisfying behavior given the different conceptualizations, albeit not identical Beven and Binley (1992). For example, Brochero et al. (2013) utilized the Pareto fronts generated with NSGA-II for selecting the "best" ensemble from a hydrologic forecasting model with a pool of 800 streamflow predictors, in order to reduce the H-EPS complexity.

In this study, the daily streamflow ensemble forecasts issued from five single-model H-EPSs over the Gatineau River (Province of Québec, Canada) are post-processed. Details about the study area, hydrologic models, and hydrometeorologic data are described in Section 2. Section 3 explains the methodology and training strategy of AKD and NSGA-II methods, in parallel with the scoring rules that evaluate the performance of the forecasts. Specific concepts associated with those scores are also introduced in this section. Predictive distribution estimation based on the five single-model H-EPSs configurations, which lack accounting for the model structure uncertainty, is presented in Section 4. The comparison of both statistical post-processing methods in improving the forecasting quality as well as enhancing the uncertainty communication are discussed and analyzed as well. Conclusion follows in Section 5.

2   The H-EPSs

Figure 1 illustrates the study area: the Gatineau River located in southern Québec, Canada. It drains 23,838 km2 of the Outaouais and Montréal hydrographic region and experiences a humid continental climate. The river starts from Sugar Loaf Lake (47° 52 54N, 75° 30 43W) and joins the Ottawa River some 400 km later. The average daily temperature is about -3°C in winter while the temperature spectrum is 10-22°C in summer (Kottek et al., 2006). The hydrologic regime of the study area is generally wet, cold, and snow-covered. The largest flood typically appears in spring or early summer (i.e., from March to June) from snowmelt and rainfall. Autumnal rainfall often leads to a lesser peak between September and November (Figure 2).

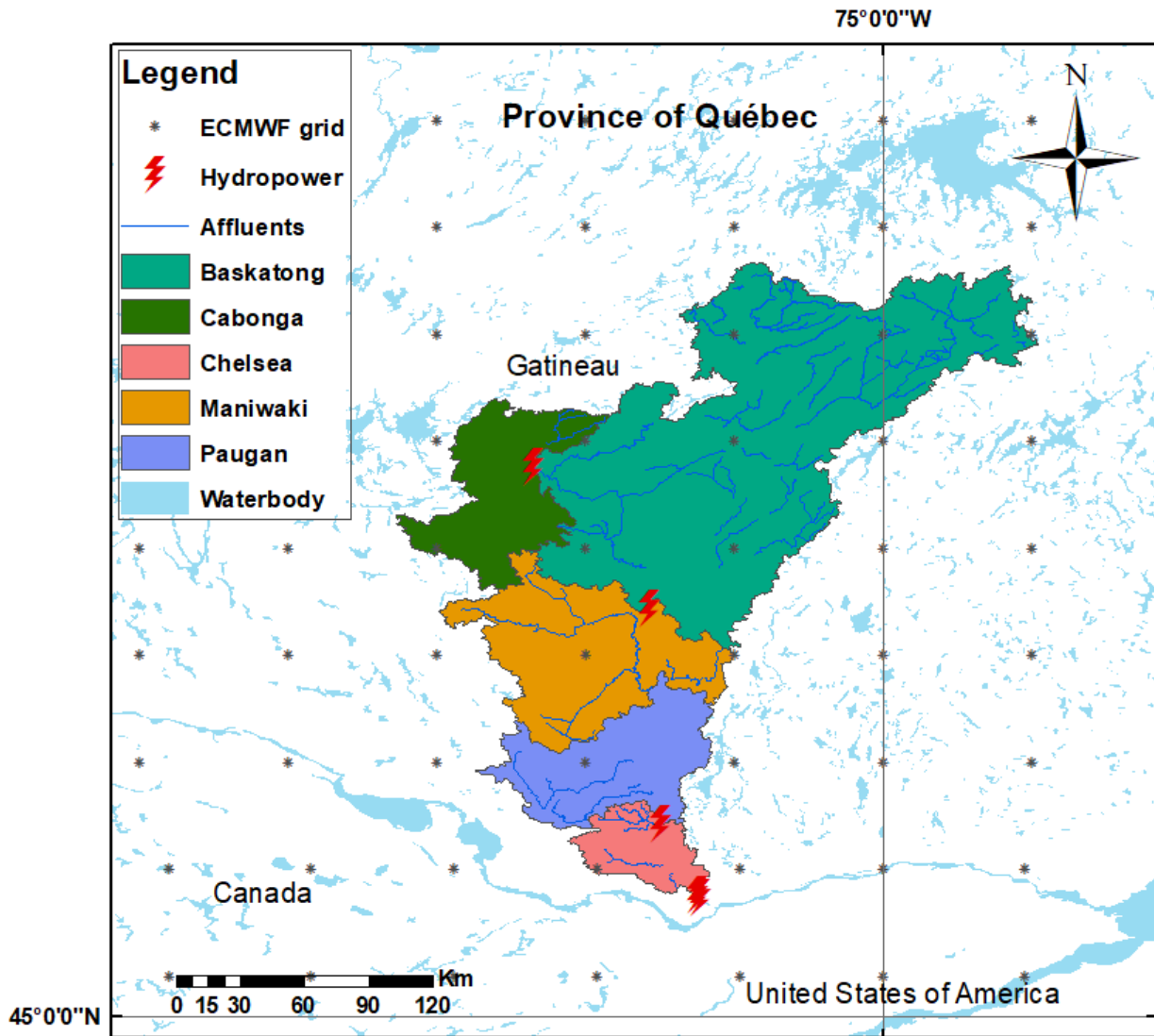



Figure 1. The five sub-catchments of the Gatineau River. The red thunder marks locate the dams while the original ECMWF grid points, before downscaling, are marked using black stars.

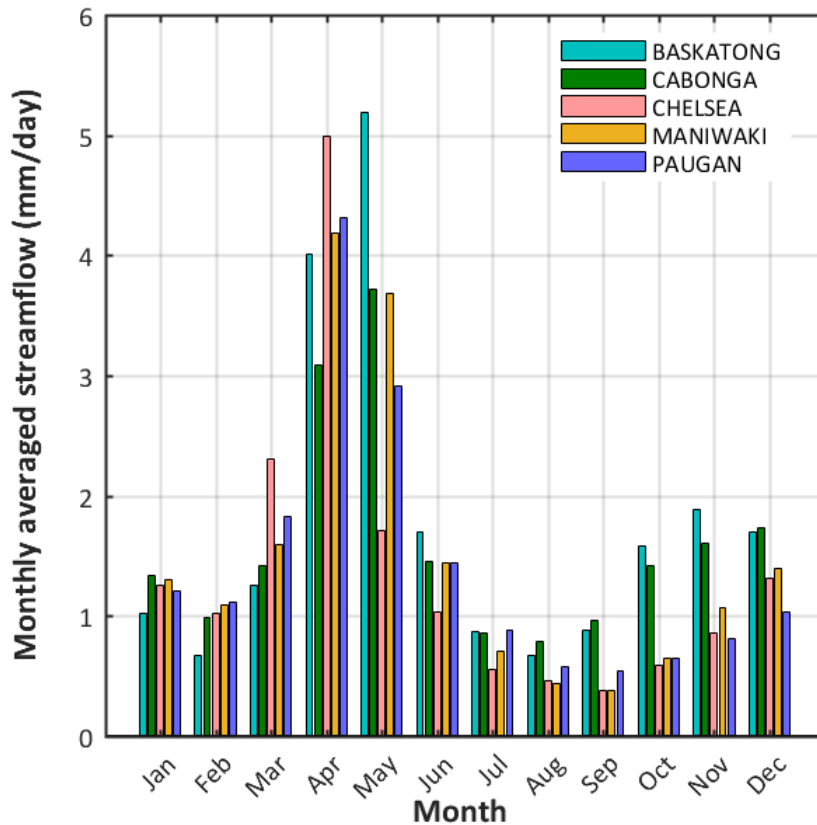



Figure 2. Hydrograph of daily streamflows (*mm/day*) averaged over each month during 33 years from 1985 to 2017.

For operational hydrologic modeling, reservoir operation, and hydroelectricity production, the whole catchment has been divided up into five sub-catchments: Baskatong, Cabonga, Chelsea, Maniwaki, and Paugan, identified by different colors in Figure 1. The sub-catchments are modelled independently from one another, in order to inform a decision model operated by Hydro-Québec (e.g., Movahedinia, 2014). All hydroclimatic time series to the project were made available by Hydro-Québec that carefully constructed them for their own hydropower operations. Dams are identified in Figure 1 as red thunder marks. The two most upper ones allow the existence of large headwater reservoirs, while the other three are run-of-the-river installations. The daily streamflow (m^3/s) time series entering the reservoirs were constructed by the electricity producer from a diversity of local information and made available to the study along with spatially averaged minimum and maximum air temperature ($°C$) and precipitation (mm) for each sub-basin.

The time series extend from January 1950 to December 2017. The study focuses on the last 33 years (1985-2017) to avoid the increased bias and variability caused by missing values within the record. Table 1 summarizes the various hydroclimatic characteristics of the Gatineau River sub-catchments. Potential evapotranspiration is calculated from the temperature-based Oudin et al. (2005) formulation.

Table 1. Hydroclimatic characteristics of five sub-catchments of the Gatineau River.

Name	Lat.	Lon.	Catchment Area (km^2)	Mean annual Q (mm)
Cabonga	47.21	-76.59	2,665	1.35
Baskatong	47.21	-75.95	13,057	1.49
Maniwaki	46.53	-76.25	4,145	1.24
Paugan	46.07	-76.13	2,790	1.29
Chelsea	45.70	-76.01	1,142	1.27

The meteorological ensemble forecasts were retrieved from the European Center for Medium-Range Weather Forecasts (ECMWF; Fraley et al. (2010)). The time series extend from January 2011 to December 2016. The meteorological ensemble forecast used the reduced Gaussian transformation to the latitude-longitude system during the THORPEX Interactive Grand Global Ensemble (TIGGE) database retrieving by bilinear interpolation (e.g., Gaborit et al., 2013). The horizontal resolution was downscaled during retrieval from the 0.5° ECMWF grid resolution to a 0.1° grid resolution. This study resorts to the 12:00 UTC forecasts only, aggregated to a daily time step over a 7-day horizon. All data are aggregated at the catchment scale, averaging grid points located within each sub-catchments.

The HydrOlOgical Prediction Laboratory (HOOPLA; Thiboult et al. (2020)) provides the modular framework to perform calibration, simulation, and streamflow prediction using multiple hydrologic models (i.e., 20 lumped models) (Perrin, 2000; Seiller et al., 2012). The empirical two-parameter model CemaNeige (Valéry et al., 2014) simulates snow accumulation and melt. Five random hydrologic models from HOOPLA are exploited in this study. Their main characteristics are summarized in Table 2. All time series were split in two following the Split-Sample Test (SST) procedure of Klemeš (1986): 1986-2006 for calibration and 2013-2017 for validation. In both cases, three prior years were used for spin-up. January 2011-December 2016 is committed to hydrologic forecasting.

Table 2. Main characteristics of the hydrologic models (Seiller et al., 2012).

Model	No. of optimized parameters	No. of reservoirs	Derived from
M01	6	3	BUCKET (Thornthwaite and Mather, 1955)
M02	4	2	GR4J (Perrin et al., 2003)
M03	9	3	HBV (Bergström et al., 1973)
M04	7	3	IHACRES (Jakeman et al., 1990)
M05	9	5	SACRAMENTO (Burnash et al., 1973)

Initial condition uncertainties within each H-EPS are accounted for by a 100-member Ensemble Kalman Filter (EnkF) that adjusts the model states distribution function given observational distributions. Meteorological uncertainties are quantified by providing the 50-member ECMWF ensemble forcing to the H-EPSs. Resulting ensemble streamflow forecasts thus consists of 5,000 members. This set-up is similar to the one described in more details by Thiboult et al. (2016). The EnKF hyperparameters selection follows the work of Thiboult and Anctil (2015). Streamflow and precipitation uncertainties are assumed proportional;

they are set to 10% and 50%, respectively. Temperature uncertainty is considered constant; it amounts to $2°C$. A Gaussian describes the streamflow and temperature uncertainty and a gamma law represents the precipitation uncertainty.

3 Methodology

This study was conducted on the base of 1-7-day ensemble streamflow forecasts issued from five single-model H-EPSs and their realizations. Both AKD and NSGA-II methods are utilized in this study as the statistical post-processing or so-called ensemble interpretation method (Jewson, 2003; Gneiting et al., 2005) to transform the raw ensemble forecast into a probability distribution.

3.1 Affine kernel dressing (AKD)

Rather than adopting the ensemble mean and the standard deviation and approximate the distribution of the raw ensemble (Wilks, 2002), the principal insight of this methodology is that the probability distribution could be fitted of the observation given the ensemble (Bröcker and Smith, 2008). AKD method interprets the ensemble by approximating the distribution of the observation given the ensemble forecasts. The ordering of the ensemble members is not taken into account (i.e., ensemble members are considered exchangeable here). Here, we denote the ensemble forecasts with m members over time by $X(t) = [x_1(t), x_2(t), \ldots, x_m(t)]$ and the observation by $y(t)$. The mean and the variance of the raw ensemble forecasts are then:

$$\mu(X) = \frac{1}{m} \sum_i x_i \tag{1}$$

$$\upsilon(X) = \frac{1}{m} \sum_i [x_i - \mu(X)]^2 \tag{2}$$

In a general form, the probability density function of $p(y; X, \theta)$ defines the interpreted ensemble (i.e., kernel dressed ensemble) given the original ensemble with free parameter vector θ:

$$p(y; X, \theta) = \frac{1}{bh} \sum_i K\left(\frac{y - ax_i - b}{h}\right) \tag{3}$$

for which the interpreted ensemble can be seen as a sum of probability functions (kernels) around each raw ensemble member. x_i represents the ith ensemble member and y is the corresponding observation. Hence, $ax_i + b$ identifies the center of each kernel using the scale parameter a and offset parameter b. h is the positive bandwidth of each kernel. Note that various

distributions could be adopted as kernels (Silverman, 1986; Roulston and Smith, 2003; Bröcker and Smith, 2008). We opted for the standard Gaussian density function with zero mean and unit variance for its computational convenience:

$$K(\cdot) = \frac{1}{\sqrt{2\pi}} exp\left(-\frac{1}{2}(\cdot)\right)^2 \tag{4}$$

The mean and the variance of the interpreted ensemble can be defined as:

$$\mu'(X) = b + a \cdot \frac{1}{m}\sum_i x_i = b + a \cdot \mu(X) \tag{5}$$

$$\upsilon'(X) = h^2 + a^2 \cdot \frac{1}{m}\sum_i [x_i - \mu(X)]^2 = h^2 + a^2 \cdot \upsilon(X) \tag{6}$$

The mapping parameters of a, b, and h are determined from the raw ensemble. The updated mean $\mu'(X)$ of the kernel dressed ensemble is a function of the raw ensemble mean $\mu(X)$, scaled and shifted using a and b. The variance $\upsilon'(X)$ of the kernel dressed ensemble is a function of the initial ensemble variance $\upsilon(X)$, scaled and shifted using a^2 and h^2. Detailed derivations of these equations are given by Bröcker and Smith (2008).

AKD provides the following solutions for determining parameters of a, b, and h are determined as functions of X:

$$b = r_1 + r_2 \cdot \mu(X) \tag{7}$$

$$h^2 = h_S^2 \cdot \left[s_1 + s_1 \cdot a^2 \cdot \upsilon(X)\right] \tag{8}$$

$$h_S = 0.5 \cdot [4/(3m)]^{1/5} \tag{9}$$

Here, h_S is Silverman's factor (Silverman, 1986). Technically, we can use some scores (e.g., mean square error, etc) to select the optimal bandwidth h for a kernel density estimation, yet this would be difficult to estimate for general kernels. Hence, the first rule of thumb proposed by Silverman gives the optimal bandwidth h which is the standard deviation of the distribution. And in this case, the kernel is also assumed to be Gaussian. The parameters $\theta = [a, r_1, r_2, s_1, s_2]$ are free parameters and usually

$r_1 = 0$, $r_2 = 1$, $s_1 = 0$ and $r_2 = 1$ are rational initial selections (Bröcker and Smith, 2008). Once the optimal free parameter vector $\theta = [a, r_1, r_2, s_1, s_2]$ is obtained, the interpreted ensemble can be set to:

$$p(y; X, \theta) = \frac{1}{bh} \sum_i K\left(\frac{y - ax_i - b}{h}\right) = \frac{1}{bh} \sum_i K\left(\frac{y - z_i}{h}\right) \tag{10}$$

$$z_i = ax_i + r_2 \cdot \mu(X) + r_1 \tag{11}$$

$$h^2 = h_S^2 \cdot [s_1 + s_2 \cdot \upsilon(X)] \tag{12}$$

Where, Z_i is the resulting kernel dressed ensemble, based on the raw ensemble X and fitted parameters a, r_1, and r_2. Bröcker and Smith (2008) stressed that this AKD ensemble transformation works on the whole ensemble rather than on each individual member. Finally, the mean and variance of the interpreted ensemble shown in Eq. (5) and Eq. (6) can be re-written as:

$$\mu'(X) = b + a \cdot \mu(X) = r_1 + (a + r_2) \cdot \mu(X) \tag{13}$$

$$\upsilon'(X) = h^2 + a^2 \cdot \upsilon(X) = h_S^2 \cdot s_1 + a^2 \cdot \left(h_S^2 \cdot s_2 + 1\right) \cdot \upsilon(X) \tag{14}$$

3.2 Nondominated sorting genetic algorithm II (NSGA-II)

Multiobjective optimization problems are common and typically lead to a set of optimal options (Pareto solution set) for users to choose from. Exploiting a genetic algorithm to find all Pareto solutions out from the entire solution space have been proposed and improved since the publication of the vector-evaluated genetic algorithm (VEGA) around 1985 (Schaffer, 1985).

There exist two main standpoints for dealing with multiobjective optimization problems: (1) define a new objective function as the weighted sum of all desired objective functions (e.g., MBGA, RWGA) or (2) determine the Pareto set or its representative subsets for a selected group of objective functions (e.g., SPEA, SPEA-II, NSGA, NSGA-II). The first approach is more trivial as it reduces to a single-objective optimization problem. Yet, the needed weighting strategy is difficult to set accurately as a minor difference in weights may lead to quite different solutions. On the other hand, Pareto-ranking approaches have been devised in order to avoid the problem of converging towards solutions that only behave well for one specific objective function. Users still have to select objective functions that are pertinent to the problem and that are not heavily correlated to one another. Readers may refer to the review of Konak et al. (2006) for more details.

Similar ideas can be utilized in this study as the goal is to achieve a "good forecast". Various efficiency criteria are needed when we verify whether an H-EPS is competent issuing accurate and reliable forecasts. *Accuracy* might be the first idea that crosses our mind that indicates that there is a good match between the forecasts and the observations. Since here we are focused on probabilistic streamflow forecast, the *accuracy* could be measured by computing the distances between the forecast densities with the observed ones (Wilks, 2011). Usually, hydrologists could rely on the Nash-Sutcliffe efficiency criterion (*NSE*, Nash and Sutcliffe (1970)) for measuring how well forecasts can reproduce the observed time series. Transforming the time series beforehand allows specializing it (i.e., NSE_{inv}, NSE_{sqrt}) for specific needs (e.g., Seiller et al., 2017). *NSE* is dimensionless and varies on the interval of $[-\infty, 1]$. A perfect model forecast output would have an *NSE* value that equals to one.

Meanwhile, *bias*, also known as systematic error, refers to the correspondence between the average forecast and the average observation, which is different from accuracy. For example, systematic *bias* exists in the streamflow forecasts that are consistently too high or too low. Hence, *NSE* simulNSEo and *bias* are utilized here as objective functions, which is to say that it is seeking to minimize the *bias* and maximize the *NSE* simulously. This brings us a multi-objective optimization question to solve.

Technically, inserting the elitism in the multi-objective optimization algorithms is not compulsory. However, it would have a strong influence that if the algorithms could preserve the best individuals (i.e., elites) that were founded during the search process and then incorporated the elitism back in the evolutionary process (Groşaelin et al., 2003). A classic, fast and elitist multiobjective genetic algorithm, the Nondominated sorting genetic algorithm II (NSGA-II; Deb et al. (2002)) is adopted for searching for the Pareto solution set. NSGA-II offers three specific advantages over previous genetic algorithms: 1) there is no need to specify extra parameters such as the niche count for the fitness sharing procedure; 2) it reduces complexity over alternative GA implementations; 3) elite individuals are well maintained and hence the effectiveness of the multiobjective genetic algorithm is largely improved.

In this study, the population is denoted by $X(t)$. Specific steps for NSGA-II are briefly introduced here:

1) Layer the whole population by using the fast nondominated sorting approach: i is initially set to 1, while z_i represents the ith solution among the m ones. Compare the domination and nondomination relationship between the individuals z_i and z_j for all the $j = 1, 2, \ldots, m$ and $i \neq j$. z_i is the nondominated solution as long as no z_j dominates it. This process is repeated until all the nondominated solutions are found and composed the first nondominated front of the population. Note that the selected individuals of the first front can be neglected when searching for subsequent fronts (i.e., marked as k_{rank}).

2) Find the crowding distance for each individual in each front. Deb et al. (2002) pointed out the basic idea of the "crowding distance" calculated in the NSGA-II is "to find the $EuclidianDistance$ between each individual in a front based on their m objectives in the m dimensional hyper space. The individuals in the boundary are always selected since they have infinite distance assignment. The large average crowding distance will result in better diversity in the population". This step ensures the diversity of the population. For example, for the first front, sort the values of the objective functions in an ascending order.

The boundary solutions (i.e., maximum and minimum solutions) are then the value at infinity. The crowding distance for other individuals can be assigned as:

$$k_{distance} = \sum_{k=1}^{m} \left(\left| \int_{n}^{j+1} - \int_{n}^{j-1} \right| \right) \tag{15}$$

where $k_{distance}$ represents the value for the kth individual and f_n^{j+1} and f_n^{j-1} are the values of the nth objective function at $j+1$ and $j-1$, separately. Thereafter, the crowding-comparison operator can be utilized based on k_{rank} and $k_{distance}$. Individual z_i will be assumed superior than z_j if $k_{rank}^{i} < k_{rank}^{j}$ or $k_{distance}^{i} > k_{distance}^{j}$, when their Pareto front ranks are equal.

3) Elitism strategy is introduced in the main loop. Offspring population Q_t is firstly generated from parent population P_t after mutation and gene cross-over. Then the above-mentioned nondominated sorting and crowding distance assignment are conducted on the composed population R_t that contain both Q_t and P_t with the size of $2m$. The first-rate nondominated solutions will be assign to the new parent population P_{t+1}. Outputs after the whole evolutionary search are the un-repeated nondomination solutions and a weight matrix can also be extracted from the solutions. Specifically, in this study, the population size is set to 50, the number of objective functions equals to 2, the boundary is from 0 to 1, the mutation probability and crossing-over rate are 0.1 and 0.7, and the maximum evolution runs are 430 times.

3.3 Verifying metrics

The performance of the post-processed forecast distributions, mostly in terms of accuracy and reliability, is assessed using scoring rules. Except for *bias* and *NSE* described above, seven other verifying scores are applied to both the raw and post-processed forecast distributions.

The overall accuracy and reliability of the probabilistic forecast can be evaluated using the Continuous ranked probability score (*CRPS*, Matheson and Winkler, 1976, Hersbach, Gneiting and Raftery, 2007). Hersbach (2000) decomposed the *CRPS* into two parts: reliability and resolution. In practice, The Mean continuous ranked probability score (*MCRPS*) is the average value of *CRPS* over the whole time series *T* and is calculated using empirical distributions. Besides, *MCRPS* is negatively oriented and the optimal *MCRPS* value is 0:

$$MCRPS = \frac{1}{T} \sum_{t=1}^{T} \int_{-\infty}^{+\infty} \left(P_t^{fcst}(y) - H\left(y_t \geq y_t^{obs}\right) \right)^2 dy \tag{16}$$

where y is the predictand and y_t^{obs} represents the corresponding observations. $P_t^{fcst}(y)$ is the cumulative distribution function of the forecasts at time step t. The Heaviside function H equals 0 (or 1) when $y_t < y_t^{obs}$ (or, $y_t \geq y_t^{obs}$).

As for the deterministic metrics, we adopt the Mean absolute error (*MAE*) and Root mean squared error (*RMSE*, e.g., Brochero et al., 2013) for verifying the average forecast error of the variable of interest. Both *MAE* and *RMSE* are negatively

oriented and range from 0 to $+\infty$. More accurate forecasts lead to lower *MAE* and *RMSE*. Note that the *RMSE* score tends to penalize the large errors more than *MAE*. In some cases that the variance corresponding to the frequency distribution in higher, the *RMSE* will have larger increase while the *MAE* remains stable.

RMSE has the benefit of penalizing large errors more so can be more appropriate in some cases

The Kling-Gupta efficiency (*KGE*; Gupta et al., 2009) also allows for a comprehensive performance assessment of the deterministic forecasts. *KGE'*, a slightly modified version of *KGE* (Kling et al., 2012), avoids any cross-correlation between the bias and the variability ratios. It is defined as:

$$KGE' = \sqrt{(r-1)^2 + (\beta-1)^2 + (\gamma-1)^2} \tag{17}$$

$$\beta = \frac{\mu_y}{\mu_o} \tag{18}$$

$$\gamma = \frac{CV_y}{CV_o} = \frac{\sigma_y/u_y}{\sigma_o/u_o} \tag{19}$$

The correlation coefficient r represents the linear association between the deterministic forecast and the observations. μ_y (μ_o) and σ_y (σ_o) are the mean and the standard deviations of the forecasts (here, the ensemble mean) and observation, respectively. *CV* is the dimensionless coefficient of variation.

The *Reliability diagram* (Stanski et al., 1989) is a graphical representation of the reliability of an ensemble forecast. It contrasts the observed frequency against the probability of ensemble forecasts over all quantiles of interest. The proximity from the diagonal line indicate how close the forecast probabilities are associated to the observed frequencies for selected quantiles. The 45° diagonal line thus represents perfect reliability, i.e., when the ensemble forecast probabilities equals the observation ones. When the plotted curve lies above the 45° line, the predictive ensemble is over-dispersed. It is otherwise under-dispersed. In addition, a flat curve represents that the forecast has no resolution (i.e., climatology).

The Spread Skill plot (*SSP* or simply refered as *spread* later, Fortin et al., 2014) assesses the ensemble spread and identifies an ensemble forecast with poor predictive skill and large dispersion that would be positively assessed by a reliability diagram. Fortin et al. (2014) stresses that the ensemble spread should match the *RMSE* of the ensemble mean when the predictive ensemble is reliable. Thus, the *SSP* complements the spread component with an accuracy aspect.

3.4 Experimental setup

Establishing and analyzing both AKD and NSGA-II predictive models to interpret single-model hydrologic ensemble forecasts for uncertainty analysis can be summarized in three steps:

(1) Determine the length of the training period. The target ensemble for interpretation has a horizon that extends from day 1 to 7. It is a well-known fact that the skill of hydrologic forecasts fades away with increasing lead time. The 4-day-ahead ensemble forecasts issued from each single-model H-EPSs and their corresponding observations are chosen as a training dataset, since located in the middle of the forecast horizon. The validation dataset thus consists of the remaining forecasts: day 1-3 and 5-7 ahead raw forecasts issued from the associated H-EPSs. Here, this specific procedure we selected is to be taken as an example. We conducted the calibration on day-4 and then tested it on other lead times to assess the robustness of the predictive models. Yet one may decide otherwise, such as implementing the calibration/validation procedures separately for each days.

(2) AKD mapping between the ensemble and observation over the training dataset. The observation time series are used to identify the free parameter vector $\theta = [a, r_1, r_2, s_1, s_2]$, minimizing the *MCRPS* to obtain the kernel-dressed ensemble. Note that AKD acts on the entire ensemble rather than on each individual member.

(3) Evaluate the Pareto fronts (i.e., nondominated solutions that minimize/maximize the *bias* and the *NSE*) and the weight matrix, applying NSGA-II over the training dataset. Sloughter et al. (2007) mentioned that the training period should be specific for each dataset or region. Here a 30-day moving window is selected so it contains enough training samples with coherent consistency. Especially, from the operational perspective, a monthly moving window is more coherent and efficient in the real world, with limited length for time series.

A general flowchart of the streamflow input, AKD and NSGA-II frameworks, and expected outputs is illustrated in Figure 3.

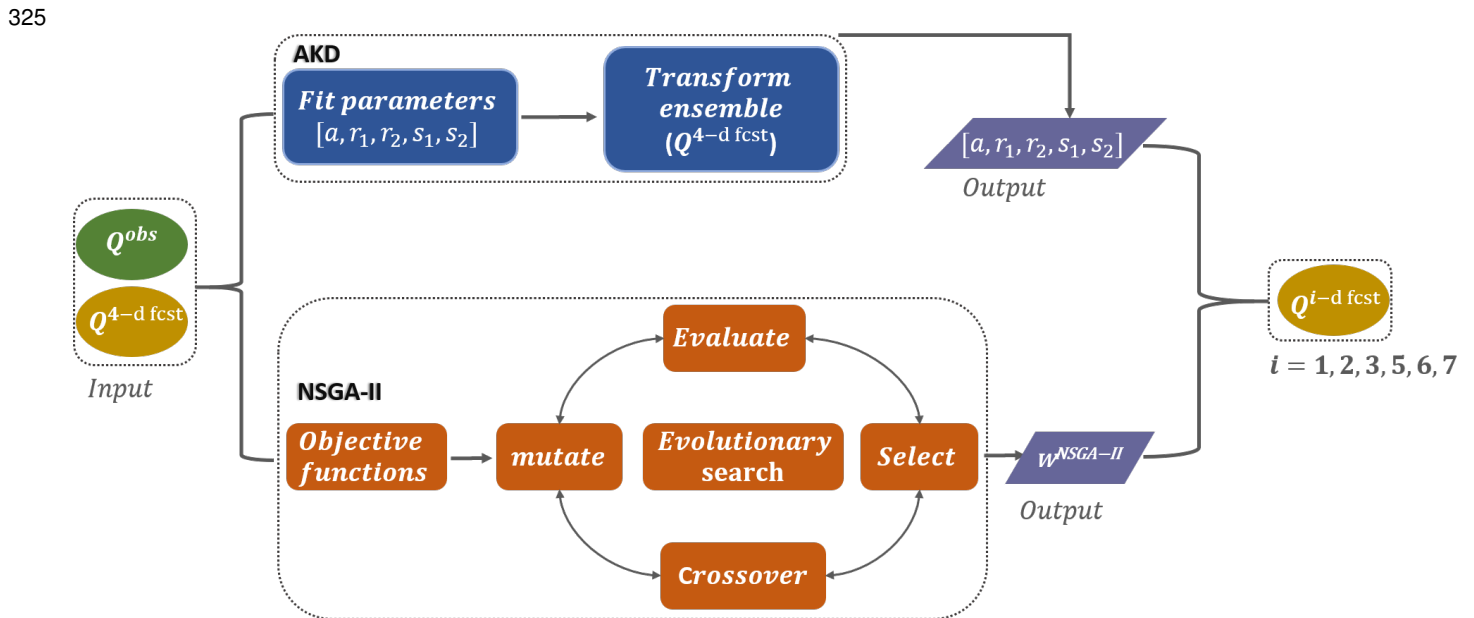



Figure 3. Schematic of the experimental setup flowchart.

4 Results and discussions

4.1 Ensemble member exchangeability

330 The issue of member interchangeability is central to this study, since for AKD each raw ensemble will be considered as a whole (i.e., indistinguishable members) whereas for NSGA-II a weight matrix is sought, which implies that different weights are assigned to each candidate members.

Interchangeability is here assessed visually, simultaneously looking at the individual *RMSE* values of all 5,000 members, 7 daily forecast horizons, and 5 H-EPSs. Figure 4 displays (typical) values for day 500 and Baskatong sub-catchment - a video

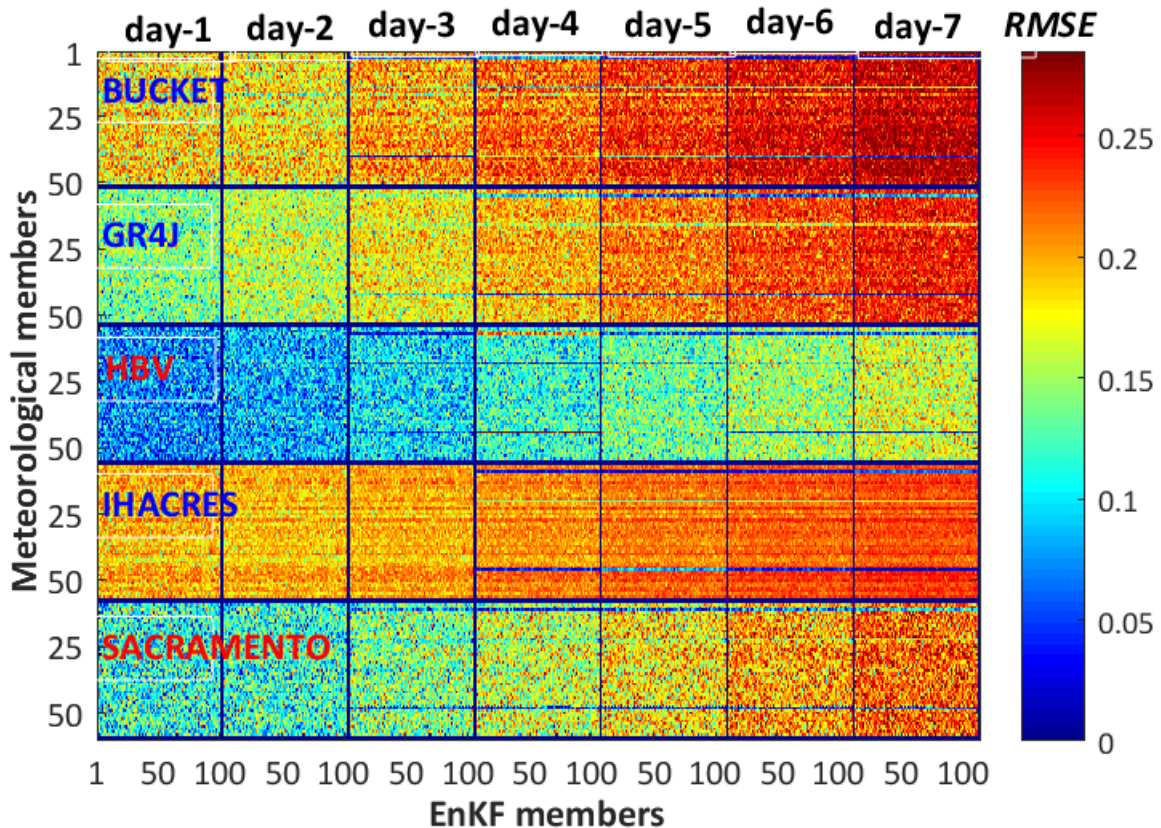
335 covering the full time series is available as a supplemental material to this paper). For each H-EPS forecast horizon boxes, horizontal lines consist of 100 EnKF members and vertical lines, of 50 meteorological members. Mosaics with redder colors represent higher values of the *RMSE*. The decreasing predictive skill of the H-EPSs with lead time is hence shown as an increasingly red mosaic.

340 **Figure 4.** Illustration of the *RMSE* values (*mm/day*) of the individual members of the forecast issued by the 5 H-EPSs for the Baskatong sub-catchment, on day 500. There are 7 daily forecasts horizons. Each box consists of 5,000 members, from 100 EnKF members (horizontal lines) and 50 meteorological members (vertical lines).

Figure 4 displays the hydrologic forecasts build upon the 50-member ECMWF ensemble forecasts. The basic idea behind Figure 4 (and its accompanying video) is to visually assess if the initial interchangeability of the weather forecasts holds for the hydrologic forecasts (i.e., horizontal lines). While the interchangeability of the probabilistic data assimilation scheme is assessed in parallel (vertical lines). One can notice in Figure 4 colorful horizontal lines within each box start to appear from day 3 and on, revealing a distinguishable character with longer lead times. At the same time, no obvious vertical lines are present in the same figure. These results suggest that the hydrologic forecasts produced in this study are fully interchangeable with respect to EnKF, but less so with respect to the weather, the latter being non-linearly transformed by the hydrologic models. This opens up the possibility of assigning weights to the hydrologic forecasts associated to the ECMWF members.

For practical reasons, as the 100-member data assimilation ensemble was deemed fully interchangeable, this component is randomly reduced to 50 members from now on in this document. This procedure simplifies the implementation of the AKD and NSGA-II post-processing computations, which results are presented next.

4.2 Uncertainty analysis

The NSGA-II Pareto front drawn in Figure 5 (model M01 over the Baskatong catchment) is quite typical. In this multiobjective evolutionary search, 35 (nondominated) Pareto solutions are identified. No objective can be improved more wi thout the sacrifice of another. The optimal *NSE* is inevitably accompanied with the highest bias (e.g., *NES* = 0.84594, *bias* = 0.034055), or vice versa. The solutions in the elbow region of the Pareto front are the compromise between both two objective functions. Pareto fronts with different numbers of solutions can be attained daily via setting the sliding window. Therefore, rather than choosing only one fixed position in the front, we opted to pick the solution randomly for respecting and exploring the diversity within. Figure 6 confirms NSGA-II convergence.

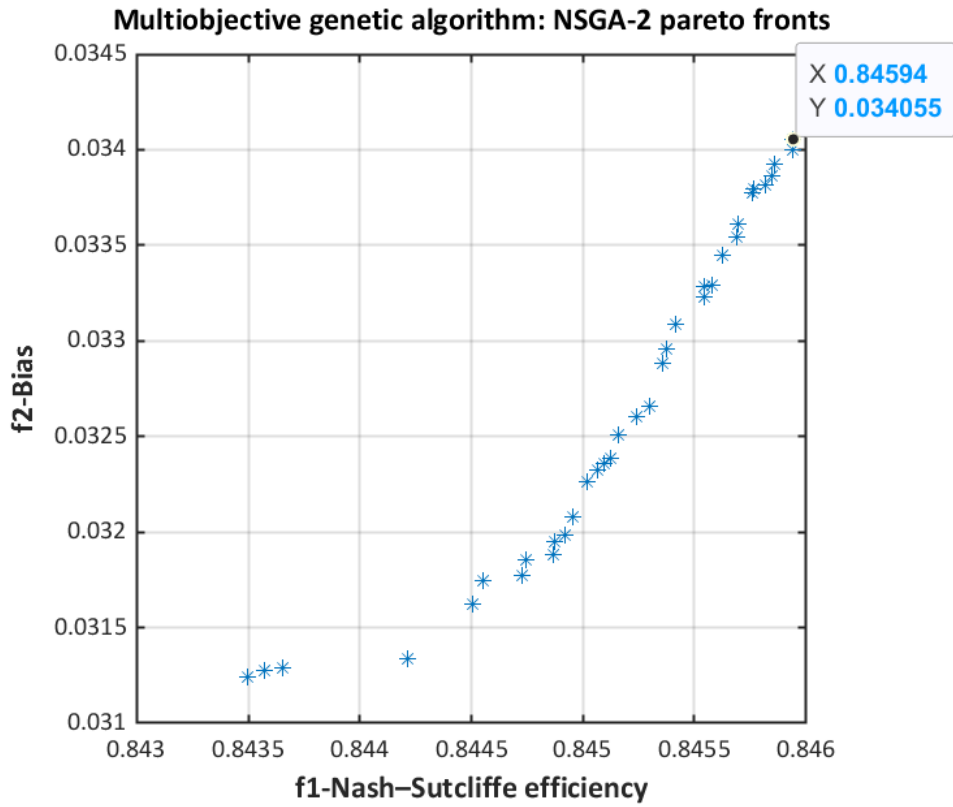
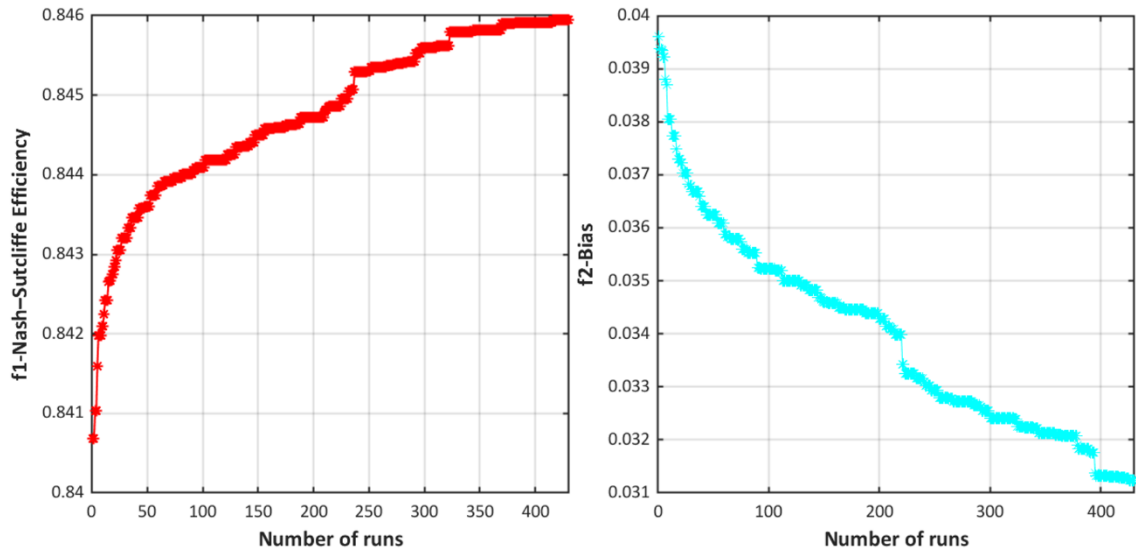



Figure 5. NSGA-II Pareto fronts of model M01 over Baskatong catchment. Horizontal and vertical axis are *NSE* and *bias*, separately.

 Figure 6. NSGA-II dynamical performance plots for both objective functions versus the number of evaluations, for model M01 over Baskatong catchment.

However, deterministic uncertainty analysis is not sufficient to compare the skill of these two post-processing methods. The accuracy and reliability are verified in terms of probabilities as well. As mentioned above, the predictive models are trained on 4-day ahead ensemble forecasts issued from each model, and corresponding observations. The 1-3 and 5-7-day ahead forecasts are used as a testing dataset. The reliability of the raw, kernel dressed and NSGA-II predictive distributions with different lead-times are displayed in the *reliability diagrams* of Figure 7. Both post-processing methods improve over the raw ensemble, especially the NSGA-II, as it achieves the best reliability. Over-dispersion exists mainly over the Baskatong catchments for NSGA-II.

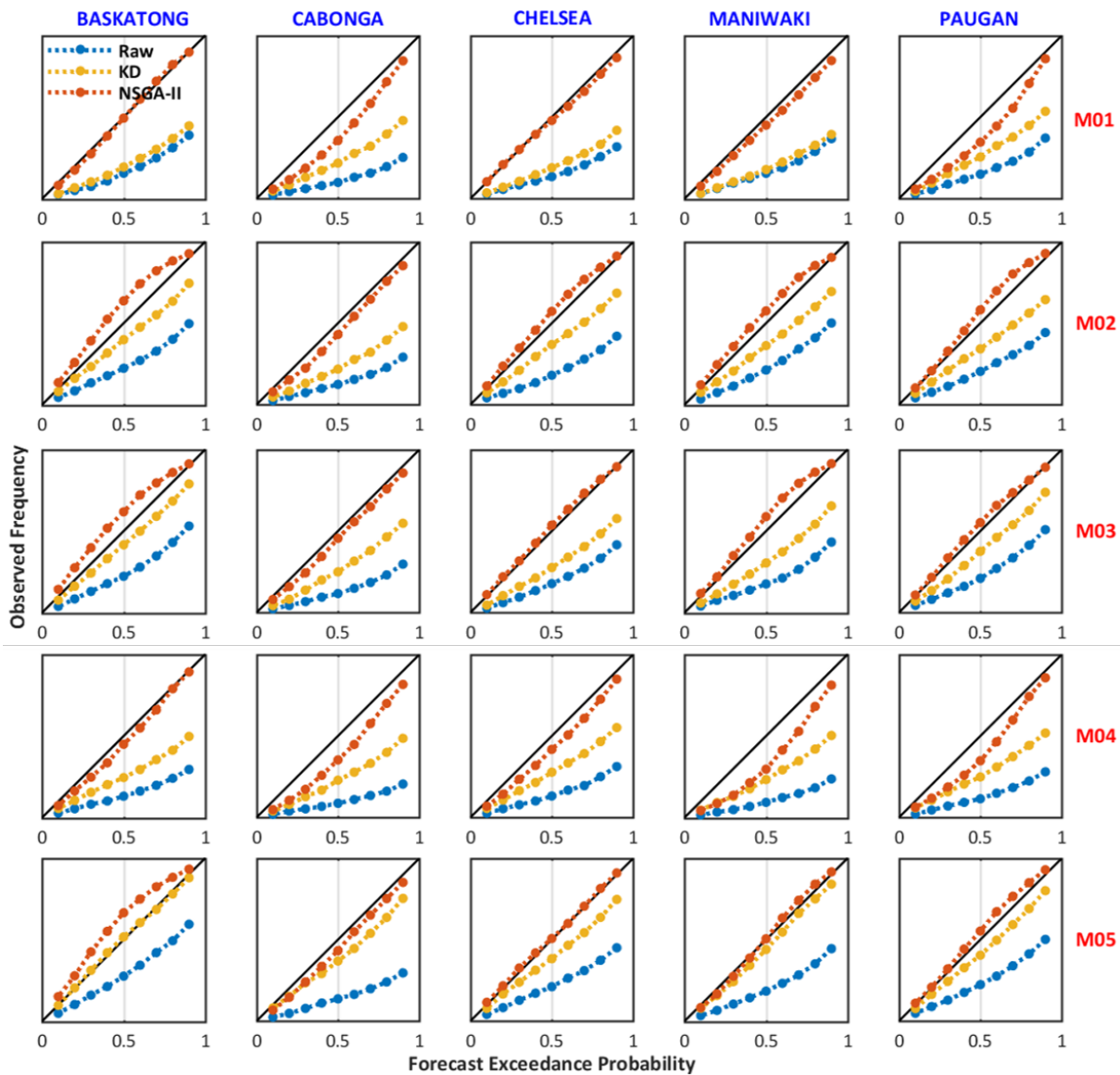



Figure 7. Forecasting reliability of the raw, AKD, and NSGA-II forecasts on the calibration data set (4-day ahead forecast) for five single-model H-EPSs over each individual catchment.

The relevant accuracy performances of the raw, AKD, and NSGA-II predictive models are summarized using radar plots in Figure 8. We can notice that the kernel dressed ensemble fails in decreasing the forecast bias. However, it adjusts the ensemble dispersion properly. As for the NSGA-II, the post-processed ensemble has an obvious improvement on both bias and ensemble dispersion. Accordingly, it demonstrates a very reliable performance shown in the reliability diagram.

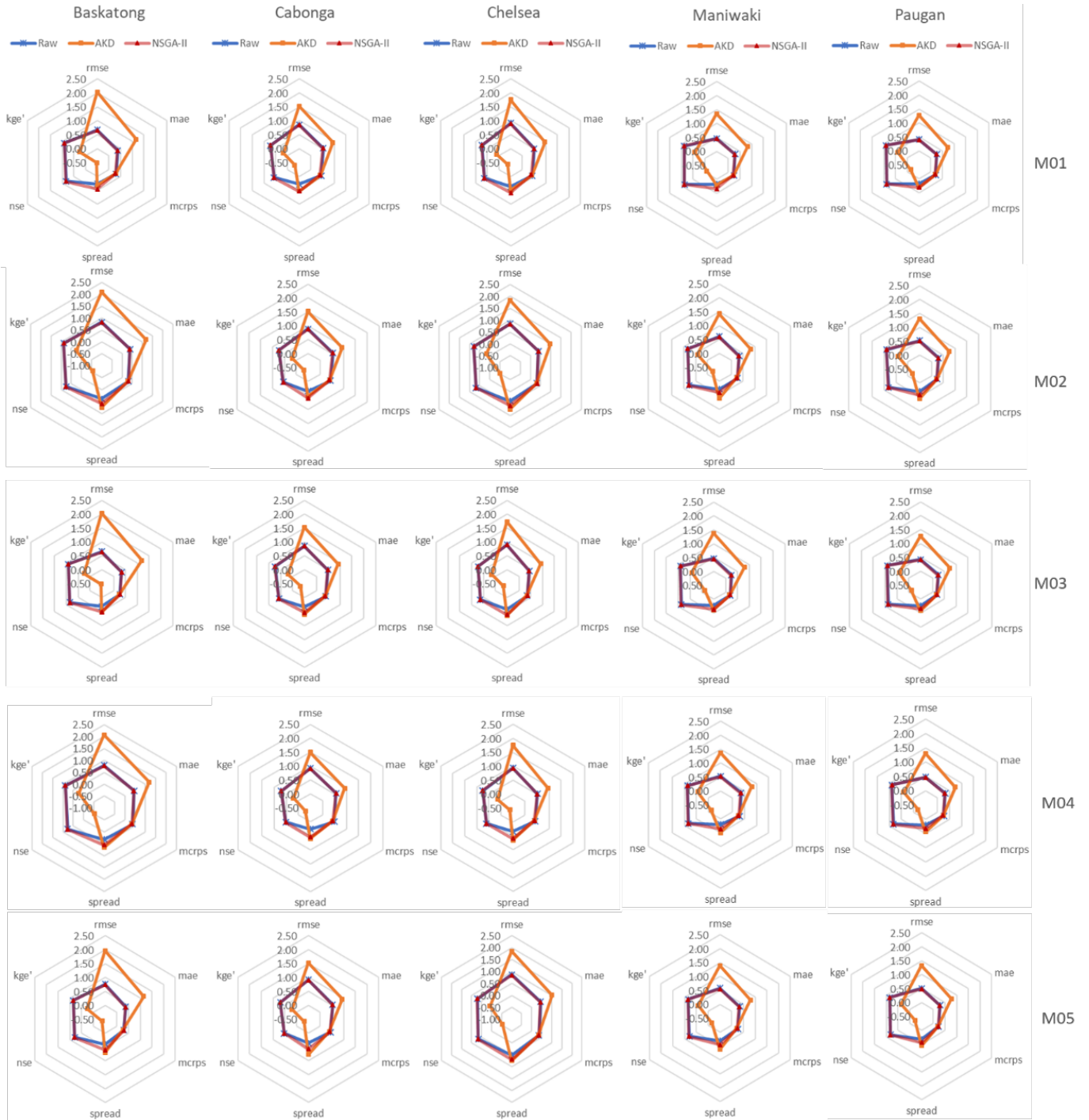



Figure 8. Accuracy performance assessment of the raw, AKD, and NSGA-II forecasts (4-day ahead) for five single-model H-EPSs over each sub-catchment of the Gatineau catchment.

385   The trained optimal free parameter vector $\theta = [\alpha, r_1, r_2, s_1, s_2]$ or weight estimates are obtained over the 4-day ahead ensemble forecasts. They are then applied to the validation data set. It comprises the 1-, 3-, 5-, and 7-day ahead raw forecasts issued from the associated H-EPSs. Figure 9 shows the reliability diagrams for raw, kernel dressed, and NSGA-II forecasts for the validation data set over five individual catchment. Therefore, there are 15 lines shown in each sub diagram. Again, raw forecasts (i.e., blue lines) display a severe under-dispersion, revealing that error growth is not maintained well in a single-model H-EPS.

390 In general, the other two statistical post-processing methods succeed in improving the forecast reliability, with the curves closer to the bisector lines. Especially, the NSGA-II (i.e., red curves) demonstrates its superior ability for maintaining the reliability with the lead time. The over-dispersion appears with most of the AKD transformed ensembles (i.e., yellow lines), especially at shorter lead times. The ensemble spread tends to a proper level as the lead time increases. Note that there is one special case that the predictive distributions of the kernel dressed ensemble are the most reliable for model M05 over almost all individual

395 catchments.

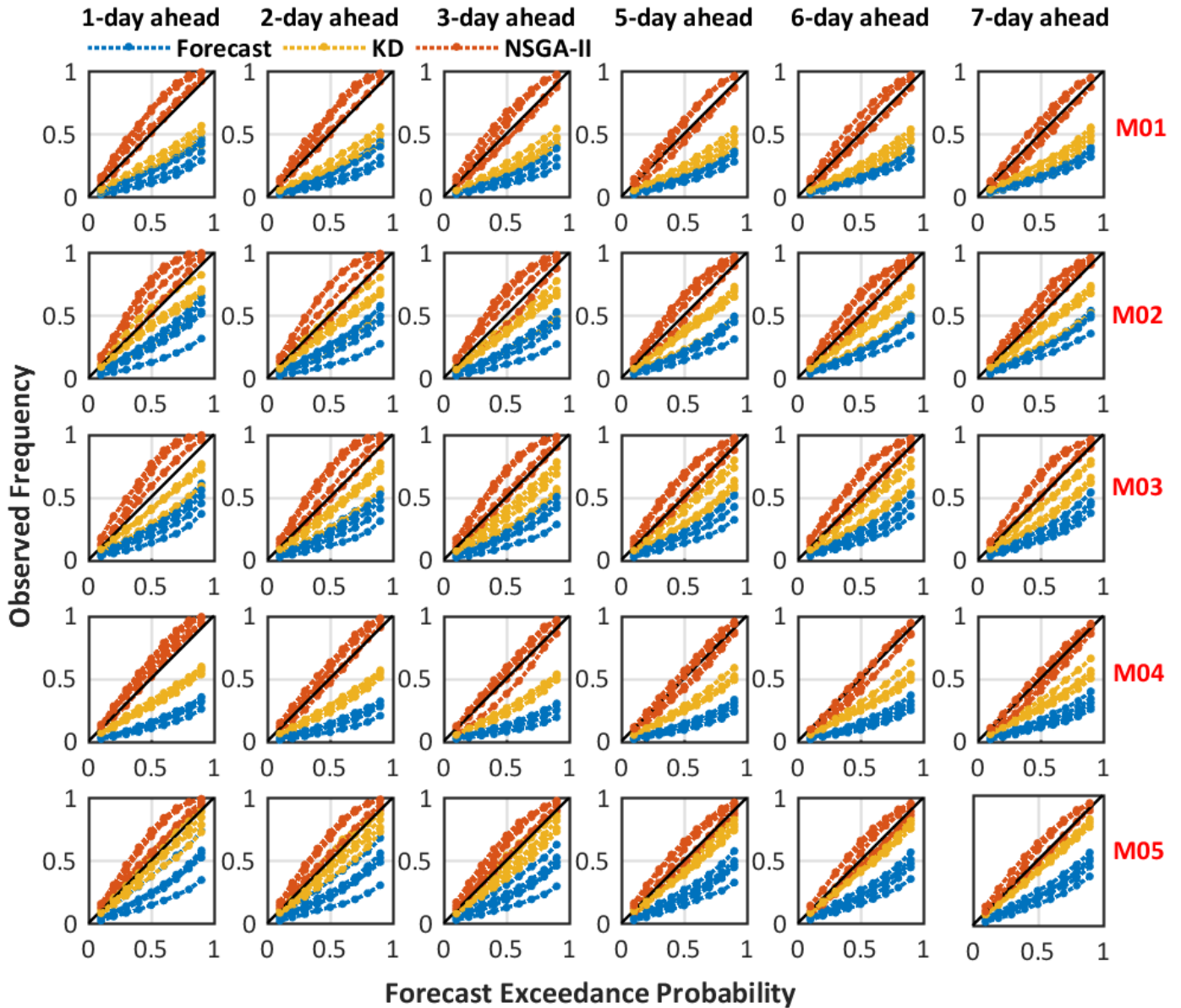



Figure 9. Comparison of the reliability of the raw, kernel dressed and NSGA-II forecasts on the validation dataset (i.e., 1-3 and 5-7-day ahead forecasts) for five singe-model H-EPSs over all catchments.

Figure 10 demonstrates the ensemble spread with different forecasting horizons on the x-axis, showing the changing performance trend. Clearly, both the kernel dressed ensemble and NSGA-II predictive forecasts have increased dispersion for all models over all catchments and result in more reliable predictive distributions. Figure 10 also provides an intuitive reference of the accuracy performance of the raw, AKD and NSGA-II interpreted ensemble forecasts in terms of the *MAE*, *MCRPS*, and the ensemble dispersion for different forecasting horizons, showing the evolution of forecasting performance. Clearly, both the

 kernel dressed ensemble and NSGA-II forecasts have increased dispersion compared to raw forecasts for all models and over all catchments. This results in more reliable predictive distributions, as shown in Figure 9.

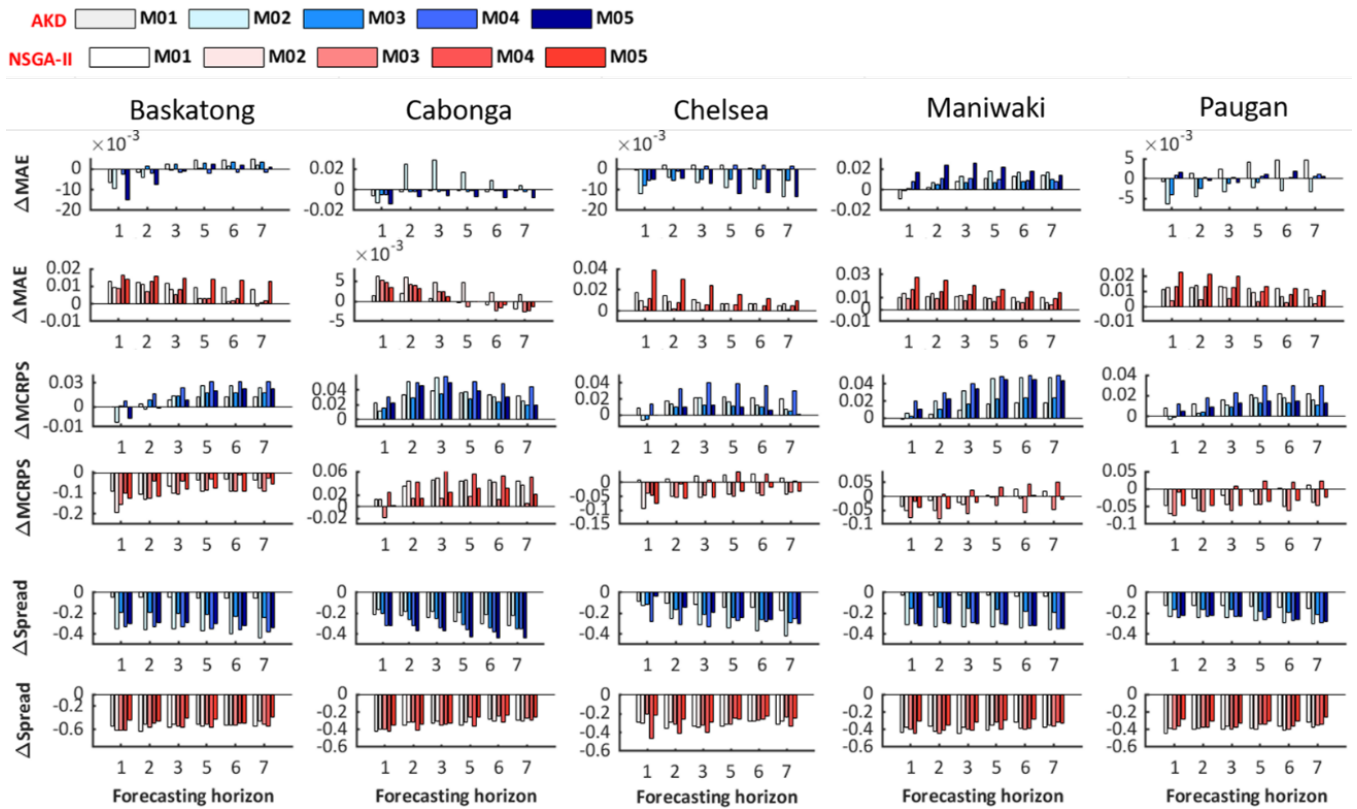



Figure 10. Comparison of the *MAE*, *MCRPS*, and ensemble dispersion of the raw, AKD, and NSGA-II forecasts (i.e., 1-3 and 5-7-day ahead forecasts) for five singe-model H-EPSs over all catchments. The x-axis for each sub-plot represents different horizons.

5   Conclusions

Hydrologic post-processing of streamflow forecasts plays an important role for correcting the overall representation of uncertainties in the final streamflow forecasts. Both the kernel ensemble dressing and the evolutionary multiobjective optimization approaches are tested in this study to estimate the probability density directly from the data (i.e., daily ensemble streamflow forecast) over five single-model hydrologic ensemble prediction systems (H-EPSs). The AKD method provides an affine mapping between the entire ensemble forecasts and the observations without any assumption of the underlying distributions. The Pareto fronts generated with NSGA-II relaxes the parametric assumptions regarding the shape of the predictive distributions and offers trade-offs between different objectives in a multi-score framework.

The single-model H-EPSs explored in this study account for both forcing uncertainty and initial conditions uncertainty by using the ensemble weather forecasts (ECMWF) and data assimilation (EnKF). Hydrologic post-processing with AKD and NSGA-II rely on very different assumptions and methodology. However, they both transform the raw ensembles into probability distributions. Results show that the post-processed forecasts achieve stronger predictive skill and better reliability than raw forecasts. In particular, the NSGA-II post-processed forecasts achieve the most reliable performances, since this method improves both bias and ensemble dispersion. However, over-dispersion may exist occasionally over the Baskatong catchment for NSGA-II. Kernel dressed ensemble succeed in adjusting the ensemble dispersion properly, but bias increases. Note that here we calibrated the models on day 4 and then tested it on the other days to assess the robustness of the procedure. The results show that both AKD and NSGA-II predictive models could offer an efficient post-processing skill and the procedure is quite robust as well. Others may try alternatives such as implementing the models separately on other lead times.

In the operational field, not only quantifying, but also communicating the predictive uncertainties in probabilistic forecasts will become an essential topic. As mentioned in the introduction, another challenge that remains is how we can bridge the communication gap between the forecasters' interpretation about probabilistic forecasts and the end-users, such as the operational hydrologists, local conservation authorities, and some other relevant stakeholders. What factor may have the strongest impact on decision-making? The different end-users may have their unique preference and demand. For instance, the reliability and sharpness (i.e., spread) could be improved simultaneously or there could be a trade-off between them. Compared to conventional post-processing method, such as AKD, NSGA-II demonstrated its superior ability for improving the forecast performance. In parallel, the use of NSGA-II opens up the opportunities to enhance the forecast quality in line with the specific needs of end-users, since it allows for setting multiple specific objective functions from scratch. This flexibility should be considered as a key part of facilitating the implementation of H-EPSs in real-time operational forecasting effectively.

Appendix A

Table A1. Hydroclimatic characteristics of five sub-catchments of the Gatineau River.

Name	Lat.	Lon.	Catchment Area (km^2)	Mean annual Q (mm)
Cabonga	47.21	-76.59	2,665	1.35
Baskatong	47.21	-75.95	13,057	1.49
Maniwaki	46.53	-76.25	4,145	1.24
Paugan	46.07	-76.13	2,790	1.29
Chelsea	45.70	-76.01	1,142	1.27

Table A2. Main characteristics of the hydrologic models (Seiller et al., 2012).

Model	No. of optimized parameters	No. of reservoirs	Derived from
M01	6	3	BUCKET (Thornthwaite and Mather, 1955)
M02	4	2	GR4J (Perrin et al., 2003)
M03	9	3	HBV (Bergström et al., 1973)
M04	7	3	IHACRES (Jakeman et al., 1990)
M05	9	5	SACRAMENTO (Burnash et al., 1973)

445 **Figure A1.** The five sub-catchments of the Gatineau River. The red thunder marks locate the dams while the original ECMWF grid points, before downscaling, are marked using black stars.

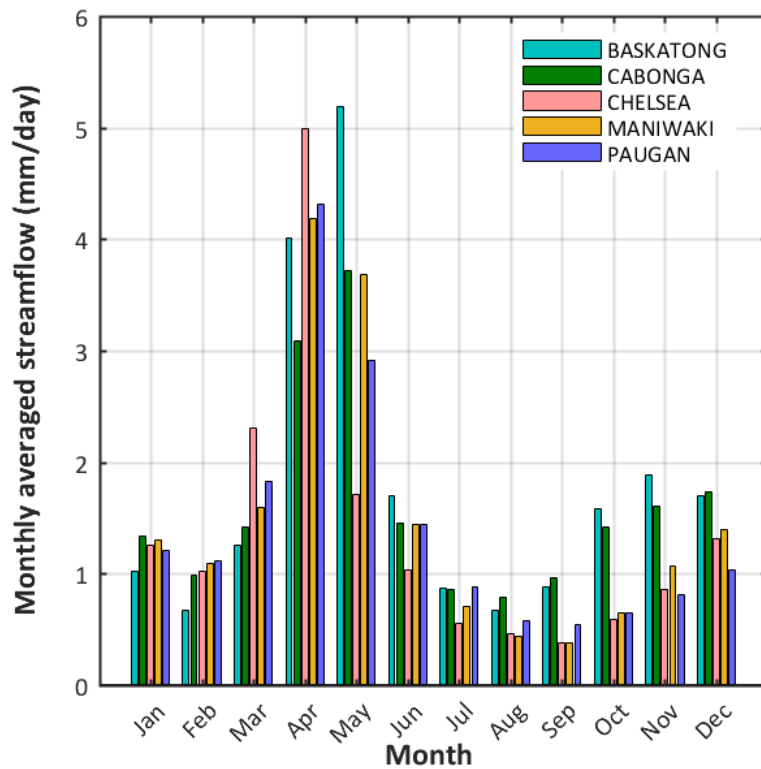
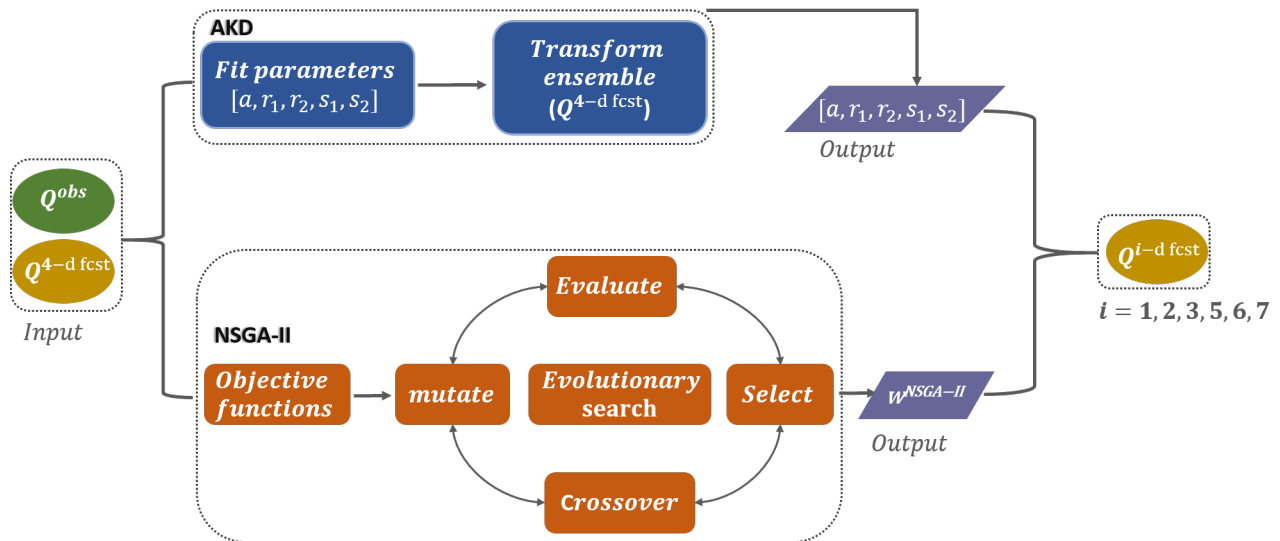



Figure A2. Hydrograph of daily streamflows (*mm/day*) averaged over each month during 33 years from 1985 to 2017.

450 **Figure A3.** Schematic of the experimental setup flowchart.

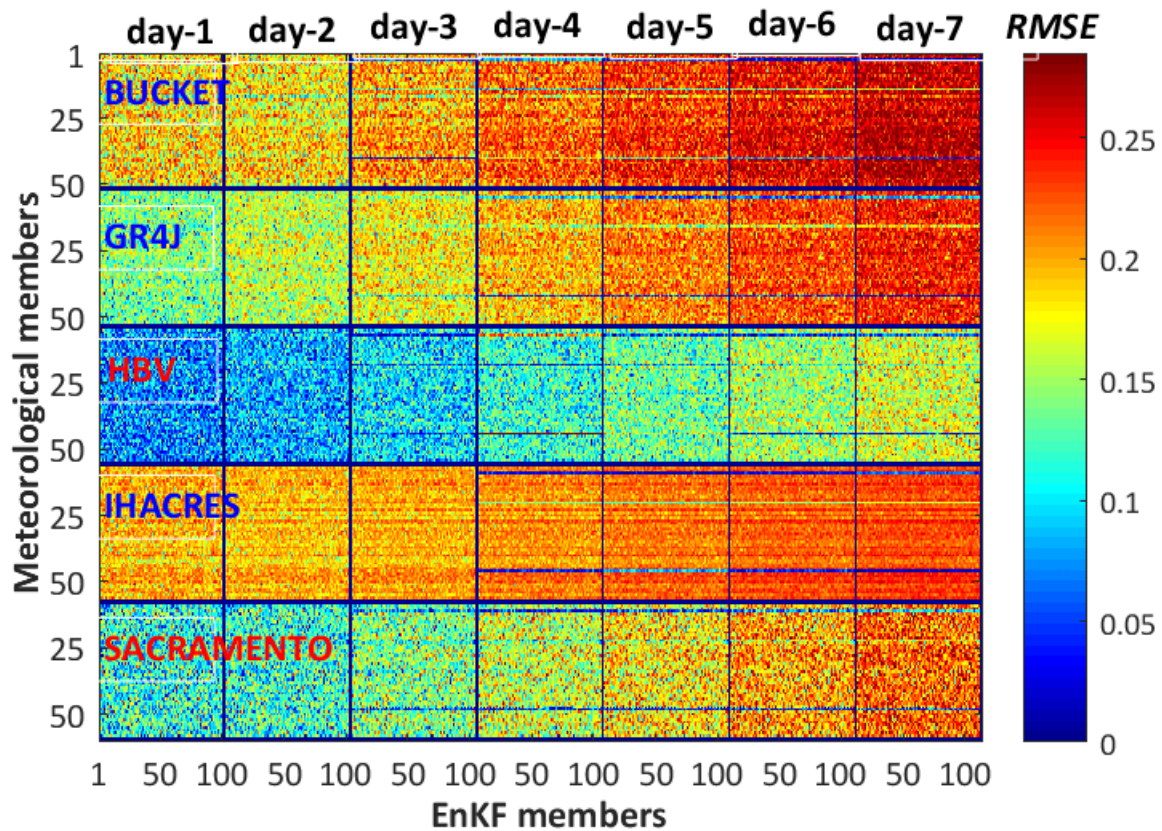



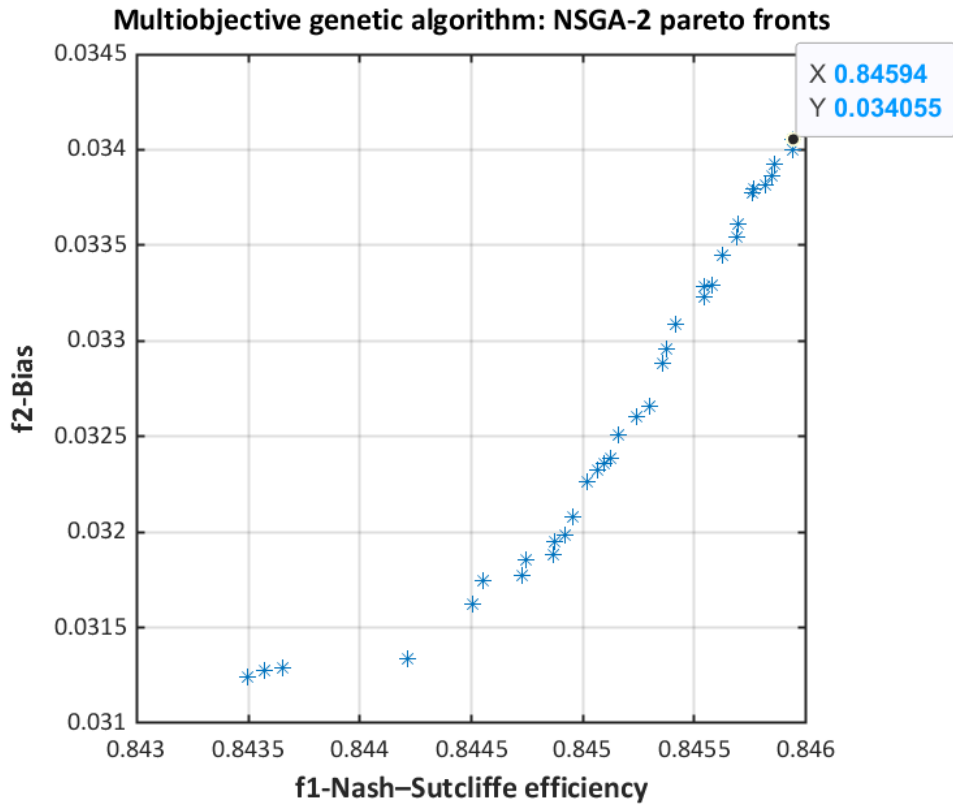
Figure A4. Illustration of the *RMSE* values (*mm/day*) of the individual members of the forecast issued by the 5 H-EPSs for the Baskatong sub-catchment, on day 500. There are 7 daily forecasts horizons. Each box consists of 5,000 members, from 100 EnKF members (horizontal lines) and 50 meteorological members (vertical lines).

455

Figure A5. NSGA-II Pareto fronts of model M01 over Baskatong catchment. Horizontal and vertical axis are *NSE* and *bias*, separately.

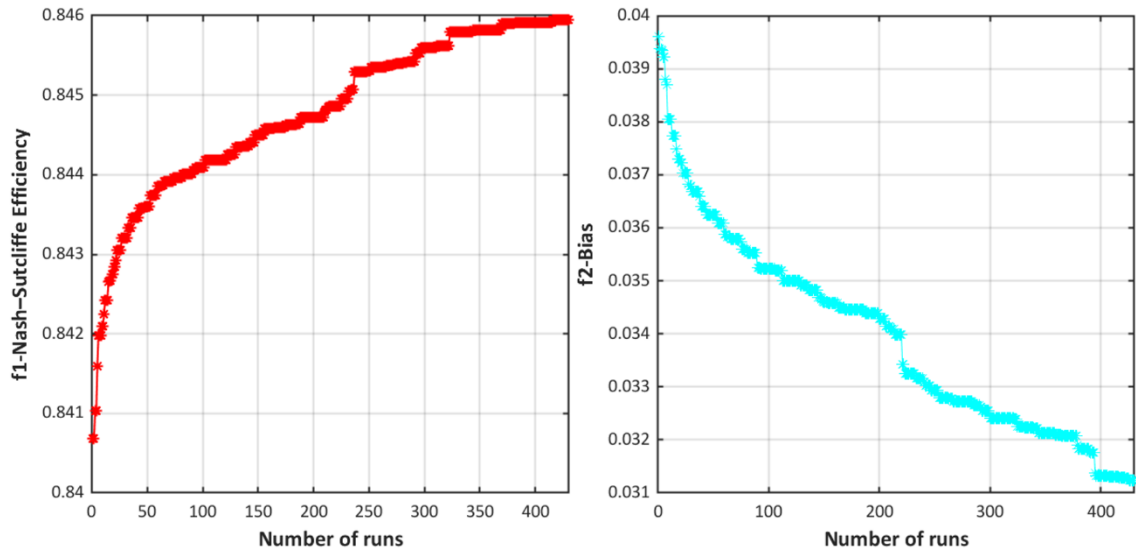



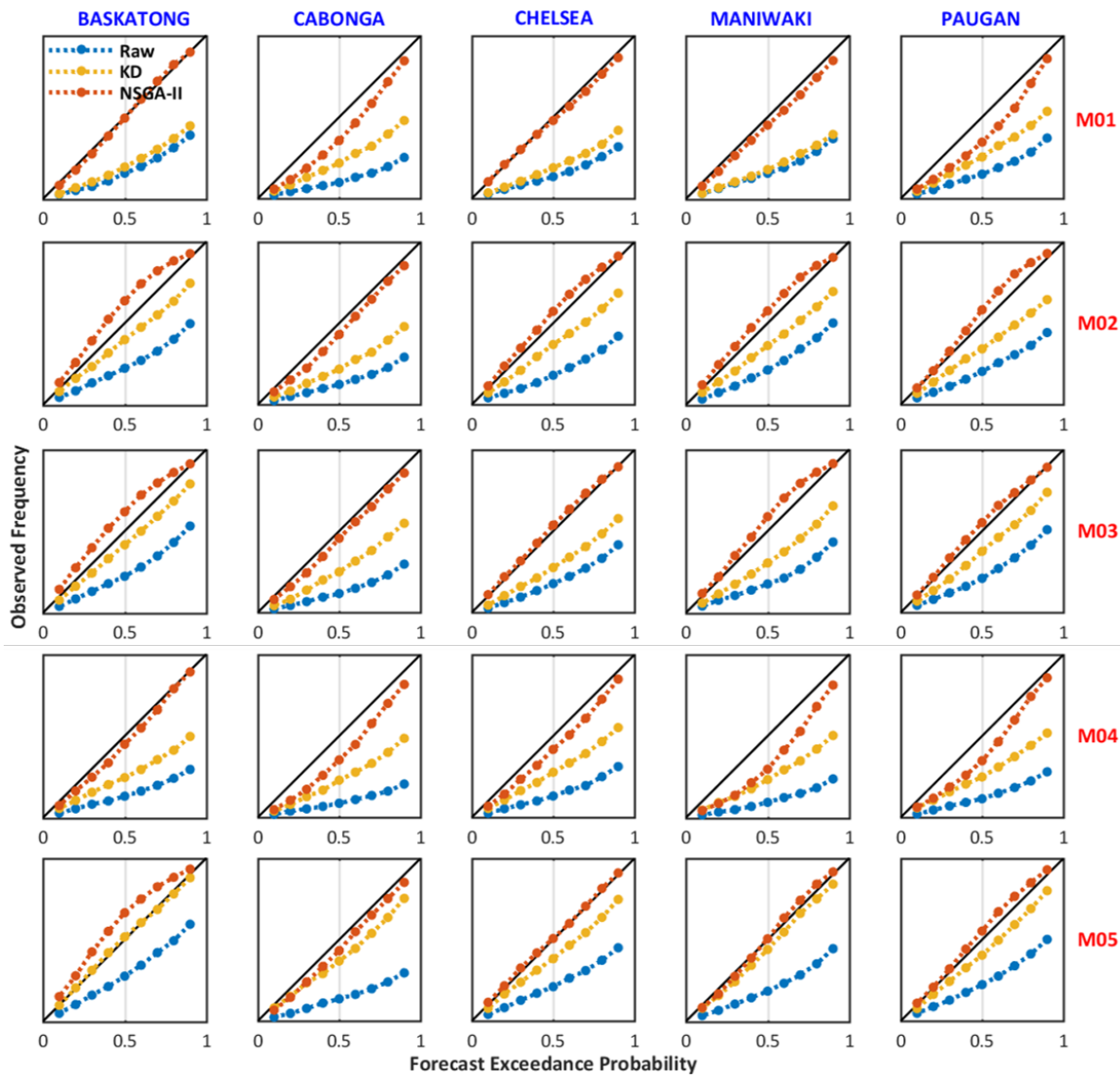
Figure A6. NSGA-II dynamical performance plots for both objective functions versus the number of evaluations, for model M01 over Baskatong catchment.

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Figure A7. Forecasting reliability of the raw, AKD, and NSGA-II forecasts on the calibration data set (4-day ahead forecast) for five single-model H-EPSs over each individual catchment.

Figure A8. Accuracy performance assessment of the raw, AKD, and NSGA-II forecasts (4-day ahead) for five single-model H-EPSs over each sub-catchment of the Gatineau catchment.
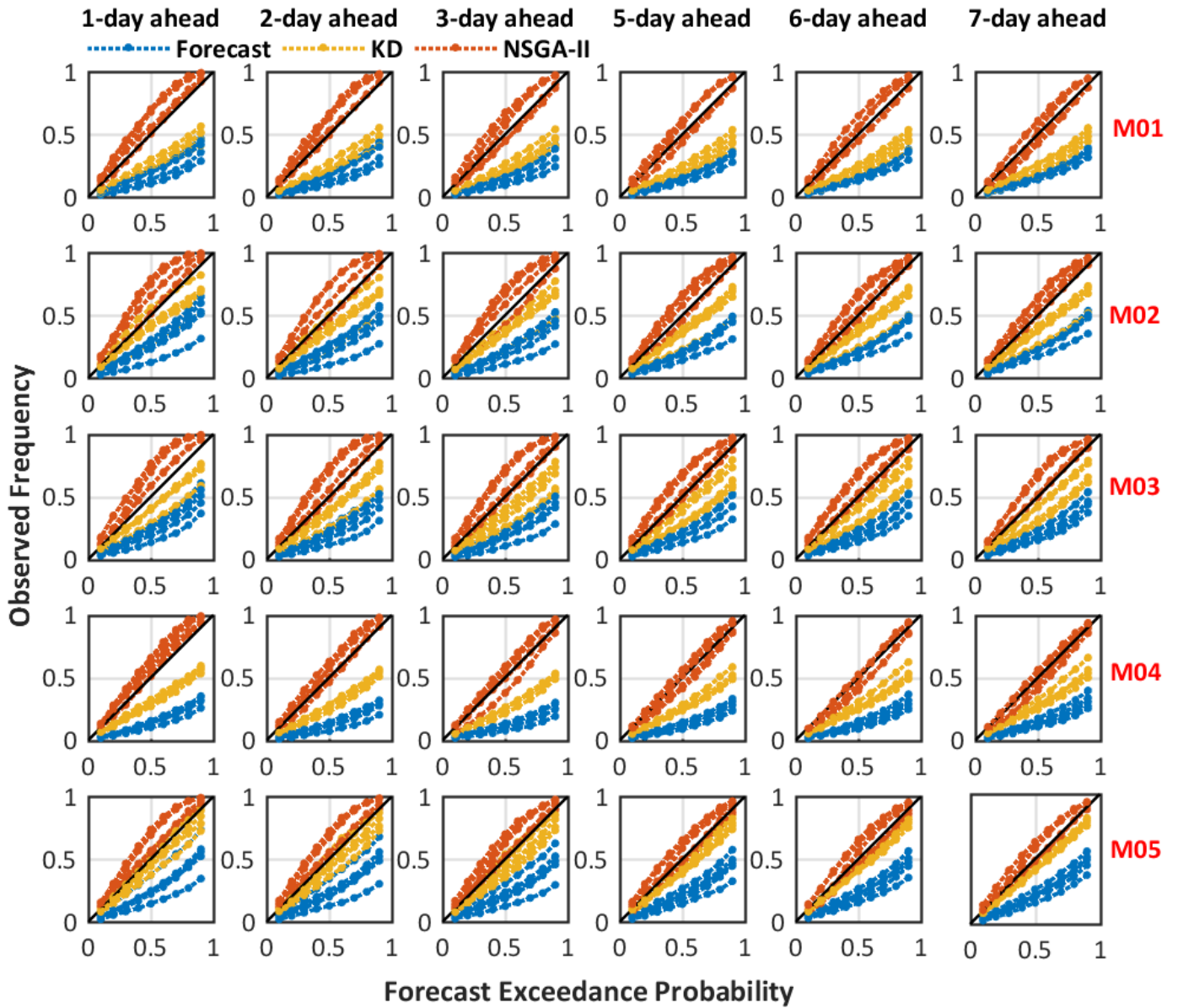
Figure A9. Comparison of the reliability of the raw, kernel dressed and NSGA-II forecasts on the validation dataset (i.e., 1-3 and 5-7-day
470   ahead forecasts) for five singe-model H-EPSs over all catchments.
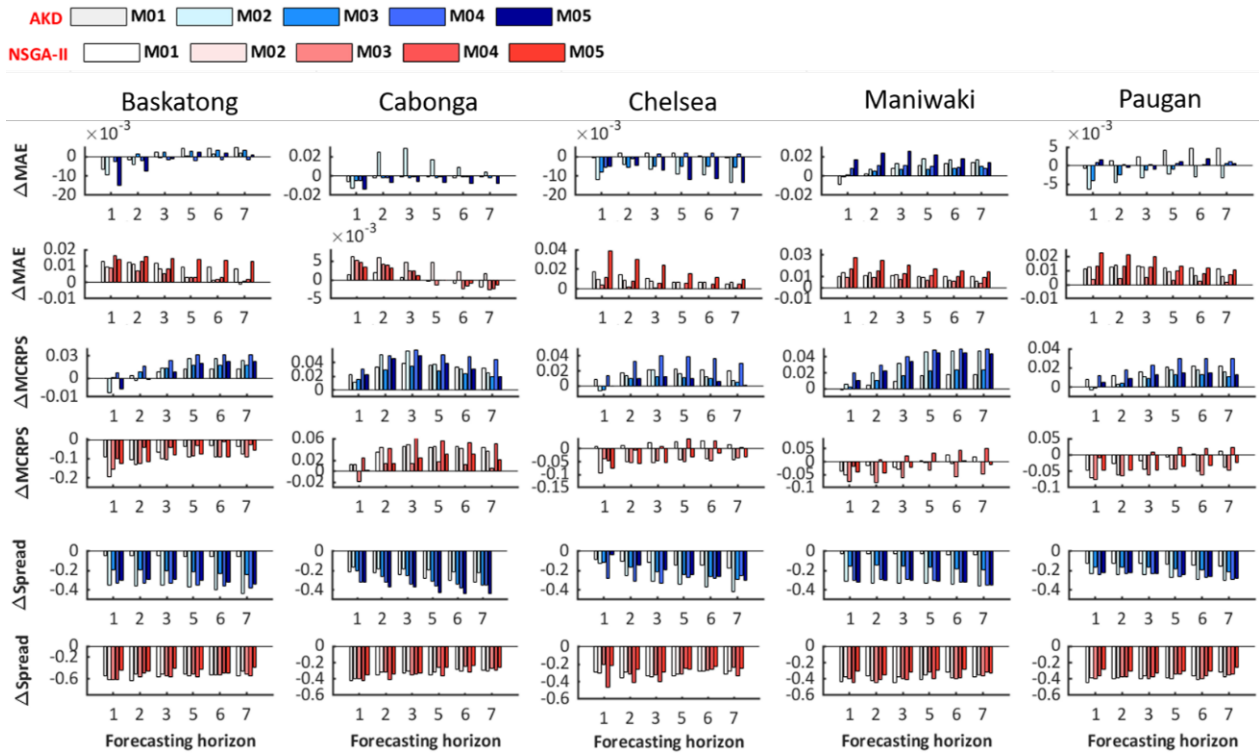
Figure A10. Comparison of the *MAE*, *MCRPS*, and ensemble dispersion of the raw, AKD, and NSGA-II forecasts (i.e., 1-3 and 5-7-day ahead forecasts) for five singe-model H-EPSs over all catchments. The x-axis for each sub-plot represents different horizons.

Author contributions.

475   Jing Xu, François Anctil, and Marie-Amélie Boucher designed the theoretical formalism. Jing Xu performed the analytic calculations. Both François Anctil, and Marie-Amélie Boucher supervised the project and contributed to the final version of the manuscript. We would like to thank Emixi Valdez, who provided the data that were used for this project. Funding for this work was provided by FloodNet. Finally, we would also like to thank the ECMWF for maintaining the TIGGE data portal and providing easy access to archived meteorological ensemble forecasts.

480   *Competing interests.*

I, Jing Xu, as the corresponding author, do hereby confirm that this manuscript has no potential conflicts of interest. My institution and I did not receive any payment or services from a third party (government, commercial, private foundation, etc.) for any aspect of the submitted wor. There is also no relationships or activities that readers could perceive to have influenced, or that give the appearance of potentially influencing for this submitted work.

485   *Acknowledgements.* This work was supported by the Natural Science and Engineering Research Council of Canada (NSERC) Canadian FloodNet (Grant number: NETGP 451456). The authors wish to thank the ECMWF for maintaining the TIGGE data portal and providing easy access to archived meteorological ensemble forecasts. HOOPLA is an open-source MATLAB toolbox available through GitHub.

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