



Transferability of climate simulation uncertainty to hydrological climate change impacts

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Abstract: Increasing number of climate models are being produced to cover the uncertainty, which makes it infeasible to use
10 all of them in climate change impact studies. In order to thoughtfully select subsets of climate simulations from a large
ensemble, several envelope-based methods have been proposed. The subsets are expected to cover a similar uncertainty
envelope as the full ensemble in terms of climate variables. However, it is not a given that the uncertainty in hydrological
impacts will be similarly well represented. Therefore, this study investigates the transferability of climate uncertainty related
to the choice of climate simulations to hydrological impacts. Two envelope-based selection methods, K-means clustering and
15 Katsavounidis-Kuo-Zhang (KKZ) method, are used to select subsets from an ensemble of 50 climate simulations over two
watersheds with very different climates using 31 precipitation and temperature variables. Transferability is evaluated by
comparing uncertainty coverage between climate variables and 17 hydrological variables simulated by a hydrological model.
The importance of properly choosing climate variables in selecting subsets is investigated by including and excluding
temperature variables. Results show that KKZ performs better than K-means at selecting subsets of climate simulations for
20 hydrological impacts, and the uncertainty coverage of climate variables is similar to that of hydrological variables. The subset
of first 10 simulations covers over 85% of total uncertainty. As expected, temperature variables are important for the snow-
related watershed, but less important for the rainfall-driven watershed. Overall, envelope-based selection of around 10 climate
simulations, based on climate variables that characterize the physical processes controlling hydrology of the watershed, is
recommended for hydrological impact studies.

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1 Introduction

In studies of climate change impacts on hydrology, multi-model ensembles (MMEs) formed by multiple Global Climate Models (GCMs) and multiple emission scenarios have been widely used to drive hydrological models (Minville et al., 2008; Vaze and Teng, 2011; Mehran et al., 2014; Chen et al., 2011b). There are two strengths of using MMEs: (1) the MME mean typically performs better in representing historical climate observations than any individual model (Gleckler et al., 2008; Pierce et al., 2009; Pincus et al., 2008; Mehran et al., 2014); and (2) the spread of a MME can be used to estimate climate change uncertainties, for example those related to GCM structure, future greenhouse gas concentrations and internal climate variability (Mendlik and Gobiet, 2016; Knutti et al., 2010; Chen et al., 2011b; Tebaldi and Knutti, 2007). While climate projection uncertainty and spread or coverage of a MME are not equivalent, the latter does provide an imperfect estimate of uncertainty and, for sake of simplicity, we use the terms interchangeably in the remainder of this study.

The number of GCM simulations available for impact studies is increasing rapidly. For instance, the Coupled Model Intercomparison Project Phase 3 (CMIP3) contains outputs from 25 different GCMs, whereas CMIP5 contains outputs from 61 GCMs (<https://pcmdi.llnl.gov>), with each GCM contributing one or more simulation runs (Taylor et al., 2012). Although it is usually advised that all available climate simulations be employed in impact studies, the extraction, storage, and computational costs associated with a large MME may be prohibitive. In practice, it is not uncommon for impact studies to instead rely on a small subset of climate simulations, the members of which are often selected manually, relying on expert judgement.

Several studies have considered more objective means of selecting subsets of climate simulations for impact studies based on different criteria. Generally, there are two main types of selection approaches. The past-performance approach weights or selects climate simulations according to their agreement with the observed near-past climate conditions (Gleckler et al., 2008; Perkins et al., 2007; Pincus et al., 2008). Climate model performance is often defined by various climate metrics. For example, Perkins et al. (2007) ranked climate models based on probability density functions of observed temperature and precipitation. Similarly, Gleckler et al. (2008) evaluated the performances of 22 GCMs according to relative errors of some climatological fields, but stressed that a wider range of metrics might give more robust results. In general, the assumption that models with good performance over the near-past provide more realistic climate change signals is questionable (Knutti et al., 2010; Reifen and Toumi, 2009), although recent work on emergent constraints suggests that it may be possible to remove models that fail to represent certain key physical processes that dictate the evolution of long-term climate projections (Klein and Hall, 2015). In practice, however, the metrics commonly used to evaluate model performance are often manually defined based on the fields of interest, which leads to substantial subjectivity within the weighting process.

Another means to select subsets of climate simulations is the envelope-based approach, which tries to cover a sufficient range of the full ensemble in terms of future climate change signals as possible (Warszawski et al., 2014; Cannon, 2015; Logan et al., 2011). For instance, Cannon (2015) used two automated multivariate statistical algorithms, K-means clustering and Katsavounidis-Kuo-Zhang (KKZ) method (Katsavounidis et al., 1994), to select subsets of CMIP5 GCMs that bracket the



overall range of changes in a suite of 27 climate extreme indices. The goal of the envelope-based approach coincides with the motivation behind the usage of a MME, namely to account for different sources of projection uncertainty, including structural uncertainty (Wilcke and Barring, 2016; Tebaldi and Knutti, 2007).

5 Some studies have proposed selection methods that combine both near-past performance and climate change envelope coverage criteria (Mendlik and Gobiet, 2016; McSweeney et al., 2012; Lutz et al., 2016; Giorgi and Mearns, 2002). For example, Lutz et al. (2016) took both model historical skill and the range of projection uncertainty in means and extremes into consideration through a three-step sequential selection process. With an emphasis on model performance, these selection methods inherit the potential flaws of the past-performance approach.

10 Regardless of underlying approach, most selection methods are only conducted on climate variables that can be calculated directly from the MME simulation outputs. Even subsets of simulations that account for most of the ensemble range in climate variables can be identified, it is not guaranteed that the same level of range coverage extends to hydrological impacts variables because of the complexity and nonlinearity of hydrological responses. For example, small perturbations in the frequency or intensity of temperature and precipitation regimes may have noticeable impacts on streamflow patterns and flood magnitudes (Muzik, 2001; Whitfield and Cannon, 2000). Consequently, whether the sufficient coverage of climate simulation uncertainty is transferable to hydrological impacts should be evaluated before applying envelope-based selection methods in hydrological impacts studies.

15 Chen et al. (2016) investigated the transferability of optimal subsets of climate simulation to hydrological impacts by using two automatic selection methods over a Canadian watershed. They concluded that selected subsets of climate simulations do not remain optimal for hydrological variables. However, the selection methods used in their study were applied to just two climate variables, mean temperature and mean annual precipitation, which is a common strategy employed by practitioners who employ envelope-based approaches (Immerzeel et al., 2013; Warszawski et al., 2014). Hydrological responses are driven both by annual climate conditions and intra-annual climate processes, which may not be described by a small number of climate variables. For example, both the magnitude and intensity of a rainfall event can affect the flood discharge in a rainfall-dominated watershed. The transferability of climate uncertainty may be diminished due to insufficient climate variables.

25 Following Cannon (2015), who considered a larger suite of climate indices, this study aims to investigate the transferability of climate simulation uncertainty to the assessment of hydrological climate change impacts by using a pool of climate variables, including seasonal means, annual means, and climate extremes. The case study is conducted over two watersheds with very different climate conditions, one of which is seasonally snow-covered and the other driven by summer monsoon rainfall with little winter snowfall. Two envelope-based approaches (K-means clustering and KKZ method) are used to select subsets of climate simulations based on different sets of climate variables. Transferability is evaluated by comparing the uncertainty coverage between the climate variables and 17 hydrological variables simulated by a hydrological model.



2 Study Area and Data

2.1 Study Area

This study was conducted over two watersheds (the Xiangjiang and Manicouagan 5 watersheds) with different climate and hydrological characteristics (Fig. 1). The Xiangjiang watershed is a monsoon-climate and rainfall-dominated watershed located in south-central of China, whereas Manicouagan 5 is a temperate-climate and seasonally snow-covered watershed located in central Quebec, Canada.

2.1.1 Xiangjiang Watershed

The Xiangjiang watershed is one of the largest sub-basins of the Yangtze River watershed (Fig. 1a). The Xiangjiang River originates from the Haiyang Mountain in Guangxi Autonomous Region and flows north to the Dongting Lake in Hunan Province, which connects to the Yangtze River. The Xiangjiang River consists of several tributaries with a surface area of approximately 94,660 km², but only the watershed with an area of 52,150 km² above the Hengyang gauging station was used in this study. The watershed has a hilly topography ranging from a maximum elevation of 2042 m above sea level to a minimum elevation of 58 m above sea level at the Hengyang station. The Xiangjiang watershed is heavily influenced by a subtropical monsoon climate with hot and humid summers and mild and dry winters. The average annual precipitation over the catchment is about 1570 mm almost entirely in the form of rainfall. Around 61% precipitation occurs from April to August, resulting in high flows during this period. The average daily maximum and minimum temperatures are around 22 °C and 15 °C, respectively. The average daily discharge at the Hengyang station is around 1400 m³/s. The peak discharge of the averaged daily hydrograph is about 4420 m³/s, mainly resulting from high intensity rainfall.

2.1.2 Manicouagan 5 Watershed

The Manicouagan 5 watershed, the largest sub-basin of the Manicouagan River watershed, is located in the center of the province of Quebec, Canada (Fig. 1b). The Manicouagan 5 River discharges into the Manicouagan reservoir, an annular reservoir within the remnant of an ancient eroded impact crater, and ends at the Daniel Johnson Dam, which is the largest buttressed multiple arc dam in the world. The drainage area of the Manicouagan 5 River is about 24,610 km², which is mostly covered by forest and has a moderately hilly topography ranging from a maximum elevation of 952 m to a minimum elevation of 350 m above sea level (Chen et al., 2016). The Manicouagan 5 watershed has a continental subarctic climate dominated by long and cold winters. The annual precipitation is fairly evenly distributed within the year and averages about 912 mm, around 45% of which is snowfall. The average daily maximum and minimum temperatures are around 2.4 °C and -7.8 °C, respectively. The average discharge of the Manicouagan 5 River is about 530 m³/s. The peak discharge of averaged daily hydrograph is around 2200 m³/s, mainly resulting from snowmelt.



2.2 Data

Both observed and simulated daily meteorological (maximum and minimum temperatures and precipitation) data over both watersheds were used in this study. All the climate data from multiple stations or grids were averaged over the watersheds.

2.2.1 Climate Simulations

5 Climate model simulation data used in this study were extracted from the CMIP5 archive (Taylor et al., 2012) for both the historical reference (1975-2004) and future (2070-2099) projection periods. Twenty-six GCMs from 15 institutions were selected to represent climate modeling uncertainty (Table 1). Two Representative Concentration Pathways (RCP4.5 and RCP 8.5) were used for each GCM to represent forcing scenario uncertainty, with the exception of CMCC-CESM, which only used RCP8.5, and MRI-ESM1, which only used RCP4.5. On the whole, an ensemble of 50 climate simulations was used in this
10 study.

2.2.2 Observations

Observed daily meteorological data used to downscale the GCM outputs and calibrate the hydrological model cover the 1975-2004 period for both watersheds. Meteorological data for the Manicouagan 5 watershed were obtained from the 10-km gridded dataset of Hutchinson et al. (2009), which was created by fitting spatially continuous functions of longitude, latitude and
15 elevation to daily station data using a trivariate thin plate smoothing spline interpolation algorithm. Discharge data at the outlet of the Manicouagan 5 River were based on mass balance calculations at the Daniel Johnson Dam. Meteorological and discharge data for the Xiangjiang watershed were observed at 100 rain gauges, 8 temperature gauges, and 1 streamflow gauge in the catchment above the Hengyang station.

3 Methodology

20 3.1 Subset Selection of GCM Simulations

Two automated envelope-based methods were used on subset selection of climate simulations. One is the K-means clustering which finds centroid simulations by partitioning the multivariate ensemble into high-density clusters, and the other is the KKZ method which sequentially selects simulations to cover the extent of an ensemble (Cannon, 2015). Both selection methods operate on multivariate data, which means that they are sensitive to the choice and scaling of climate variables.

25 3.1.1 Climate Variables

Since the hydrological response of a watershed depends not only on annual mean temperature and precipitation but is also sensitive to intra-annual climate variability (e.g. seasonal means or extremes), subset selection should be based on a set of climate variables that includes annual and seasonal averages as well as extremes. The World Meteorological Organization's



Expert Team on Climate Change Detection and Indices (ETCCDI) has recommended a set of core climate indices that can be easily derived from daily meteorological data series (http://etccdi.pacificclimate.org/list_27_indices.shtml). The ETCCDI indices are designed to monitor changes in the frequency and intensity of climate extreme events and characterize the variability of extremes (Zhang et al., 2011). Here, we assume that the ETCCDI indices are sufficient to characterize climate extremes that lead to hydrological impacts.

Specifically, this study used a set of 31 climate variables as shown in Table 2 (21 ETCCDI extreme indices and 10 seasonal or annual mean indices), including 16 temperature variables and 15 precipitation variables. Since the focus of this study is on the capability of selected GCM subsets to cover uncertainty of climate change signals, changes in climate variables (relative change for precipitation and absolute change for temperature and duration) between the historical reference period (1975-2004) and the future projection period (2070-2099) were calculated for 50 climate simulations over the two study watersheds. Changes in each climate variable were standardized to zero mean and unit standard deviation to eliminate influences from different magnitudes and units between variables. These changes in climate variables are referred to as simulated climate change signals. Once changes were calculated, subsets could be selected based on the multivariate space formed by the climate variables.

3.1.2 K-means Clustering

The K-means clustering is an unsupervised algorithm to partition clusters in multivariate data so as to minimize within-cluster sums of squared errors (SSE) (Hartigan and Wong, 1979). The ensemble of 50 simulations was divided into a user-specified number clusters and each cluster was represented by its centroid simulation. The SSE was characterized by the Euclidean distances from simulations to their corresponding cluster centroids in this study. The climate simulations closest to the centroids were selected as the subsets. Some studies have applied this method to select subsets of climate simulations (Logan et al., 2011; Cannon, 2015; Houle et al., 2012). Due to sensitivity of the K-means clustering to initial cluster centroid positions, it was run 10000 times with different initializations and the best solution with lowest SSE was kept. A disadvantage of the K-means clustering is that it needs to be run independently when the size of subset changes. The selected climate simulations are not ordered, which makes it inconvenient for end-users to change the subset size for different applications.

3.1.3 KKZ Method

The KKZ method was originally designed by Katsavounidis et al. (1994) as an initialization technique for identifying initial seed centroids in the K-means clustering, and was introduced by Cannon (2015) in the selection of climate simulations. This method prefers the peripheral simulations in the multivariate space. The specific procedure is as follows:

1. The climate simulation closest to the centroid of whole ensemble is selected as the first simulation;
2. The simulation farthest from the first selected simulation is selected as the second representative simulation; and
3. Following simulations are selected according to their distance to previously-selected simulations. Specifically, for each remaining simulation, its distance to the nearest previously-selected simulation is calculated. Then, the simulation with the



largest calculated distance among remaining simulations is selected as the next representative simulation. This step can operate recursively until all simulations are selected.

Compared to the K-means clustering, the selection result of KKZ method is incremental and deterministic. However, it is more susceptible to selecting outliers than K-means clustering. In addition, a random selection, repeated 100 times to minimize the influence of its stochastic nature, was conducted as a baseline to evaluate the K-means clustering and KKZ method.

3.2 Generation of Climate Scenarios

GCM outputs are typically on a coarse spatial grid and contain systematic biases that preclude their direct use in hydrological modeling (Mpelasoka and Chiew, 2009; Chen et al., 2011a; Chen et al., 2011b; Minville et al., 2008; Vaze and Teng, 2011). It is thus necessary to bias correct and downscale GCM outputs before running the hydrological model. The main objective of this study is to investigate the transferability of climate simulation uncertainty; hence, there is no need to use a complicated downscaling method. A commonly used change factor method, namely the Daily Scaling (DS) method proposed by Harrold and Jones (2003), was used in this study. This method assumes that climate change signals simulated by GCMs are credible and can be used to perturb observations to obtain future daily series. The DS method adjusts the observed daily series using the differences in distributions of simulated temperature/precipitation between the future period and the reference period. The specific steps are:

1. Distributions (represented by 100 quantiles in this study) of daily temperature and precipitation simulated by GCMs are calculated for both reference and future periods in each calendar month (e.g., January, February, etc.);
2. Scaling factors are estimated as the differences (for temperatures) or ratios (for precipitation) in distributions of precipitation or temperature between reference and future periods for each calendar month; and
3. Scaling factors are added (for temperatures) or multiplied (for precipitation) to corresponding distributions of observed daily temperature or precipitation for each calendar month.

The use of the DS method preserves the simulated climate change signal. It is based on differences in probability distributions between the reference and future periods, which are only caused by climate change signals. In addition, the consideration of quantile-dependent changes in the precipitation distribution is important in hydrological impact studies, because more runoff is generated in high-intensity precipitation events (Harrold and Jones, 2003; Chiew et al., 2009). However, temporal sequencing in the future period is assumed to be the same as in the observed data. Changes in, for example, wet/dry spell lengths are not informed by the GCM simulations.



3.3 Hydrological Response Simulation

3.3.1 Hydrological Modeling

The GR4J-6, which is a 6-parameter, lumped and conceptual hydrological model, was employed to simulate the hydrological impacts. The GR4J-6 model consists of the GR4J rainfall-runoff model and the CemaNeige snow accumulation and melt routines (Arsenault et al., 2015). The GR4J is a reservoir-based model developed on the basis of the GR3J model (Edijatno et al., 1999; Perrin et al., 2003). This model routes runoff through a production reservoir, two linear unit hydrographs and a non-linear routing reservoir. This model has four parameters to be calibrated, which accounts for runoff production, groundwater, runoff routine and unit hydrograph, respectively. In an evaluation of hydrological models, Perrin et al. (2003) found that GR4J outperformed 19 models over a large sample of catchments.

Due to its lack of snow accumulation and snowmelt algorithms, the GR4J model cannot be directly used in snow-related watersheds. Thus, the general snow accounting routine proposed by Valéry et al. (2014), CemaNeige, was added. CemaNeige depends on the range of daily temperature to determine the snowfall fraction in precipitation, and the updating of snowpack and snowmelt relies on a degree-day approach that has two free parameters (cold content factor and snowmelt factor). In addition, evapotranspiration in the GR4J-6 was estimated by the Oudin formulation (Oudin et al., 2005).

The input data for GR4J-6 includes basin-averaged maximum and minimum air temperature and precipitation. The shuffled complex evolution optimization algorithm (Duan et al., 1992) was used to calibrate model parameters to maximize Nash-Sutcliffe Efficiency (NSE) (Nash and Sutcliffe, 1970). The periods of observation data used for model calibration and validation are shown in Table 3. The optimally chosen sets of parameters yield a NSE greater than 0.87 over both watersheds. The observed and simulated mean hydrographs in Fig. 2 show the applicability of GR4J-6 over two watersheds. In addition, the GR4J model was also calibrated in the Xiangjiang watershed. Results showed that absence of the CemaNeige snow module would not influence the performance of GR4J-6 in the rainfall-dominated Xiangjiang watershed (Table 3).

3.3.2 Hydrological Variables

To examine the performance of subset selection in terms of hydrological response uncertainty, this study used a set of 17 hydrological variables based on Water Resources Indicators (WRIs), Indicators of Hydrologic Alteration (IHAs) and quantiles of daily flow series (Table 4). WRIs have been used in many hydrological impact studies to assess streamflow alteration due to natural and anthropogenic climate change (Eum et al., 2017; Shrestha et al., 2014; Chen et al., 2011b). IHAs are used to examine the temporal alterations of key streamflow hydrograph components (Eum et al., 2017; Richter et al., 1996; Shrestha et al., 2014). Quantiles of daily flow series have been used to describe the characteristics of flow regimes (Mu et al., 2007; Wilby, 2005).

Similar to climate variables, changes in hydrological variables between the reference (1975-2004) and future (2070-2099) period were calculated. To remove the influence of systematic biases between the observations and simulations, simulated runoff values instead of gauge observations were used as flow data in the reference period. The first year of each period was



used to spin-up the hydrological model and was excluded when calculating the hydrological variables. Once the projected changes in hydrological variables were calculated, the uncertainty coverage of subsets could be compared between climate variables and hydrological variables to evaluate the transferability of climate simulation uncertainty.

3.4 Data Analysis

5 A criterion called the Percentage of Spread Coverage (PSC) is used to measure the uncertainty coverage of a subset relative to the coverage of all simulations. For a given variable and subset, PSC was calculated by dividing the variable's range in the subset by the variable's range in all simulations. Figure 3 shows examples of PSC when 5 climate simulations are selected by KKZ method. Since it is difficult to illustrate results in more than 3 dimensions, examples are limited to 1, 2 and 3 variables. In Fig. 3a, points represent the changes in 'WiT' (seasonal average temperature in winter) for 50 GCM simulations. The larger squares represent the same variable for a subset of 5 climate simulations selected by KKZ. The PSC is calculated by dividing the temperature range of the selected subset, 6.19°C, by that of the whole ensemble, 6.49°C. Therefore, for this specific variable the PSC (uncertainty coverage) of the subset is 95.36%. Similarly, every variable has a corresponding PSC associated with a subset of a given size; examples for 'WiR' (seasonal total precipitation in winter) and 'Rx1day' (annual maximum 1-day precipitation) are shown in Fig. 3b-c. For the random subset selection method, the reported PSC is the mean value of 100
15 PSCs, each calculated for a different random subset of the specified size.

4 Results

4.1 Transferability of Climate Uncertainty

As an illustrative example, the uncertainty transferability from one climate variable to one hydrological variable in the Xiangjiang watershed is shown in Fig. 4. The larger squares represent the 5 and 10 climate simulation subsets selected by the
20 KKZ method. The subfigures on the top display the PSC for 'Rx5day' (maximum consecutive 5-day precipitation), whereas those on the bottom display the PSC for 'Qx7day' (7-day maximum flow). The reason for choosing these two variables is that there is a generally accepted linkage between high-intensity precipitation and high flow in a rainfall-driven watershed. Although this particular choice of climate and hydrological variables is, in some ways, unfair because the overall selection process is based on a high-dimensional multivariate climate space, these subfigures still illustrate the process of uncertainty
25 transferability from climate simulations to hydrological impacts. Here, the PSC of the climate variable increases from 66.45% to 92% as the number of selected simulations goes from 5 to 10; at the same time, the PSC of the hydrological variable increases from 80.53% to 94.59%. In this case, the uncertainty coverage of the subsets in terms of the climate variable is well translated to uncertainty coverage of the hydrological variable.

Figure 5 expands the example above from 1 to 2 dimensions. In this case, the subfigures on the top show a two-
30 dimensional space formed by the changes in two climate variables, 'ARav' (annual total precipitation) and 'Rx1day' (maximum 1-day precipitation), whereas those on the bottom show changes in two hydrological variables, 'MD' (annual mean



flow) and ‘HPD’ (mean duration of high pulses). It should be noted that the subsets of climate simulations are the same as in the 1-dimensional example above. As the number of selected simulations increases from 5 to 10, the mean PSC for the two climate variables increases from 67.24% to 91.98%, while the mean PSC for the two hydrological variables increases from 76.33% to 98.06%. The increases are mostly due to selection of outlying simulations in the top right corner of the plots (the 7th and 10th selected simulations). There is strong consistency between locations of selected simulations in 2-dimensional climate space and hydrology space. For example, the 5th, 7th and 10th selected simulations are close to each other in both climate space (Fig. 5b) and hydrology space (Fig. 5d). Accordingly, the uncertainty coverage tends to translate well from climate variables to hydrological variables in this 2-dimensional example. However, PSC increases are not consistent in all cases. For example, selection of the simulation on the left edge of Fig. 5b (the 8th selected simulation) substantially improves the PSC of ‘Rx1day’, but does not lie on the edge of Fig. 5d and hence does not contribute to improvements in PSC of either hydrology variable. This may be due to the nonlinearity of the hydrological model or an imperfect explanatory relationship between the climate and hydrological variables.

The discussion above is limited to results for 5 and 10 simulation subsets for one watershed selected using the KKZ method. In the study as a whole, subset sizes from 1 to 50 simulations were evaluated in terms of transferability for two watersheds and envelope-based methods (K-means and KKZ). PSCs for all 31 climate variables and 17 hydrological variables were calculated for both selection methods and watersheds. Figure 6 shows distributions of climate and hydrological PSCs for 5, 10, 20, 30 and 40 simulation subsets. For the Xiangjiang watershed (Fig. 6a-b), PSCs for the climate variables are similar to those for the hydrological variables. For the Manicouagan 5 watershed (Fig. 6c-d), PSCs of the hydrological variables are consistently slightly smaller than those for the climate variables. Overall, the tendency of the hydrological PSCs to increase with subset size is comparable to that for the climate PSCs in both watersheds. In other words, as the size of subset becomes larger, the improvement in PSCs of the hydrological variables is similar to that of the climate variables. When comparing the two envelope-based methods, KKZ tends to outperform K-means clustering.

Given the large number of climate and hydrological variables under consideration and the challenges inherent in communicating information about multi-dimensional data, two summary criteria are used to generalize subset coverage results in this study. The first criterion is the average PSC for all climate or hydrological variables. Following Cannon (2015), the second criterion is the percentage of variables that reach a 90% PSC threshold (PSC90p).

Figure 7 presents the average PSC and PSC90p for climate variables (solid lines) and hydrological variables (dashed lines) when selected subsets contain K simulations ($K = 1$ to 50) over the two watersheds. Generally, the KKZ method performs better than K-means clustering for both evaluation criteria and both watersheds, and the two automated envelope-based methods outperform the random selection. For the Xiangjiang watershed (Fig. 7a), the 9 simulation KKZ subset reaches an average PSC of 90% for climate variables, while K-means and random selection require 19 and 27 simulations, respectively, to reach this threshold. For hydrological variables, the KKZ method still shows the best performance. To reach an average PSC of 90%, KKZ and K-means clustering require 10 and 38 simulations, respectively. In contrast to results for the climate variables, K-means clustering only performs better than random selection for the hydrological variables when the subset size



does not exceed 29. In the case of the Manicouagan 5 watershed (Fig. 7c), the KKZ method again outperforms K-means clustering and random selection.

In addition, as more simulations are selected, the average PSC increases rapidly when the subset has less than 10 simulations for both watersheds, while the rate of increase slows when the number is larger than 10. For KKZ, the subset of 5 10 simulations covers over 85% of uncertainty for climate and hydrology variables in both watersheds; selecting more than 10 climate simulations leads to little change in uncertainty coverage. For these two watersheds, a subset of 10 simulations selected using KKZ appears to be optimal for reducing computational costs while incurring the smallest possible loss of uncertainty information. In addition, the performance of the KKZ method is maintained for larger subsets, while the performance of K-means clustering fluctuates. In other words, a larger subset selected by the K-means clustering may not have a greater 10 uncertainty coverage than a smaller subset. The recursive nature of the KKZ method effectively guarantees that average PSC increases monotonically with subset size.

The focus of this study is the transferability of climate simulation uncertainty to uncertainty in hydrological impacts. For a given method this can be inferred from the difference in average PSC and PSC90p between climate and hydrological variables. For Xiangjiang watershed, the average PSC of climate variables is close to that of hydrological variables for all 15 selection methods (Fig. 7a). Especially for the KKZ method, differences in average PSC are less than 5% (with the exception of $K = 2$ and 9). The differences in climate and hydrology uncertainty coverage are slightly larger when the K-means clustering or random selection is used. For the criterion of PSC90p (Fig. 7b), transferability is somewhat less apparent due to the more rigorous 90% PSC threshold. Although differences in PSC90p between climate and hydrological variables are sometimes 20 large, especially for the K-means clustering, the PSC90p of hydrological variables still exhibits similar overall tendency and behaviour as the climate variables. In general, subsets of climate simulations that are selected based on a large number of relevant climate variables are effective at transferring uncertainty coverage into the realm of hydrological impacts. However, this transferability is method dependent; results are less variable and more consistent for KKZ than K-Means clustering.

Figure 7c-d presents results for average PSC and PSC90p in the Manicouagan 5 watershed. On the whole, the selection methods behave similarly in terms of transferability as in the Xiangjiang watershed, but the uncertainty coverage of the subsets 25 for the hydrological variables is reduced slightly. Degraded transferability is most apparent in larger differences in PSC90p between the climate and hydrological variables. As noted above, however, this criterion is much more stringent than average PSC.

4.2 Impact of Temperature Variables

The climate variables in Table 2 can be categorized into two groups: temperature variables and precipitation variables. Each 30 variable is given equal weight in the subset selection, regardless of inter-variable correlations, and all variables are assumed to exert the same influence on the hydrological variables. However, the impacts of climate variables on flow regimes may not be the same in watersheds with different hydroclimatic characteristics. For example, warmer temperatures lead to earlier spring floods in northern seasonally snow-covered watersheds (such as the Manicouagan 5 watershed) (Whitfield and Cannon, 2000;



Chen et al., 2011b; Minville et al., 2008), whereas changes in temperature have little impact on the timing of floods in rainfall-dominated watersheds (such as the Xiangjiang watershed). Since the importance of temperature is different for the two study watersheds, a question is raised: Can the transferability of climate uncertainty in Xiangjiang watershed be improved if irrelevant temperature variables are removed? To answer this question, temperature variables (the first 16 variables in Table 2) were removed and subset selection was conducted again using the 15 precipitation variables. The average PSC and PSC90p were then calculated to compare with original results that includes temperature variables. Results from the precipitation analysis are shown in Fig. 8.

For Xiangjiang watershed (Fig. 8a-b), removing temperature variables from the subset selection leads to improved uncertainty coverage for the hydrological variables, especially for K-means clustering. The K-means clustering now performs better than random selection in most cases. For KKZ, average PSC for the hydrological variables exceeds 90% with a subset of only 4 simulations, whereas the same level of coverage required 9 simulations when considering both temperature and precipitation. However, the effect of removing temperature variables is the opposite for the Manicouagan 5 watershed (Fig. 8c-d). Here, coverage performance for the hydrological variables is reduced substantially when temperature variables are not considered. The contrasting effects are consistent with the processes that generate runoff in the two watersheds. As mentioned above, the Manicouagan 5 watershed is seasonally snow-covered – snow accumulation and snowmelt are the dominant processes that contribute to runoff generation – and hence it is sensitive to changes in temperature. However, temperature variables are not relevant in the rainfall-dominated Xiangjiang watershed. The different impacts of temperature variables in the two watersheds highlights the necessity of carefully choosing climate variables for subset selection based on physical process knowledge.

4.3 Transferability of Multi-model Mean

In addition to the overall spread in the projected climate change signal, policymakers are also concerned with the MME mean when communicating hydrological climate change impacts. Therefore, the selection methods are also evaluated in terms of their ability to preserve the multi-model mean of the full MME. It bears noting that the CMIP5 MME considered in this study is an ensemble of opportunity. Models are not statistically independent, for example due to shared physical parameterizations, and multiple simulations may be contributed by the same model. Also, the two envelope-based methods make very different assumptions about the underlying nature of the statistical distribution of the ensemble. The KKZ method is not biased towards dense regions in the multivariate space, preferring uniform coverage, whereas the K-means method, which assumes a mixture of multivariate normal clusters with equal variance, will tend to select simulations that lie in regions populated by a large number of simulations. These characteristics will have implications for preservation of the MME mean.

In order to generalize the MME mean over multiple variables, standardized changes in each variable are averaged across variables and selected simulations to obtain a dimensionless criterion (referred to as averaged standardized mean change). For different sized subsets selected by the three selection methods, corresponding climate and hydrological averaged standardized mean changes were calculated and compared with values for the whole ensemble. Because projected changes are pre-processed



by standardizing to zero mean and unit standard deviation, the averaged standardized mean change of the whole ensemble is zero by construction. Therefore, if the averaged standardized mean change of a subset is close to zero, the MME mean change simulated by that subset is similar to that simulated by the entire ensemble. Figure 9 shows the averaged standardized mean changes in climate and hydrological variables when K simulations ($K = 1$ to 50) are selected for the two watersheds. When averaged over a large number of random trials, mean values will, by definition, lie close to zero for the random selection method; thus, the envelope of results across all 100 random selections are presented as blue and pink shaded areas in each subfigure for climate and hydrological variables, respectively. Figure 9a-b presents results for subsets when temperature variables are included in the selection process, whereas Fig. 9c-d presents results when temperature variables are excluded.

Overall, when gauged against the range of variability in the 100 random selections, subsets selected by both statistical methods perform well in reproducing the MME mean of the entire ensemble, with K-means clustering performing slightly better than the KKZ method. When looked at in more detail, in the Xiangjiang watershed, the averaged standardized mean changes of subsets in climate variables tend to differ slightly from those in hydrological variables when temperature variables are included (Fig. 9a,c). For example, when 5 simulations are selected using the KKZ method, the averaged standardized mean change for climate variables is 0.21 whereas it is -0.26 for hydrological variables. Subsets selected by the KKZ method often have higher means than the whole ensemble for climate variables, while they have lower values for hydrological variables. In other words, a subset with positive changes in climate variables gives negative changes in hydrological variables, which means that selected subsets have poor transferability in terms of MME mean. However, when temperature variables are not included in the selection process, performance and transferability are both improved. In the Manicouagan 5 watershed, by contrast, differences between average changes in climate variables and hydrological variables are smaller when temperature variables are included (Fig. 9b,d). Again, this highlights the importance of selecting the appropriate climate variables when performing ensemble subset selection.

5 Discussion

In order to recommend a practical subset of climate simulations for end-users who handle the assessment of climate change impacts on hydrology, various selection methods have been proposed based on different criteria (Mendlik and Gobiet, 2016; Cannon, 2015; Gleckler et al., 2008; Lutz et al., 2016; McSweeney et al., 2012; Warszawski et al., 2014; Perkins et al., 2007). Even though these methods usually perform well in terms of the climate variables to which they are applied, their performance in terms of hydrological impacts needs to be verified. In normal usage, for example, envelope-based methods may only consider changes in mean temperature and annual precipitation (Immerzeel et al., 2013; Murdock and Spittlehouse, 2011; Warszawski et al., 2014), which will have a strong influence both on the overall measurement of climate uncertainty and subset selection results in terms of hydrological impacts. By not considering relevant climate variables, there may be a loss of information when transferring climate uncertainty to hydrological uncertainty (Chen et al., 2016). When one considers the fact that it is often hard to determine a one-to-one correspondence between climate and hydrological variables, it may be reasonable



to use a large suite of climate variables. However, this may result in the inclusion of irrelevant and redundant variables that could compromise performance.

Therefore, this study assessed the transferability of climate simulation uncertainty to the hydrological world by K-means clustering and KKZ methods using a large number of climate and hydrological variables, including both seasonal and annual means and extremes. Multiple variables, when selected carefully, can improve the transferability of climate simulation uncertainty to hydrology impacts. Although the introduction of multiple climate variables may lead to irrelevant or redundant information, this can nonetheless give a more useful and reasonable selection for the purpose of covering an overall range of future climate change and its hydrological impacts.

This study also evaluated the impact of variable selection by comparing uncertainty transferability in a rainfall-dominated watershed and a seasonally snow-covered watershed when including and excluding temperature variables. The different impacts of temperature variables over two watersheds indicate that climate variables, if not chosen with consideration of runoff generating processes, can affect the performance of the subset selection algorithms. In the rainfall-dominated Xiangjiang watershed, inclusion of temperature variables, which play little role in generating runoff, leads to a small loss of performance, whereas in the snow-related Manicouagan 5, exclusion of temperature variables resulted in a large loss of performance. This is reflected in results both for ensemble spread and MME mean. Thus, it is important to choose proper climate variables that characterize the physical processes controlling hydrology of the watershed for subset selection. Although the results emphasize the impacts of temperature variables, the judgement on relevant climate variables in this study is somewhat subjective. Some automated variable selection procedure may provide a more objective selection on relevant climate variables, such as redundancy analysis or multivariate sparse group lasso (Li et al., 2015).

In terms of methodology, the results of this study reveal two strengths of the KKZ method over K-means clustering. First, the KKZ method selects simulations on the boundaries of the climate simulation ensemble and, as a result, it is better able to cover overall climate uncertainty, as measured by average PSC and PSC90p, of the ensemble than K-means clustering. Second, uncertainty coverage of the KKZ method for climate variables increases monotonically as more climate simulations are selected, whereas the K-means clustering is unstable. This is because climate simulations are added incrementally, in a recursive fashion, by the KKZ method as subset size increases, whereas K-means clustering needs to be run independently for each subset. Consequently, K-means clustering produces a disordered sequence of solutions. The results of this study show that these two strengths of the KKZ method are retained for hydrological impacts. Therefore, in the aspect of overall uncertainty coverage, the KKZ method outperforms K-means clustering. Performance in terms of MME mean were also evaluated in this study. Results show that the subsets selected by K-mean clustering produce a more similar MME mean to the whole ensemble, although differences between the two methods are small. This result is expected because K-means clustering selects representative simulations for each cluster according to their closeness to the cluster centroid, which is the multivariate mean.

The two envelope-based methods in this study are from a single branch of selection methods whose purpose is to cover the spread (uncertainty) in projected changes of an ensemble. The model ranking approach is another common way to select model simulations, usually based on historical model performance, measures of statistical independence, and other evaluation



metrics. Some studies have investigated the impact of assigning weights to climate models on climate projections or hydrological impacts (Chen et al., 2017; Christensen et al., 2010). They concluded that weighting methods have little influence on the ensemble mean and uncertainty, and it is more appropriate to consider GCMs as being equiprobable.

Some studies have argued that certain GCMs may not be independent from one another because of shared code or parameterization schemes (Evans et al., 2013; Knutti et al., 2010). In an ensemble of opportunity like CMIP5, this dependence may lead to high-density regions in climate variable space and hence influence the selection of models by methods like K-means clustering. On the other hand, the KKZ method is designed to select simulations that lie on the edges of the ensemble. If these simulations are outliers because their projections are not credible, for example due to poor process representation, and then their selection may not be warranted. Therefore, previously removing any obviously dependent or ill-behaving GCMs through model weighting methods may improve the rationality of these two equal-weighting selection methods in regional impact studies.

6 Conclusion

In this study, the transferability of climate simulation uncertainty to climate change impacts on hydrology was investigated over two watersheds with different climate and hydrological regimes based on multiple climate variables. Main conclusions are summarized as follows:

- (1) In terms of uncertainty coverage, both the KKZ method and K-means clustering are effective at selecting subsets of climate simulations that represent the range of the climate change signal. However, when it comes to hydrological impacts, the KKZ method always performed better than random selection, while K-means clustering sometimes performed worse than random selection.
- (2) Both K-means clustering and the KKZ method are capable of reproducing the MME mean of the whole ensemble, although K-means clustering performed slightly better than the KKZ method in some cases.
- (3) The uncertainty of climate simulations based on multiple climate variables can be transferred to the assessment of hydrological impacts uncertainty. In other words, selected subsets can generate similar uncertainty coverage in terms of both climate simulation and hydrological impacts.
- (4) In order to cover an adequate range of climate simulation and hydrological impacts uncertainty with less computational costs, selection of about 10 simulations from the ensemble of 50 simulations is required. Little improvement is gained when the number of simulations is increased beyond 10.
- (5) The choice of climate variables affects the transferability of climate uncertainty to hydrological uncertainty. Thus, the climate and hydrological regimes of a watershed should be considered when choosing variables used to subset climate model simulations for hydrological impact studies.



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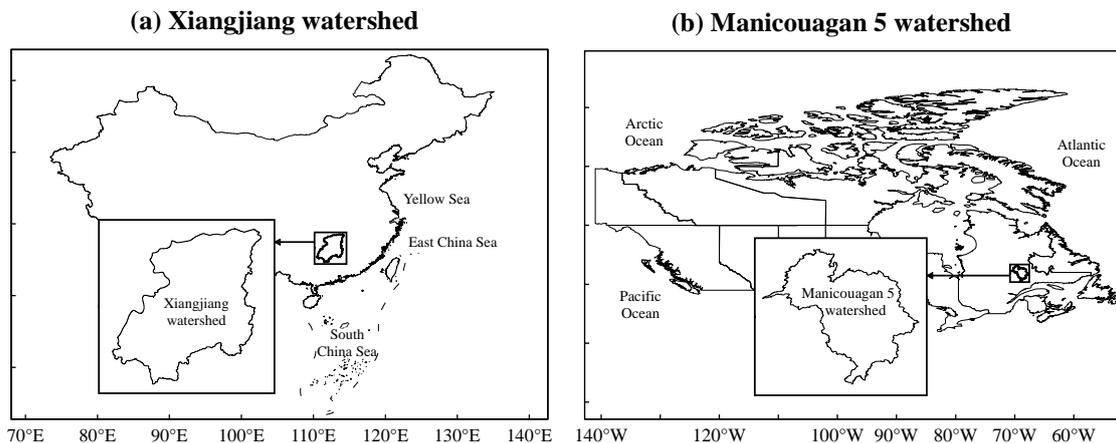


Figure 1: Location maps of the (a) Xiangjiang and (b) Manicouagan 5 watersheds.

**Table 1: Basic information about the CMIP5 models**

Institution	Model name	Resolution (Lon. × Lat.)
Commonwealth Scientific and Industrial Research Organization (CSIRO) and Bureau of Meteorology (BOM), Australia	ACCESS1.0	1.875 × 1.25
	ACCESS1.3	1.875 × 1.25
Beijing Climate Center, China Meteorological Administration	BCC-CSM1.1	2.8 × 2.8
	BCC-CSM1.1(m)	1.125 × 1.125
College of Global Change and Earth System Science, Beijing Normal University	BNU-ESM	2.8° × 2.8
Canadian Centre for Climate Modelling and Analysis	CanESM2	2.8 × 2.8
Centro Euro-Mediterraneo per I Cambiamenti Climatici	CMCC-CMS	1.875 × 1.875
	CMCC-CM	0.75 × 0.75
	CMCC-CESM	3.75 × 3.7
Centre National de Recherches Météorologiques/Centre Européen de Recherche et Formation Avancée en Calcul Scientifique	CNRM-CM5	1.4 × 1.4
Commonwealth Scientific and Industrial Research Organization in collaboration with Queensland Climate Change Centre of Excellence	CSIRO-Mk3.6.0	1.8 × 1.8
LASG, Institute of Atmospheric Physics, Chinese Academy of Sciences; and CESS, Tsinghua University	FGOALS-g2	1.875 × 1.25
NOAA Geophysical Fluid Dynamics Laboratory	GFDL-CM3	2.5 × 2.0
	GFDL-ESM2G	2.5 × 2.0
	GFDL-ESM2M	2.5 × 2.0
Met Office Hadley Centre (additional HadGEM2-ES realizations contributed by Instituto Nacional de Pesquisas Espaciais)	HadGEM2-CC	1.875 × 1.25
	HadGEM2-ES	1.875 × 1.25
Institute for Numerical Mathematics	INM-CM4	2.0 × 1.5
Institut Pierre-Simon Laplace	IPSL-CM5A-LR	3.75 × 1.9
	IPSL-CM5A-MR	2.5 × 1.25
	IPSL-CM5B-LR	3.75 × 1.9
Japan Agency for Marine-Earth Science and Technology, Atmosphere and Ocean Research Institute (The University of Tokyo), and National Institute for Environmental Studies	MIROC-ESM-CHEM	2.8 × 2.8
	MIROC-ESM	2.8 × 2.8
Atmosphere and Ocean Research Institute (The University of Tokyo), National Institute for Environmental Studies, and Japan Agency for Marine-Earth Science and Technology	MIROC5	1.4 × 1.4
Meteorological Research Institute	MRI-ESM1	1.125 × 1.125
	MRI-CGCM3	1.1 × 1.1


Table 2: Definitions of 31 climate variables. The final column indicates whether the change in a given variable is expressed in the form of relative difference (CT = change type)

Category	Index	Description	CT
ETCCDI extreme indices	TXx	Annual maximum value of daily maximum temperature	
	TXn	Annual minimum value of daily maximum temperature	
	TNx	Annual maximum value of daily minimum temperature	
	TNn	Annual minimum value of daily minimum temperature	
	TX10p	Percentage of days when daily max temperature < 10th percentile	
	TX90p	Percentage of days when daily max temperature > 90th percentile	
	TN10p	Percentage of days when daily min temperature < 10th percentile	
	TN90p	Percentage of days when daily min temperature > 90th percentile	
	WSDI	Warm spell duration index: Annual count of days with at least 6 consecutive days when TX>90th percentile	
	CSDI	Cold spell duration index: Annual count of days with at least 6 consecutive days when TN<10th percentile	
DTR	Daily temperature range: Monthly mean difference between daily max and min temperature		
Seasonal or annual mean indices	Tav	Annual average temperature	
	SpT	Seasonal average temperature in spring	
	SuT	Seasonal average temperature in summer	
	AuT	Seasonal average temperature in autumn	
WiT	Seasonal average temperature in winter		
ETCCDI extreme indices	R1mm	Annual count of days when precipitation \geq 1mm	
	R10mm	Annual count of days when precipitation \geq 10mm	
	R20mm	Annual count of days when precipitation \geq 20mm	
	CDD	Maximum length of dry spell, maximum number of consecutive days with daily precipitation < 1mm	
	CWD	Maximum length of wet spell, maximum number of consecutive days with daily precipitation \geq 1mm	
	Rx1day	Annual maximum 1-day precipitation	%
	Rx5day	Annual maximum consecutive 5-day precipitation	%
	SDII	Simple precipitation intensity index	%
	R95pTOT	Annual total precipitation when daily precipitation > 95th quantile	%
R99pTOT	Annual total precipitation when daily precipitation > 99th quantile	%	
Seasonal or annual mean indices	ARav	Annual total precipitation	%
	SpR	Seasonal total precipitation in spring	%
	SuR	Seasonal total precipitation in summer	%
	AuR	Seasonal total precipitation in autumn	%
	WiR	Seasonal total precipitation in winter	%



Table 3: Nash-Sutcliffe Efficiency (NSE) of hydrological models in the calibration and validation over two watersheds

Country	Watershed name	Area (km ²)	Hydrological Model	Calibration period	NSE calibration	Validation period	NSE validation
China	Xiangjiang	52150	GR4J-6	1975-1987	0.912	1988-2000	0.871
			GR4J	1975-1987	0.912	1988-2000	0.872
Canada	Manicouagan 5	24610	GR4J-6	1970-1979	0.926	1980-1989	0.881

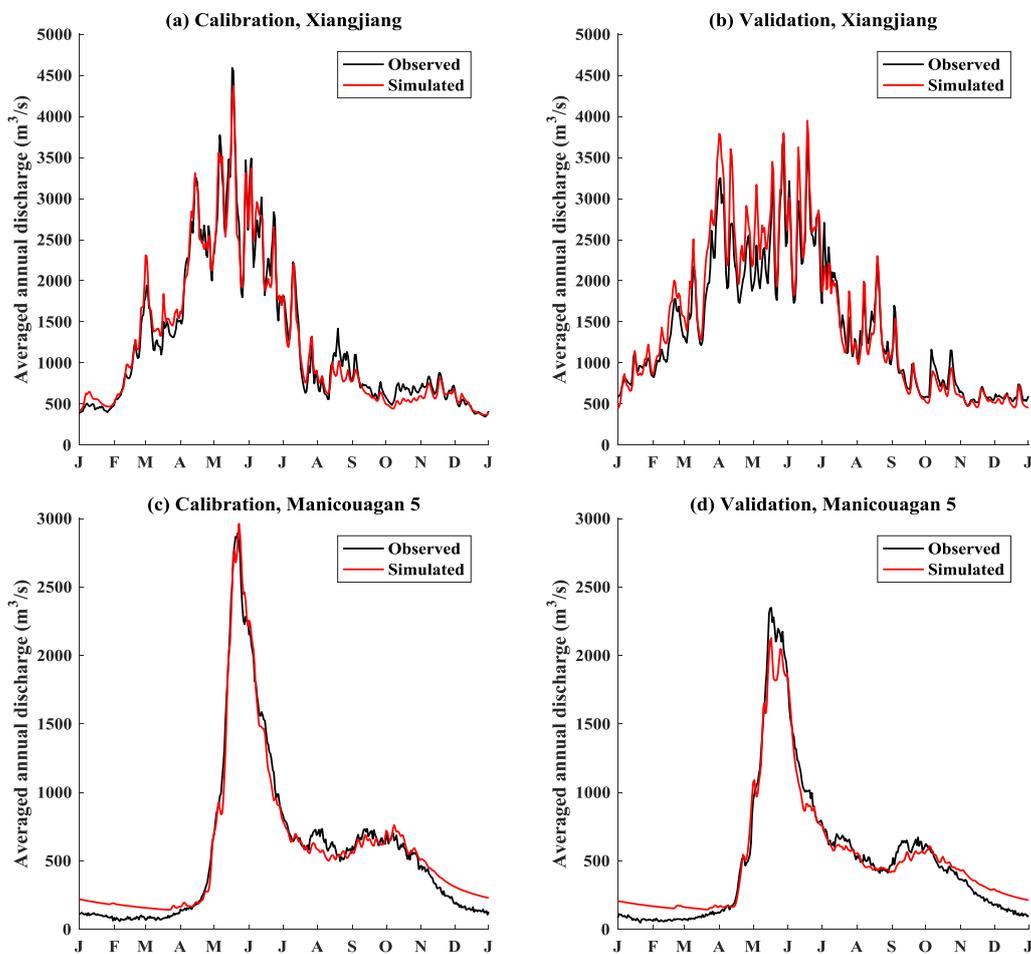


Figure 2: Observed and simulated mean hydrographs for (a, c) calibration and (b, d) validation periods over the (a, b) Xiangjiang and (c, d) Manicouagan 5 watersheds.



Table 4: Definitions of 17 hydrological variables. The final column indicates whether the change in a given variable is expressed in the form of relative difference (CT = change type)

Category	Index	Description	CT
Water Resources Indicators (WRIs)	MD	Annual mean flow	%
	SpMD	Seasonal mean flow in spring	%
	SuMD	Seasonal mean flow in summer	%
	AuMD	Seasonal mean flow in autumn	%
	WiMD	Seasonal mean flow in winter	%
	tCMD	Centre of timing of annual flow	
Quantiles of daily flow	Q5	5th quantile of daily flow series	%
	Q50	50th quantile of daily flow series	%
	Q95	95th quantile of daily flow series	%
Indicators of Hydrological Alteration (IHAs)	Qx1day	Annual mean 1-day maximum flow	%
	Qx3day	Annual mean 3-day maximum flow	%
	Qx7day	Annual mean 7-day maximum flow	%
	tQx	Julian date of annual 1-day maximum	
	LPC	Number of low pulses (annual median -25th percentile) in a year	
	HPC	Number of high pulses (annual median +25th percentile) in a year	
	LPD	Mean duration of low pulses in a year	%
HPD	Mean duration of high pulses in a year	%	

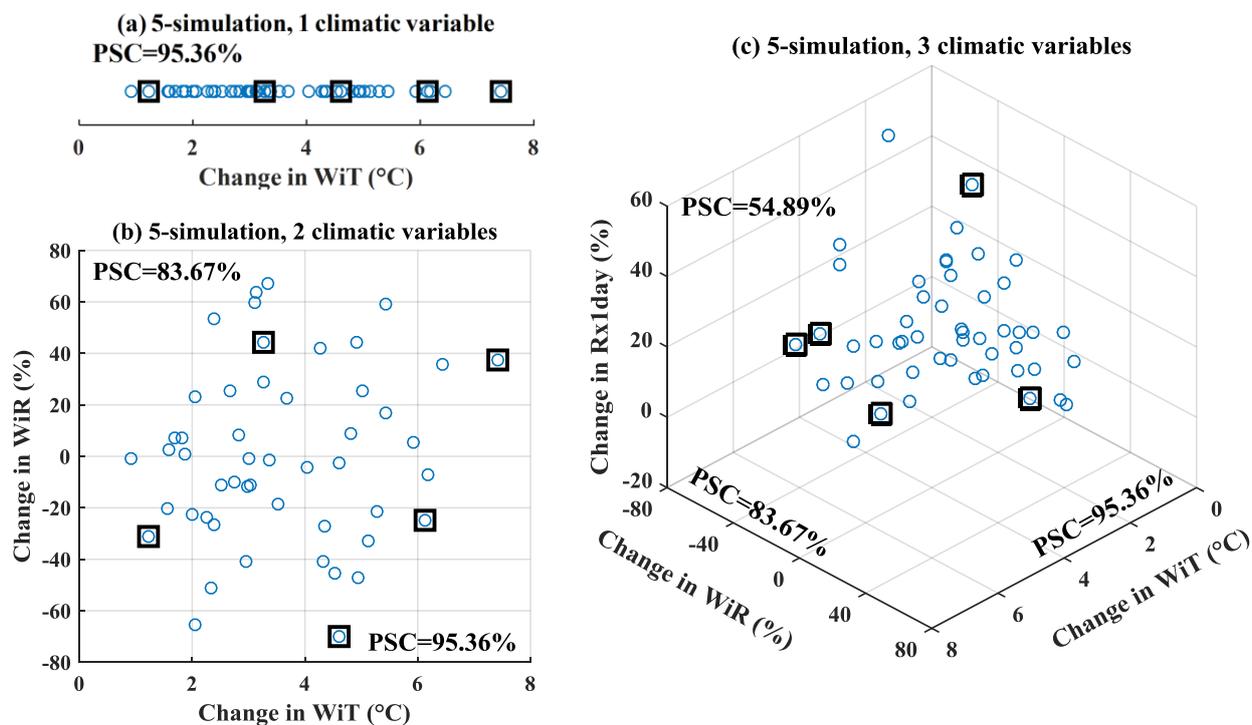


Figure 3: Examples of PSCs when selecting 5 climate simulations over the Xiangjiang watershed using the KKZ method. The PSCs of each variable are presented beside the corresponding axes.

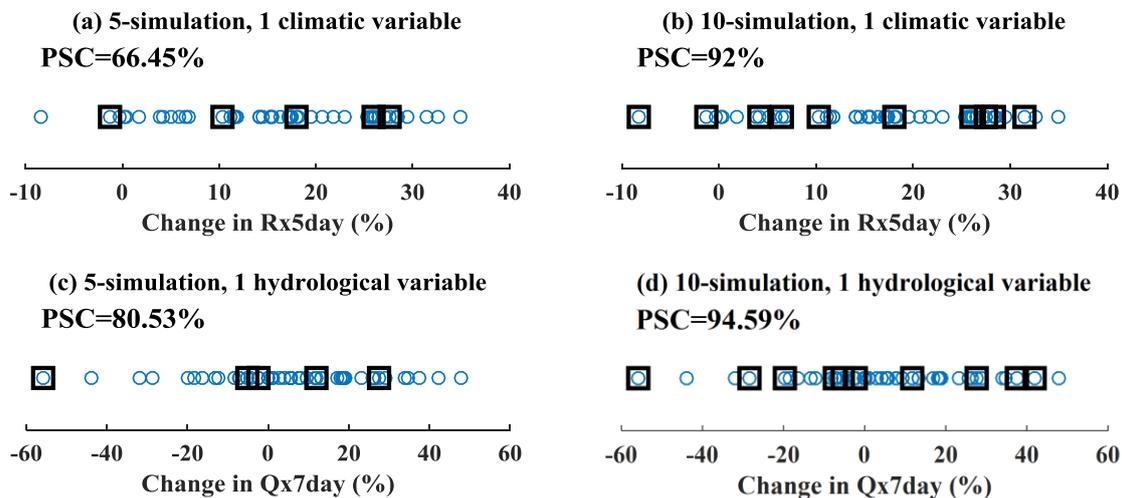


Figure 4: Examples of the transferability of climate uncertainty to hydrological impacts based on 1 variable when selecting (a, c) 5 and (b, d) 10 climate simulations over the Xiangjiang watershed using the KKZ method. The PSCs of each variable are presented in the top left corner.

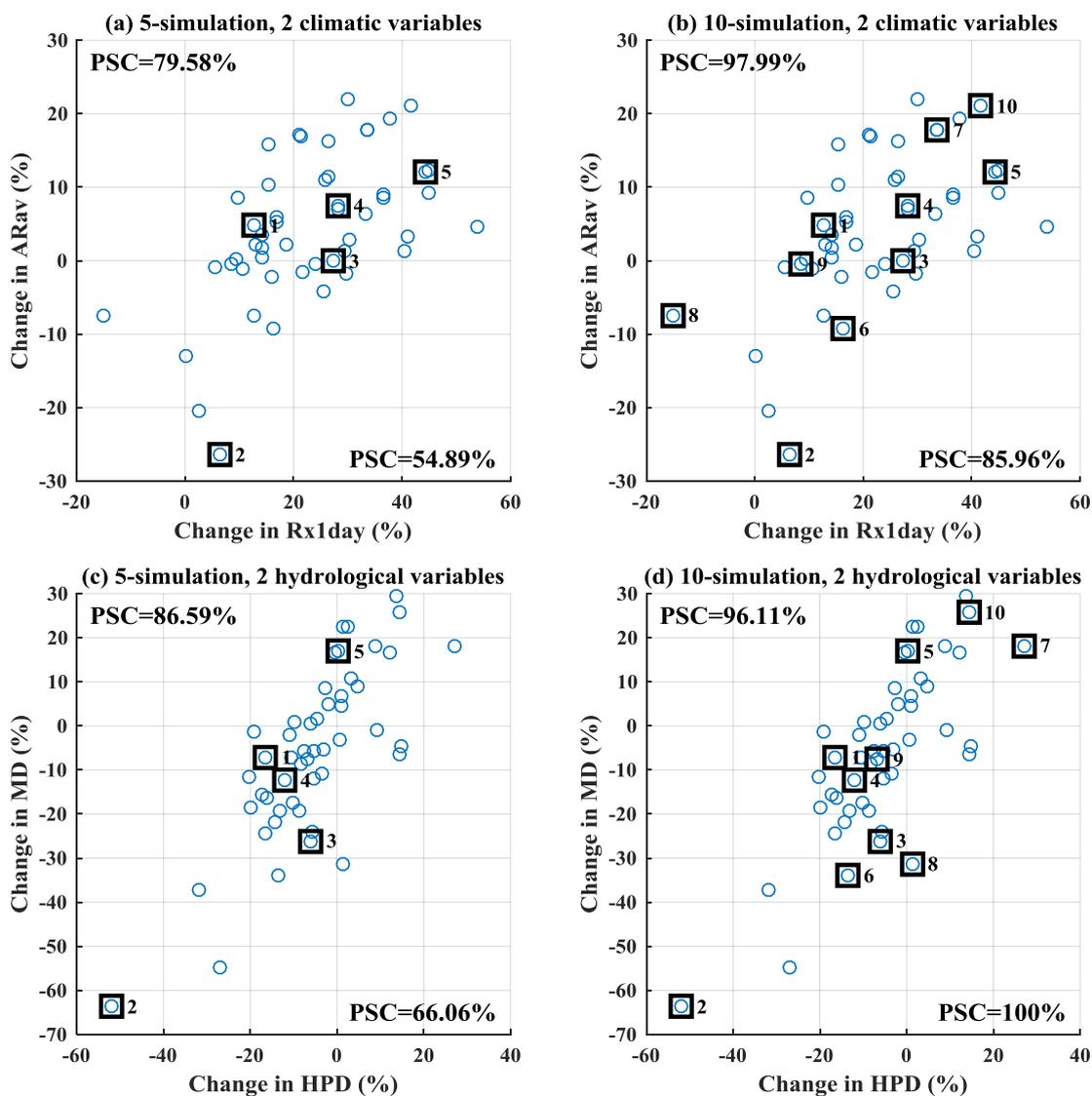


Figure 5: Examples of the transferability of climate uncertainty to hydrological impacts based on 2 variables when selecting (a, c) 5 and (b, d) 10 climate simulations using the KKZ method. The PSCs of each variable are presented beside the corresponding axes.

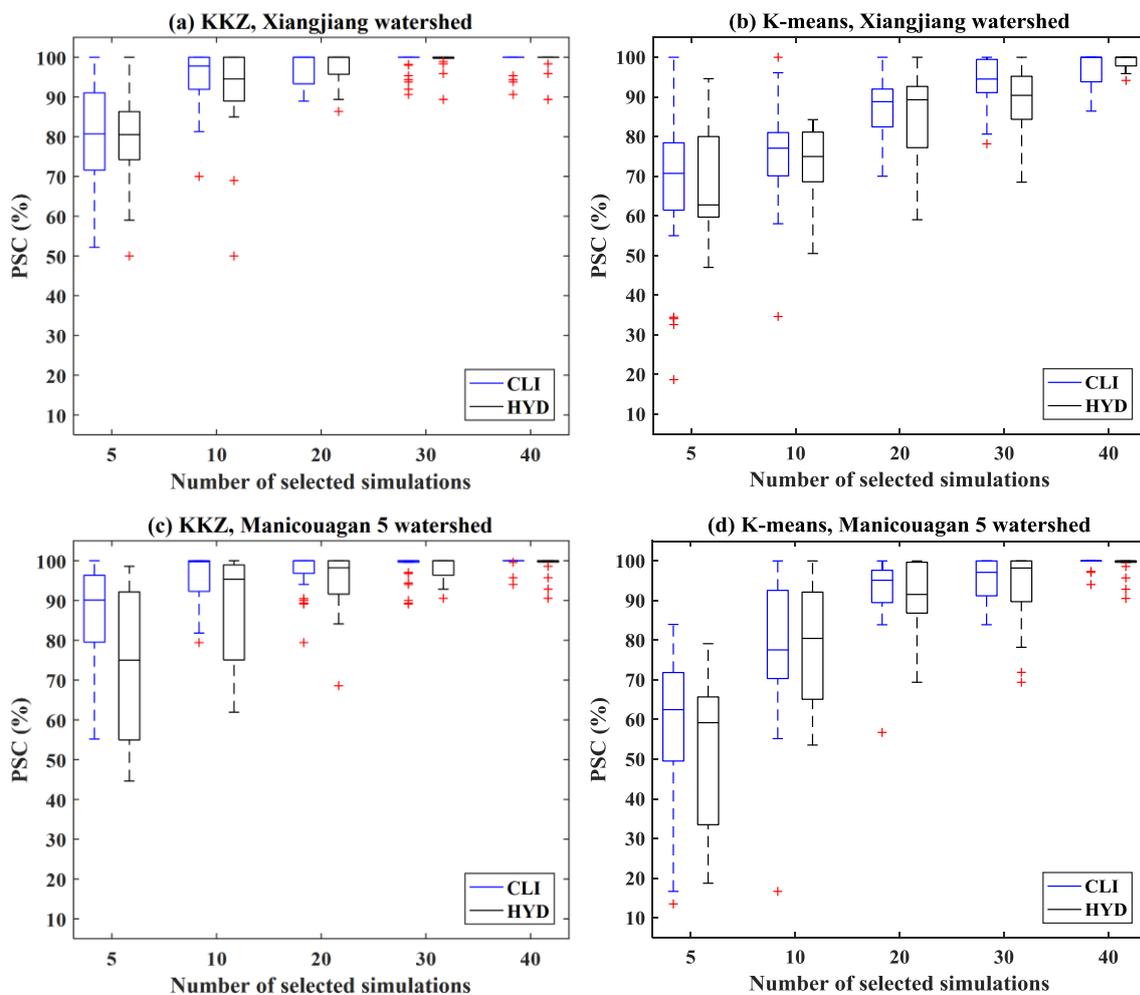


Figure 6: Boxplots of the PSCs of 31 climate variables (CLI) and 17 hydrological variables (HYD) when selecting different numbers of climate simulations over two watersheds using KKZ method and K-means clustering.

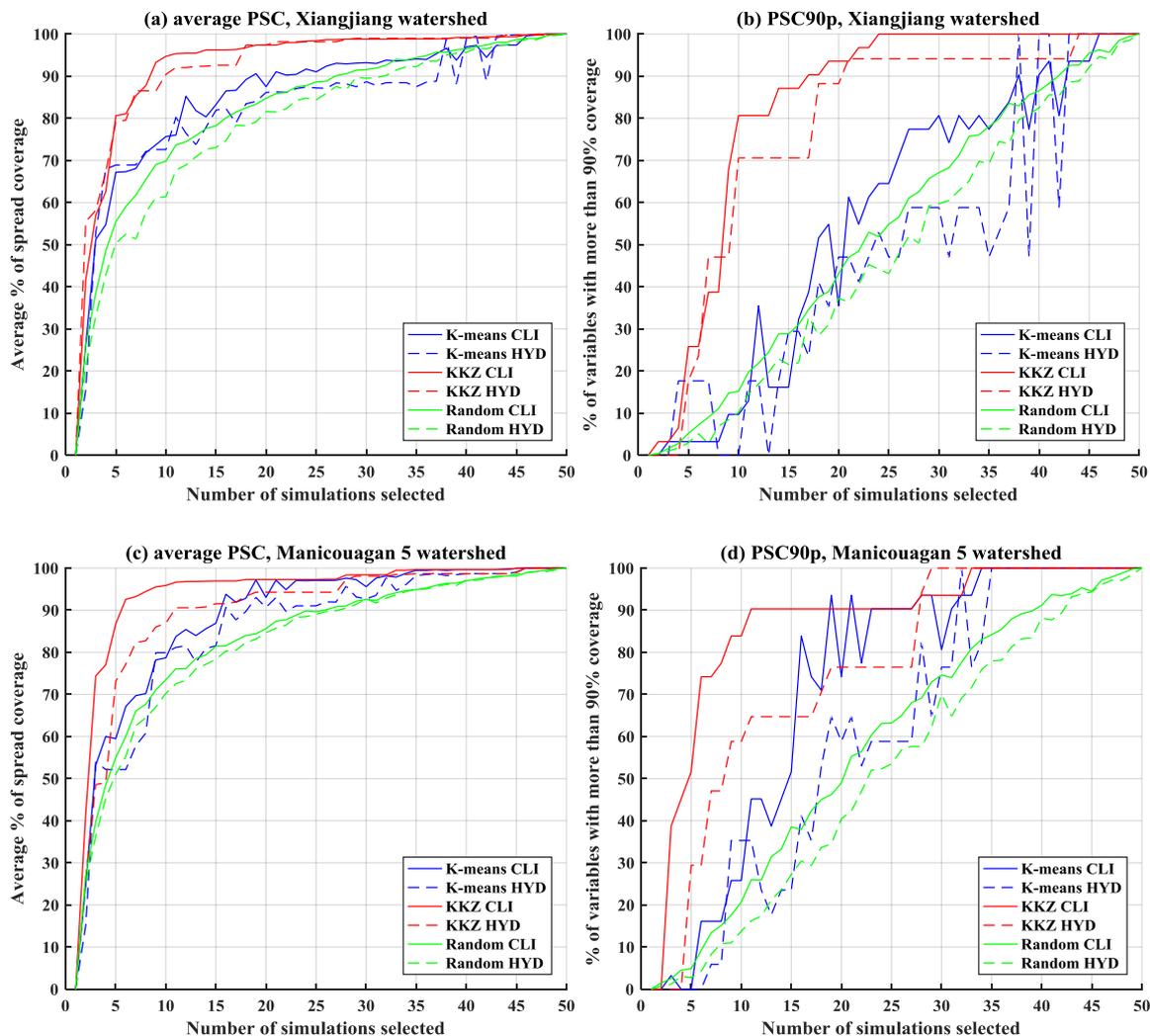


Figure 7: The (a, c) average PSC and (b, d) PSC90p for three different selection methods (K-means, KKZ and random selection) over the (a, b) Xiangjiang watershed and the (c, d) Manicouagan 5 watershed (CLI = climate variables and HYD = hydrological variables).

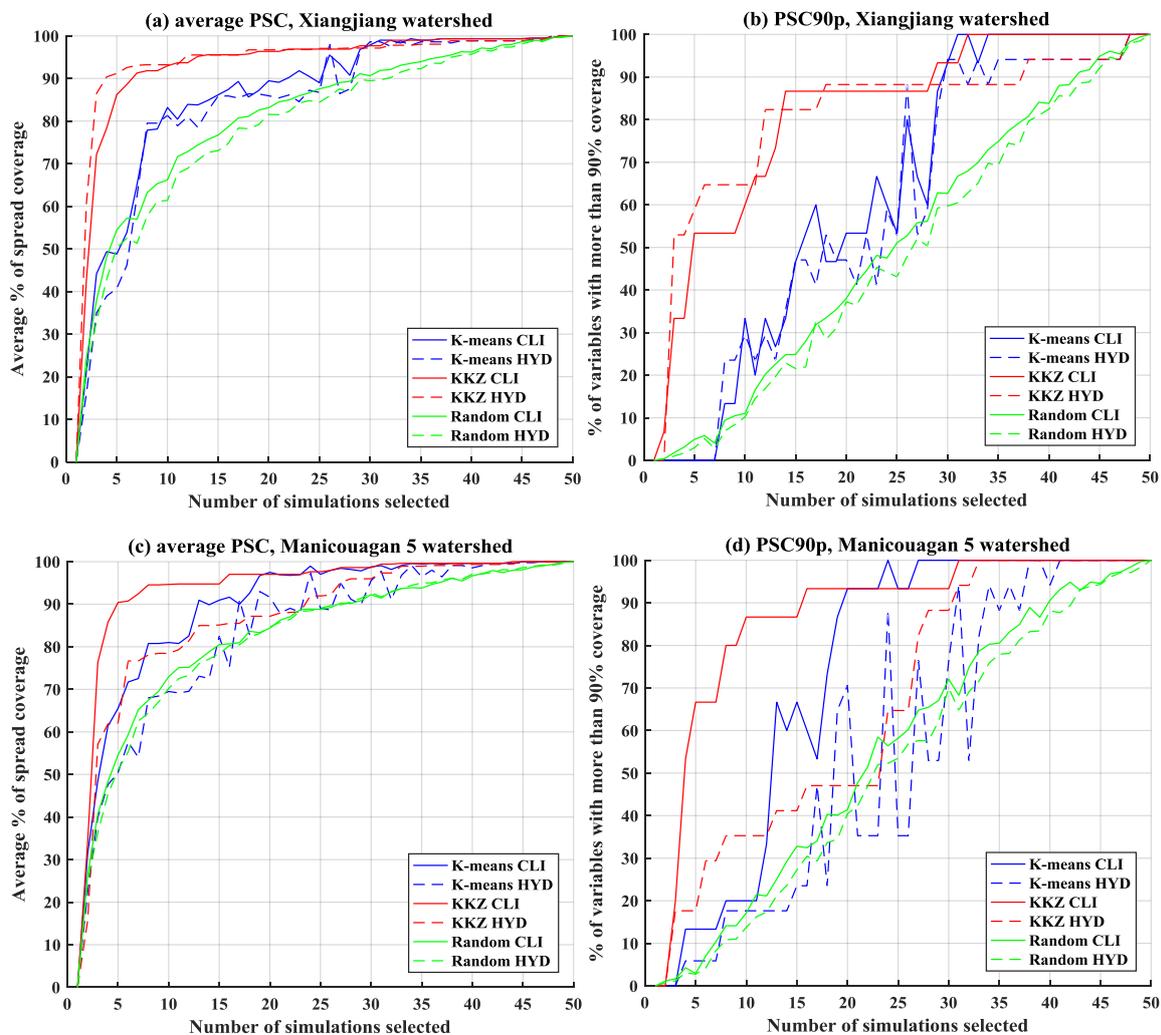


Figure 8: The (a, c) average PSC and (b, d) PSC90p for three different selection methods (K-means, KKZ and random selection) over two watersheds when temperature variables are excluded in the process of simulation selection (CLI = climate variables and HYD = hydrological variables).

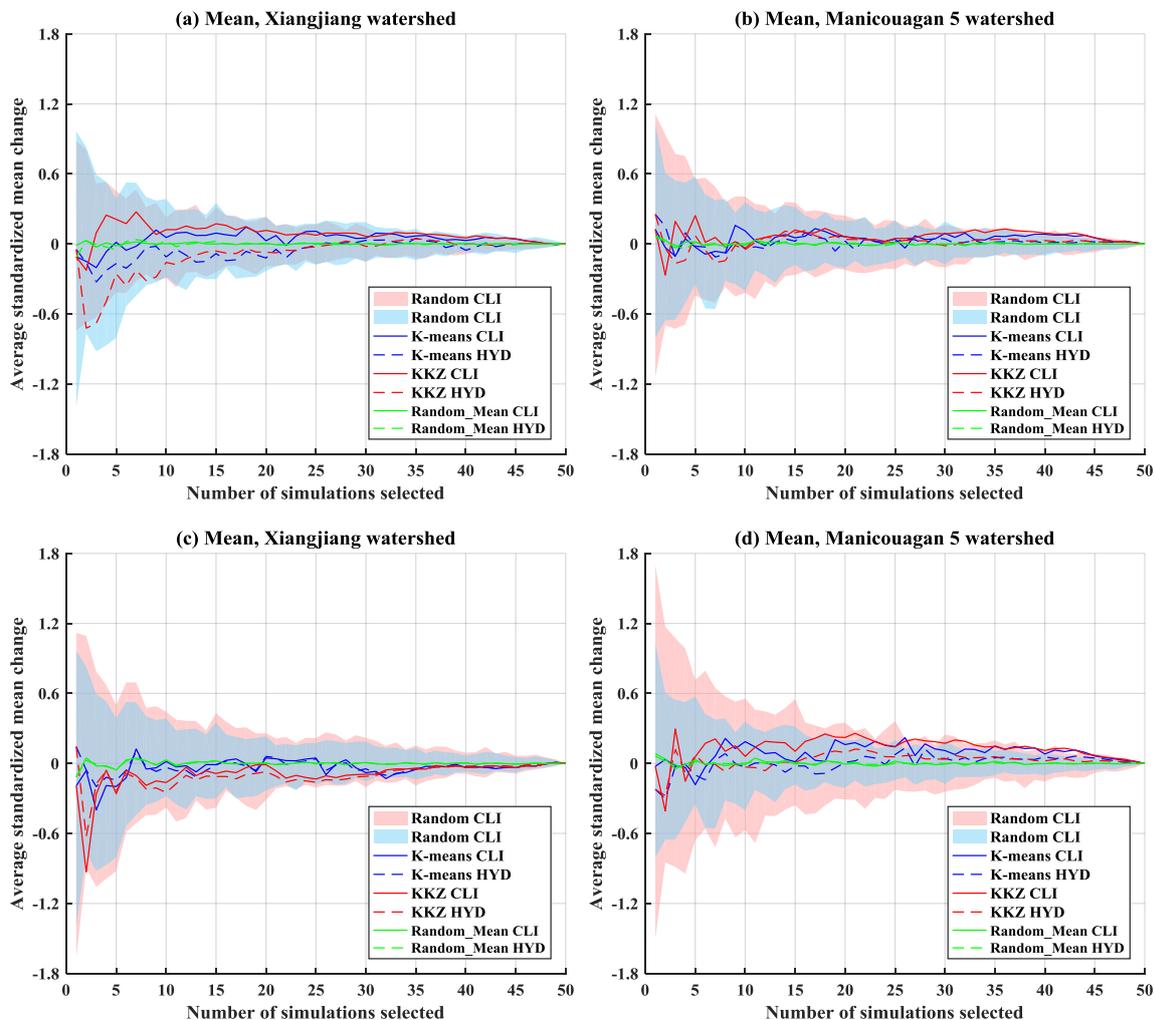


Figure 9: Averaged standardized mean changes in climate (CLI) and hydrological (HYD) variables of subsets selected by three selection methods (K-means, KKZ and random selection) over the Xiangjiang and Manicouagan 5 watersheds when temperature variables are (a, b) included or (c, d) excluded in the process of selection. The pink and blue panels are the envelopes resulting from 100 random selections.