1	Performance dependence of multi-model combination methods					
2	on hydrological model calibration strategy and ensemble size					
3						
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13						
14	Abstract:					
15	The multi-model combination is a technique to improve the performances of hydrological					
16	streamflow simulations. An area that has not been investigated much is the performance dependence					
17	of combination techniques on the hydrological model calibration strategy and ensemble size. This					
18	study aims at investigating the joint effect of the hydrological models, calibration strategies and					
19	ensemble sizes on combination abilities for selecting the most appropriate multi-model combination					
20	method. The ensemble members were constructed by applying four hydrological models and four					
21	objective functions over 383 catchments in China. The ensemble members were combined by using					
22	nine commonly used methods, which are Equal Weights (EWA), Akaike Information Criterion					
23	(AICA), Bayes Information Criterion (BICA), Bates and Granger (BGA), Granger Ramanathan A,					

24 B, and C (GRA, GRB, and GRC), Bayesian Model Averaging (BMA) and Multi-model Super

25 Ensemble (MMSE). The GRC is found as the best multi-model combination method for 26 hydrological simulations. Adding ensemble members by either multiple hydrological models or 27 calibration strategies could help to improve the simulation abilities. Specifically, the increase of 28 ensemble members can obviously enhance the performance of multi-model combinations when the 29 ensemble size is less than six, while only limited improvement is achieved when the ensemble size 30 is more than nine. The combination of ensemble members with various calibration strategies is hard 31 to compensate for the weakness of hydrological model structures. As well, the application of a single 32 calibration strategy in ensemble members only emphasizes single discharge periods and neglects 33 other important discharge periods. This study found that various models with different objective 34 functions are more robust and efficient. The combination performs better than any individual model 35 in terms of Nash-Sutcliffe efficiency (NSE) for approximately 70% catchments, but the multi-36 model combination is less efficient in terms of low-flow simulations. 37

37 Keywords: multi-model combination method; ensemble modeling; calibration strategy;
 38 ensemble size; joint effect

39

40 1. Introduction

41	Hydrological models are essential tools for addressing a wide spectrum of hydrological and
42	water resources problems, including water resources planning, drought and flood control, simulation
43	at ungauged locations, and impact studies for climate or land-use changes (Kotsuki et al., 2014;
44	Kudo et al., 2017; Lane et al., 2019; Wang et al., 2020; Zhang et al., 2014). Over the last decades, a
45	large number of hydrological models have been developed, ranging from lumped conceptual models
46	to physically-based distributed models (Arnold et al., 1998; Chiew et al., 2002; Edijatno et al., 1999;
47	Liang et al., 1994; Xu, 2021; Zhao et al., 1980). The performance of those models varies for diverse
48	catchments characterized by different climate, land use and topography, according to the strengths
49	and weaknesses of the modeling (Mendoza et al., 2016; Pechlivanidis et al., 2011; Vansteenkiste et
50	al., 2014a; Zhang et al., 2020). It is hard to determine a priori which model is most appropriate for
51	a given application over widely differing characteristics of catchments. A single model is not able
52	to consistently outperform the others for all catchment characteristics and heterogeneous
53	climatology (Arsenault et al., 2015; Kumar et al., 2015; Velazquez et al., 2010). Several studies
54	(Arsenault et al., 2015; Velázquez et al., 2011; Zhang et al., 2020) found that multi-model
55	combinations are more robust and efficient than their individual members with the concept of using
56	ensemble to reducing errors with an optimal bias and variance trade-off.

A wide range of methods can be used to generate a multi-model combination solution. The simplest example is the calculation of the arithmetic mean of the input models (commonly referred to as the Equal Weights Averaging (EWA)). More sophisticated techniques employ weighted schemes, with differential weightings applied to each input model reflecting their relative advantages or limitations. There are some popular techniques used to obtain the optimal set weights
for multi-model combinations like multiple linear regression (Arsenault et al., 2015; Granger and
Ramanathan, 1984; Kumar et al., 2015), machine learning algorithms (Jeong and Kim, 2009;
Shamseldin et al., 1997; Zaherpour et al., 2019), Bayesian model averaging (Neuman, 2003) and
Information Criterion Averaging (Akaike, 1974; Schwarz, 1978). The challenge in ensemble
modeling is to determine the ensemble size and to identify the best averaging method (Arsenault et
al., 2015; Buizza and Palmer, 1998; Kumar et al., 2015).

68 Many studies (Jeong and Kim, 2009; Shamseldin et al., 1997; Sun and Trevor, 2018; Zaherpour 69 et al., 2019) have attempted to identify the best multi-model combination method for hydrological 70 simulations. Shamseldin et al. (1997) applied three methods (simple arithmetic mean, constrained 71 ordinary least-squares weighting, and neural network) to combine four hydrological models for 11 72 catchments and found the constrained ordinary least-squares weighting and neural network are more 73 robust and efficient than the simple arithmetic mean in terms of the Nash-Sutcliffe efficiency (NSE). 74 Broderick et al. (2016) analyzed the performance of four ensemble averaging techniques using four 75 hydrological models for 37 Irish catchments. They concluded that GRA is the best ensemble 76 averaging technique, and the averaging methods performed better for the NSE as opposed to bias 77 metrics. In addition, some studies investigated the effect of ensemble size on the performance of 78 multi-model ensemble simulations. For example, Arsenault et al. (2015) compared nine multi-model 79 averaging approaches using 12 hydrographs (4 models \times 3 metrics) over 429 catchments. They 80 found that GRC performs better than other averaging methods and no catchment requiring more 81 than seven ensemble members to maximize the NSE with this method. Kumar et al. (2015) 82 compared ten different multi-model ensemble methods using eight hydrological models to select

the best multi-model ensemble method for the discharge estimation over a catchment of the Mahanadi river basin in India. They showed that the constrained multiple linear regression is the most suitable multi-model ensemble method in terms of NSE, root mean square error (RMSE) and Pearson's correlation coefficient (R), and five ensembles show the best performance for the study area.

88 The method of multi-model combination is usually used to extract as much information as 89 possible from a group of existing models, which may produce a better overall simulation, as each 90 simulation of the group provides specific information. In addition to the selection of the hydrological 91 models, the process of parameter identification is also a crucial step in streamflow modeling. The 92 calibration strategies (which here mean choice of objective functions) reflect the goodness of fitting 93 between hydrological model simulations and observations, which can substantially influence the 94 model parameters and the streamflow projections (Krysanova et al., 2018; Lane et al., 2019; 95 Mizukami et al., 2019; Seiller et al., 2017). The hydrological models with various structures and 96 calibration strategies have certain capacities to predict the streamflow. In general, the hydrological 97 simulations achieve maximum accuracy in terms of specific hydrological properties using a 98 particular metric, but that might limit the modeling skill in other aspects (Arsenault et al., 2015; 99 Mizukami et al., 2019; Seiller et al., 2017). For example, the most widely used calibration strategies, 100 such as Nash-Sutcliffe efficiency (NSE) and Kling-Gupta efficiency (KGE), emphasize high flow 101 events and their timing (Gupta et al., 2009; Mizukami et al., 2019; Nash and Sutcliffe, 1970). Those 102 metrics calculated on the natural logarithm of the flow values put more weight on low flows 103 (Pushpalatha et al., 2012; Seiller et al., 2017). The use of multi-model combination scheme is 104 expected to benefit from the variation of the parameter sets derived from objective functions targeted 105 at different hydrological processes to produce a better overall simulation. Although the influence of 106 calibration strategies exists in hydrological modeling, the impacts of hydrological model calibration 107 strategies on the performance of multi-model combinations and their joint effects with ensemble 108 sizes are not clear. Moreover, there is no consensus in the hydrological community in terms of the 109 selection of particular multi-model ensemble sizes to ensure good model performances.

110 This study aims to investigate the joint effect of ensemble sizes and hydrological model calibration strategies on combination abilities for selecting the most appropriate multi-model 111 112 combination method. Specifically, nine commonly used multi-model combination techniques are 113 compared over 383 catchments in China using ensemble members derived from 4 hydrological 114 models calibrated with 4 objective functions. The rest of the paper is organized as follows. Section 115 2 presents a brief introduction of the study data and the methodology, including the hydrological 116 models, the calibration strategies, the multi-model combination techniques, and the details of the 117 evaluation technique used in this study. The results are presented in Section 3, followed by the 118 discussion and conclusion in Section 4.

- 119 2. Data and Methodology
- 120 2.1 Study region and data

121 This study used a gridded meteorological dataset $(0.5^{\circ} \times 0.5^{\circ})$ over China for the period of 122 1961–2016, which contains four climate variables, including daily precipitation, daily maximum, 123 minimum and mean air temperatures to represent observed data. This dataset was generated from 124 2,472 in-situ gauge stations across China by thin-plate spline interpolation method and GTOPO30 125 (Global 30 Arc-Second Elevation) data sampling and is considered as the latest gridded meteorological data with the highest spatial resolution in China. This dataset has been commonly
used in many hydro-climatological studies in China (Gu et al., 2020; Li et al., 2019; Yin et al., 2020),
and downloaded from the China Meteorological Data Sharing Service System
(<u>http://www.cma.gov.cn</u>).

130 The daily streamflow series over 383 catchments in China were used (Figure 1). These 131 catchments with a wide range of climatic conditions and hydrological regimes span over all the nine 132 major river basins in China. Based on climate type and physical geography, this study region was 133 divided into four major climate regions: continental climate zone of Northwest (NW), the highland 134 climate zone of Southwest (Tibetan Plateau, SW), the temperate monsoon region of Northeast (NE), 135 and the tropical and subtropical monsoon region of Southeast (SE) (Ding, 2013; Wu et al., 2016). 136 NE is the driest region according to the average aridity index value (Figure 2). The size of the 137 catchments ranges from 612 km² to 995,343 km². The streamflow dataset covers the 1961–2016 138 period with a maximum length of 52 years and a minimum length of 22 years. The average annual 139 precipitation of the catchment varies greatly with clear gradients depending on the region. The mean 140 annual precipitation is more than 1400 mm in the southern region, while it is less than 600 mm in 141 the northern region.

142

<Figure 1>

143

<Figure 2>

144 2.2 Hydrological models

A wide range of hydrological models is used for different application purposes. Some studies
 compared the performance of lumped and distributed models for outlet streamflow simulation and

147 found that two types of models may lead to similar accuracy (Kumar et al., 2015; Lobligeois et al., 148 2014; Vansteenkiste et al., 2014b), even for quite large catchments (Merz et al., 2009). Considering 149 the scope of this study, the lumped model (the most common model type used by hydrologists for 150 water resources assessment, flood forecasting, and impact of climate change studies) was chosen, 151 and the distributed model with expensive computations was excluded. Four lumped models with 152 different complexity were used, i.e., modèle du Génie Rural à 4 paramètres Journalier (GR4J) 153 (Edijatno et al., 1999; Perrin et al., 2003), hydrological model of école de technologie supérieure 154 (HMETS) (Martel et al., 2017), simple HYDROLOG (SIMHYD) (Chiew et al., 2002), and 155 Xinanjiang (XAJ) (Zhao, 1992; Zhao et al., 1980). Those models have been widely used in 156 streamflow simulation and have been shown to be relatively efficient (Arsenault et al., 2015; 157 Broderick et al., 2016; Jones et al., 2006; Liang et al., 2013; Mathevet et al., 2020). Table 1 briefly 158 summarized the basic information for these hydrological models.

159 The four models have different numbers of parameters and are different in model structures 160 and underlying mechanisms. For example, the physical process is described in more detailed and 161 complex mechanisms in HMETS, SIMHYD and XAJ than in the most parsimonious structure GR4J 162 with only four free parameters. The main feature of the runoff generation of HMETS and XAJ is 163 using the saturation excess flow mechanism based on the soil moisture content of the aeration zone 164 reaching its field capacity. While SIMHYD considers both infiltration excess runoff and saturation 165 excess runoff in streamflow production calculated by an interception store, a nonlinear soil moisture 166 store. For the simulation of evaporation, XAJ uses a three-layer evaporation model, while HMETS 167 and SIMHYD use a one-layer model. Additionally, GR4J and HMETS consider the incorporation 168 of groundwater exchange by surface water-groundwater interaction functions, but XAJ and 169 SIMHYD do not have this consideration.

Since GR4J, XAJ and SIMHYD do not simulate snow accumulation or melt processes, a snow module (CEMANEIGE) with 2 free parameters (Valéry et al., 2014) was combined with the original model to make it applicable in seasonally snow-covered catchments in northern China. The basic inputs of these four models are catchment-averaged precipitation and temperature/potential evapotranspiration over the entire basin for the computation of discharge. The potential evapotranspiration was estimated using a temperature-based method proposed by Oudin et al. (2006a).

- 177 <Table 1>
- 178 2.3 Calibration and evaluation metrics

This study used four objective functions to calibrate the four hydrological models over 383 catchments. The four calibration strategies are the widely-used Nash–Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970), the NSE computed on natural logarithm and square root of the flow values (NSE(ln) and NSE(sqrt)), and percent bias (PBias). NSE, NSE(ln) and NSE(sqrt) all range from negative infinity to 1, with a value of 1 indicating perfect fitting. The PBias' value being closer to zero indicates the better simulating performances.

Different calibration strategies were included in the combination since they emphasize different aspects of hydrological streamflow properties. The original NSE without discharge transformation puts great emphasis on high flows (Li et al., 2019; Mizukami et al., 2019). The natural logarithm of discharge transformation (NSE(ln)) is to optimize the performance for low flow segments (Seiller et al., 2017). The analysis of NSE(sqrt) well balances simulated streamflow

190	without too much emphasis on low or high flow (Oudin et al., 2006b), and the PBias emphasizes
191	the total water balance. Regardless of the objective function, the hydrological models optimized the
192	parameter using the Shuffled Complex Evolution-University of Arizona (SCE-UA) algorithm
193	(Duan et al., 1992). A cross-validation method that divided the complete record of each catchment
194	(Arsenault et al., 2015; Yang et al., 2020) into odd and even years for model calibration and
195	validation was used, to reduce the influence from the non-stationarity of hydro-climatological
196	conditions. In this process, the first year in the calibration period was used for model warm-up.
197	In addition to using NSE, NSE(ln), NSE(sqrt) and PBias as evaluation metrics to represent the
198	overall performance of simulations, the high and low flows were also analyzed based on the
199	discharge segments of flow duration curves (FDC) to identify the influence of ensemble method on
200	the performance of various flow components. Following previous studies (Laaha and Blöschl, 2006;
201	Pfannerstill et al., 2014; Yilmaz et al., 2008), the flow exceedance probability of 70% was used to
202	represent the low flow, and the mid-flow segment was shifted from 20% to 70%. The very high-
203	flow range was defined between 0% and 5%, and the high-flow range between 5% and 20%. The
204	performance of the model simulations within these FDC segments was analyzed using PBias
205	(PBiasFSV), noted by PBiasFSV-5, PBiasFSV-20, PBiasFSV-mid, and PBiasFSV-low. The basic
206	information of those metrics which were used for evaluating the performance of the different
207	hydrograph phases was shown in Table 2.

208

<Table 2>

209 2.4 Multi-model averaging methods

210 There are several methods available in the literature for developing the multi-model

combination. Here, we compared the performance of nine commonly used deterministic ensemble
techniques for creating multi-model ensembles. The selected methods include Equal Weights
Averaging (EWA), Akaike Information Criterion Averaging (AICA), Bayes Information Criterion
Averaging (BICA), Bates and Granger Averaging (BGA), Granger Ramanathan A Averaging (GRA),
Granger Ramanathan B Averaging (GRB), Granger Ramanathan C Averaging (GRC), Bayesian
Model Averaging (BMA) and Multi-model Super Ensemble (MMSE). The general model for
averaging methods can be expressed as:

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$$Q_{ens} = \sum_{i=1}^{n} W_i \cdot Q_{simi}$$

where Q_{ens} is the ensemble simulation, Q_{simi} is the individual simulation, and W_i is the weight of the ensemble member.

A description of the selected averaging methods was given in the Appendix. The basic characteristics of the nine multi-model averaging techniques were summarized in Table 3.

3. Results

225 3.1 Performance of the individual members

The performances of the 16 ensemble members over 383 catchments in the calibration and validation were analyzed using the evaluation of NSE, NSE(ln), NSE(sqrt), and PBias representing the average simulated abilities and using the PBias of four different FDC segments (PBiasFSV-5, PBiasFSV-20, PBiasFSV-mid and PBiasFSV-low) representing the high and low flows, as presented in Figure 3. The result shows that the evaluation metrics in the validation period are consistent with those in the calibration period, which indicates the hydrological simulations are robust and transferable.

233 The ensemble members with calibration strategies closely related to the evaluation metrics 234 work best, as expected. Models calibrated with NSE(sqrt) maintain good performances in terms of 235 NSE and NSE(ln) evaluation with median values around 0.7 and 0.8. All ensemble members show 236 the absolute value of PBias being less than 10%, but the models calibrated with PBias yield inferior 237 performance in terms of NSE-based evaluation metrics. According to the FDC segment evaluation 238 values (Figures 3e-3h), the models calibrated with NSE show good performance for high flow 239 segments that obtain the best score for 38% and 42% of catchments in terms of the PBiasFSV-5 and 240 PBiasFSV-20, respectively (Table 4). The models calibrated with NSE(ln) put high weight on low 241 flows and obtain the best score at a frequency of 42% catchments. Models calibrated with NSE(sqrt) 242 emphasize middle flows, which obtain the best score at a frequency of 38% catchments. Those 243 results confirmed the specialization of the objective functions for specific parts of the hydrographs. 244 This figure also demonstrates that hydrologic models perform differently with respect to 245 different calibration strategies and evaluation metrics. For example, calibrated with NSE, both HMETS and GR4J with median NSE(ln) value of 0.6 perform better than SIMHYD and XAJ with 246 247 median NSE(ln) value of 0.3 and 0.5. In addition, HMETS and GR4J tend to overestimate the midle

and low flow segments, while the other two models (i.e., SIMHYD and XAJ) tend to underestimate
those flows. Comparing the hydrological models, XAJ generally performs best for the evaluation
metrics, followed by HMETS, GR4J and SIMHYD.

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When looking at four sub-regions based on the median value of evaluation metrics (Figure 4),

252	different models show similar spatial patterns in terms of NSE-based metrics with better
253	performances in the wetter southern catchments (SW and SE) than in drier northern catchments
254	(NW and NE). However, the performance of the four hydrological models is not the same. GR4J
255	and SIMHYD perform better than XAJ and HMETS in terms of NSE-based metrics over SW when
256	using NSE(ln) as the objective function.

- 258 <Figure 4>
- 259 <Table 4>

260 3.2 Performance of the multi-model averaging methods

The nine multi-model combination methods were applied to calculate the optimal weights based on the observed and the 16 simulated streamflow series. The performance of those methods over 383 catchments in the validation period is presented in Figure 5. The result shows that the differences of the ensemble simulations are evident not just in how well the averaging methods but also in the evaluation metrics used.

For NSE metric, almost all multi-model combination methods show similar performances with median values around 0.8 except for EWA, BGA, and BMA with median values less than 0.75. For NSE(ln) metric, EWA, BGA, and BMA perform better than others with median values around 0.8, followed by GRA, GRB and GRC with median values around 0.75. Almost all averaging methods show similar performances in terms of NSE(sqrt) metric with median values exceeding 0.81. For PBias and PBiasFSV-5, GRA, GRB, GRC and MMSE show similar performances and outperform

272	others, followed by AICA and BICA. For PBiasFSV-20, PBiasFSV-mid and PBiasFSV-low, GRC
273	performs the best, followed by GRA, GRB and MMSE. In general, all simulations tend to
274	underestimate the high flow but overestimating the mid and low flows.
275	Among various averaging methods, GRA, GRB, GRC, and MMSE show similar performance,
276	since they derived from the same optimal weighting group. The AICA and BICA perform poorly in
277	terms of NSE(ln) and PBiasFSV-low metrics compared with other averaging methods, as they put
278	almost all weights on the individual member with minimum RMSE. It can also be seen that the
279	BMA, EWA, and BGA without bias-correction show worse performances in terms of PBias-based
280	measures, especially for PBias, PBiasFSV-5 and PBiasFSV-low.
281	Overall, the GRA, GRB, GRC, and MMSE consistently outperformed other combination
282	methods in terms of the eight evaluation metrics, and GRC provided the best performances,
283	especially in terms of PBias and PBiasFSV. Therefore, GRC is considered as the best multi-model
284	averaging method for hydrological simulations in this study.
285	<figure 5=""></figure>
286	3.3 Impact of the hydrological model, calibration strategy, and ensemble size on multi-
287	model combinations
288	This section investigated the joint influence of the hydrological models, calibration strategies
289	and ensemble size on the performance of GRC. The selection of ensemble members is based on
290	multiple hydrological models calibrated with a single objective function, a single hydrological
291	model calibrated with multiple objective functions, and multiple hydrological models calibrated
292	with multiple objective functions. Figure 6 shows the median performance value over 383

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293 catchments in the validation period to represent the overall ability of those combinations.

294 The performance of multiple hydrological models calibrated with a single objective function 295 varies depending on the selection of objective function and is improved along with the increase of 296 hydrological model numbers (areas numbered 2 in Figure 6). Areas numbered 3 in Figure 6 show 297 the performances of a hydrological model with multiple objective functions. Though using multiple 298 objective functions could improve the combination abilities, the performances still depend on the 299 selection of hydrological models, as each hydrological model has its own advantages and limitations. 300 For example, the combinations based on SIMHYD generally perform worse than others in terms of 301 NSE and NSE(sqrt) but perform better in terms of NSE(ln), PBias and PBiasFSV-low. In addition, 302 a single model is not able to consistently outperform others for all catchments with various hydro-303 climatic regimes. The combinations of multiple hydrological models calibrated with various 304 objective functions taking advantage of all ensemble members generally perform more robust and 305 efficient than combinations only using a single calibration or a single hydrological model in terms 306 of all NSE-based metrics (areas numbered 4 in Figure 6).

Overall, either using multiple hydrological models or multiple calibration strategies could improve the multi-model combination performances in terms of NSE-based metrics but is less efficient in PBias-based evaluation metrics. The above results also indicate that the influence of increasing hydrological models on combination is larger than increasing model calibration strategies, and the effect of the individual simulation is decreasing along with the increase of ensemble members. The qualitative comparison of different combinations and individual simulations would be analyzed later (Section 3.4). 314

<Figure 6>

315	The combinations with ensemble sizes ranging from 2 to 16 ensemble members are generated
316	by re-sampling the ensemble members 100 times from all combination members to investigate the
317	effect of ensemble size on simulating abilities. Figure 7 shows the relationship between the
318	ensemble size and the combination performances. The 0.05 and 0.25 quantiles of NSE, NSE(ln) and
319	NSE(sqrt) values correspond to the poor efficiency modeling, while 0.75 and 0.95 quantiles
320	correspond to simulations with good performance. The median performance is represented by
321	quantile 0.50 (red lines). The absolute values of PBias and four PBiasFSV being infinite to zero
322	indicating better performances. This result indicates that the performance is improved along with
323	the increase in ensemble sizes, and the effect of ensemble size on the low quantile values is larger
324	than that on the high quantile. In general, the performance of the multi-model combinations is
325	sensitive to the ensemble size and the selection of ensemble members when the member is less than
326	six. The influence of enlarging ensemble numbers on simulation performances could be ignored
327	when the ensemble member is more than nine. In other words, when the ensemble member is more
328	than nine, neither enriching the hydrological model nor increasing calibration strategies show
329	limited improvement in simulating abilities, as larger ensemble sizes mean each individual member
330	with smaller weights and limited influence on the combination.

331

<Figure 7>

In order to investigate whether all ensemble members contribute to the performance of the combination, the frequency of the individual member being selected in the best-performed combinations of all catchments is calculated and plotted in Figure 8. Here, the ensemble sizes of the

335	combinations are nine since the results from Figure 7 concluded that the effect of increasing
336	ensemble numbers more than nine could be ignored. Figure 8 shows that all individual members
337	have similar chancies of being selected in the best-performed combinations in terms of different
338	evaluation metrics, indicating all ensemble members contribute to enhancing the combination
339	simulation.
340	<figure 8=""></figure>
341	3.4 Comparison of the multi-model combination and ensemble members
342	The performances of GRC and the ensemble members were compared using the cumulative
343	distributions of NSE, NSE(ln), NSE(sqrt), absolute values of PBias and PBiasFSV over the 383
344	catchments in the validation period (Figure 9). Here, five combinations are represented, including
345	four hydrological models calibrated with a specified objective function (i.e., H4-NSE, H4-NSE(ln),
346	H4-NSE(sqrt) and H4-PBias) and four hydrological models calibrated with four calibration
347	strategies (i.e., H4C4).
348	It is apparent that the multi-model combinations, either using multiple hydrological models or
349	using multiple calibration strategies, outperform the individual member in terms of those
350	performance metrics, except for NSE(ln) and PBiasFSV-low. The combinations of four hydrological
351	models calibrated with four calibration strategies perform the best and show 85% catchments have
352	NSE values exceeding 0.6, and 75% catchments have NSE values exceeding 0.7 (Figure 9a). In
353	addition, 91% catchments have NSE(sqrt) values exceeding 0.6, and 73% catchments have NSE(sqrt)
354	values exceeding 0.7 (Figure 9b). The absolute value of PBias is less than 10 for more than 95%
355	catchments, and that is less than 5 for 78% catchments. In addition, the absolute values of PBiasFSV-

5, PBiasFSV-20, and PBiasFSV-mid are less than 10 for 55%, 80% and 80% of catchments, respectively. However, the combinations are less efficient in terms of NSE(ln) and PBiasFSV-low evaluation than the individual members using NSE(ln) calibration, since the averaging methods based on minimum RMSE are more sensitive to flood peaks than low-flow period.

361 Table 5 shows the rate at which the averaging simulation surpasses the best individual member 362 in terms of four average performance metrics and four FDC segment metrics over the 383 catchments in the validation period. Here, the "best individual member" value is selected from the 363 364 16 members independently for each catchment. The results show that four hydrological models calibrated with four calibrations (H4C4) perform more robustly than other combinations in terms of 365 366 various performance metrics. The combination of four hydrological models calibrated with a 367 specified objective only performs efficiently for the specific parts of the hydrographs. The combinations perform better than the best individual member for about 70% catchments in terms of 368 369 NSE and for about 55% catchments in terms of NSE(sqrt). On the contrary, combinations show less 370 efficiency for performance values in terms of NSE(ln) and PBias.

Figures 10(a) and 10(b) show the geographic distribution of the NSE value in the validation period from the best individual member and combinations. The spatial patterns are consistent with better performances in the wetter southern catchments than in the drier northern catchments. For catchments with annual precipitation larger than 600 mm, 82% catchments obtain NSE value exceeding 0.7, and the combination outperforms the best individual in 82% cases. However, for catchments with annual precipitation less than 600 mm, only 51% catchments obtain NSE value

377	exceeding 0.7, and the combinations outperform the best individual only in 45% cases (Figures 10c
378	and 10d). Since hydrological simulations are big challenges for the arid catchments, especially when
379	using lumped models, which cannot represent the rainfall and loss variability that tends to be higher.
380	The multi-model combinations have less benefit when the ensemble members cannot accurately
381	simulate the streamflow.
382	<table 5=""></table>
383	<figure 10=""></figure>
384	4. Discussion and conclusion
385	The multi-model combination is a technique widely used to improve the performance of
386	hydrological streamflow simulations, as it extracts potentially useful information from a group of
387	existing models. The commonly used multi-model combination usually takes information from
388	different hydrological models while neglects the additional information from calibration strategies.
389	This study investigated the joint effect of hydrological models, calibration strategies and ensemble
390	sizes on combination abilities for selecting the appropriate multi-model combination method. This
391	study compared different multi-model ensemble methods by combining the simulated discharge
392	with four hydrological models and four different calibration strategies.
393	Generally, the hydrological model performances were similar in terms of geographic
394	distribution, with better performances in wetter catchments than drier catchments. Nevertheless,
395	there were some obvious differences between those models. GR4J and HMETS with surface water-

- 396 groundwater interaction functions performed better than XAJ and SIMHYD in terms of NSE(ln)
- 397 value. This is consistent with Pushpalatha et al. (2011) and Fleckenstein et al. (2006), who found

398 that the lumped model with the incorporation of groundwater exchange functions improves the 399 predictions of low flows.

400 One of the other goals was to compare the nine multi-model averaging methods. Overall, GRA, 401 GRB, GRC, and MMSE with similar methods for optimal weight showed consistent performances 402 and performed better than other combination methods. GRC with bias-correction showed better 403 performances in terms of PBias and PBiasFSV metrics than other combination methods and was 404 considered as the best multi-model averaging method for hydrological simulations in this study. As 405 AICA and BICA put all weights on the individual model with a minim root-mean-square error, they 406 performed similarly to the best-performing individual model. BGA, without the consideration of the 407 biases from ensemble members, only performed slightly better than EWA, which is consistent with the previous study (Arsenault et al., 2015). This study also found that BMA, which was widely used 408 409 in previous ensemble studies (Li et al., 2019; Zhang et al., 2020), performs similarly to BGA in 410 terms of PBias-baed evaluation metrics. BMA is recommended to apply on ensemble simulations, 411 whereas it is sometimes difficult to effectively remove bias from the predictions of complex 412 streamflow simulation (Madadgar and Moradkhani, 2014), which is related to the poor performance 413 in inters of PBias evaluations.

In addition, this study found that adding ensemble members by either increasing hydrological models or increasing calibration strategies could improve the simulation abilities, but the combinations of taking advantage of different hydrological models and objective functions were more robust and efficient in terms of different hydrological properties and hydro-climatic regimes. In addition, this study found that the increase of ensemble members could obviously improve the 419 multi-model combination performance when the ensemble size is less than six, but has limited 420 effects when the ensemble size is more than nine. This is consistent with Kumar et al. (2015) and 421 Arsenault et al. (2015), who found that four and seven ensemble members are efficient for multi-422 model combinations.

Comparing the combinations and individual simulations, the combinations of different 423 424 hydrological models with various objective functions performed better than any individual model 425 for around 70% of 383 catchments in terms of NSE scores. In contrast, the combinations were less 426 efficient than the best individual members in terms of low-flow simulations. This study also found 427 that the multi-model combinations perform better for wetter catchments than for drier catchments. 428 The frequencies of ensemble simulation outperforming the best individual simulation in terms of NSE were 82% catchments in wetter regions with precipitation more than 600 mm/year and 45% 429 430 catchments in drier regions with precipitation less than 600 mm/year.

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439 Appendix: Multi-model ensemble methods

440 A description of the multi-model averaging methods is presented here.

- 441 1. Equal Weights Averaging (EWA)
- In the EWA (Shamseldin et al., 1997), the equal weight is simply assigned to each of theensemble members. This is expressed mathematically as:

444
$$\mathbf{w} = \frac{1}{N} \tag{A1}$$

445 where N is the number of ensemble models.

446 2. Akaike and Bayes information criteria averaging (AICA and BICA)

AICA (Akaike, 1974) and BICA (Schwarz, 1978) methods combine ensemble members based
on both performance and model complexity. Weight represents a trade-off between reducing the
simulated error while tending toward less complex, which is calculated as:

450
$$\mathbf{w} = \frac{\exp\left(-\frac{1}{2}l\right)}{\sum_{i=1}^{N} \exp\left(-\frac{1}{2}\mathbf{I}_i\right)}$$
(A2)

451 where I is the information criterion estimated based on the mean of the logarithm of the ensemble

452 member variances and the number of calibration parameters, and is calculated as:

453
$$I = -2\log(L) + q(p)$$
 (A3)

454 where L and q(p) are the maximum likelihood of ensemble member and the penalty term, 455 respectively.

- 456 The difference between the AICA and BICA methods lies in the penalty term calculation. The457 penalty terms of AICA and BICA are estimated by equations (A4) and (A5):
- $q = 2p \tag{A4}$

$$q = p\log(k) \tag{A5}$$

where p donates the number of calibrated parameters in the members, and k donates the sample size(here is the number of time steps).

463 The BGA (Bates and Granger, 1969) method aims to produce a combined ensemble by 464 minimizing the Root Mean Square Error (RMSE) between the observations and simulations. The 465 model weighting vector is estimated according to:

466
$$W = \frac{\frac{1}{RMSE^2}}{\sum_{i=1}^{N} \frac{1}{RMSE_i^2}}$$
(A6)

467 4. Granger Ramanathan A, B and C (GRA, GRB and GRC)

468 The GRA (Granger and Ramanathan, 1984) approach minimizes the RMSE setting weights
469 based on the ordinary least squares (OLS) algorithm. The weights are estimated by:

470
$$W = \left(Q_{sim}^{T} Q_{sim}\right)^{-1} Q_{sim}^{T} Q_{obs}$$
(A7)

471 where Q_{obs} is the observation. The GRB variant is similar to the GRA method, but the OLS 472 algorithm is constrained such that the sum of the weights to unity. The GRC variant is unconstrained,

473 but the averaged streamflow is bias-corrected through the use of a constant term.

474 5. Bayesian Model Averaging (BMA)

BMA (Neuman, 2003) determines the weights of each member through the use of the ensemble
members' probability distribution functions (PDFs). The combined distribution is bias-corrected,
and the difference between the distributions is minimized. According to BMA, the posterior

478 probability of the predictand (y) is described as:

479
$$p(y | Q_{obs}) = \sum_{i=1}^{N} P(Q_{simi} | Q_{obs}) p(y | Q_{simi}, Q_{obs})$$
(A8)

where $p(y | Q_{simi}, Q_{obs})$ is the posterior predictive distribution of y on the condition of the given sample Q_{obs} and each individual model Q_{simi} ; $P(Q_{simi} | Q_{obs})$ is the optimal model on the condition of the given sample Q_{obs} denoted the weight (w_i) of each ensemble member. The mean and variance of y are given:

484
$$E[y \mid Q_{\text{obs}}] = \sum_{i=1}^{N} P(Q_{simi} \mid Q_{\text{obs}}) \int_{-\infty}^{+\infty} yp(y \mid Q_{simi}, Q_{\text{obs}}) dy = \sum_{i=1}^{N} w_i \eta_i$$
(A9)

485
$$\operatorname{Var}[y \mid Q_{\text{obs}}] = \sum_{i=1}^{N} w_i (\eta_i - \sum_{i=1}^{N} w_i \eta_i)^2 + \sum_{i=1}^{N} w_i \sigma_i^2$$
(A10)

$$w_i = P(Q_{simi} \mid Q_{obs}) \tag{A11}$$

487 where w_i is the weight of the ensemble member and sum to unite; η and σ are the expectation 488 and variance of y, respectively, on the condition of the given sample Q_{obs} .

489 6. Multi-model Super Ensemble (MMSE)

MMSE (Krishnamurti et al., 2000) uses the logic of bias reduction along with variance
 reduction through using the mean of observational value and the combination of ensemble member,
 respectively. According to this method, the ensemble discharge is estimated as:

493
$$Q_{MMSE,j} = \bar{Q}_{obs} + \sum_{i=1}^{N} w_i [Q_{sim,i,j} - \bar{Q}_{sim,i}]$$
(A12)

where w_i is the weight of ith model, which is estimated by the unconstrained least square technique
(Eq. (A1)).

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Replies to Referee #1

Performance dependence of multi-model combination methods on

hydrological model calibration strategy and ensemble size

Yongjing Wan, Jie Chen, Chong-Yu Xu, Ping Xie, Wenyan Qi, Daiyuan Li, Shaobo Zhang

We would like to thank the referee for constructive comments and suggestions. All comments are very helpful for improving this paper and beneficial to our research in general. We have provided detailed point-by-point responses to each comment below and have revised the manuscript accordingly. For clarity, comments are given in black, and our responses are given in blue. Please note that the page and line numbers mentioned in reviewers' comments refer to the original version, while in our reply, they refer to the revised version.

The authors have paid careful attention to the reviewers' comments and significantly improved the paper. I have a few minor suggestions in annotations in the attached file. The paper, especially the latest revisions, would benefit from a proof reading for English quality.

Reply: We sincerely thank the reviewer for the positive evaluation of our manuscript and for providing insightful comments. All comments in annotations in the attachment have been addressed as follows. The English has been carefully revised.

Line 103. Perhaps this is expected, if the metric on which the multi-model average is assessed is some generic metric like NSE. If the metric is more specific like high flows, then we do not expect the combination derived from using different objective functions to work better than simply using a high-flow objective. This is a critical point that needs to be made clear.

Reply: We agree with the reviewer. The use of multi-model combination scheme is expected to benefit from the variation of the parameter sets derived from objective functions targeted at different hydrological processes for producing a better overall simulation.

We have made a clear declaration in line 105 of the revised manuscript.

Line 195. This is poorly written. Needs a new sentence; and needs written more clearly and checked by an English speaker.

Reply: We have made a clear declaration in line 195 of the revised manuscript.

Line 277. Unclear what this means.

Reply: Sorry for the confusion. This sentence has been modified as: Among various averaging methods, GRA, GRB, GRC, and MMSE show similar performance, since they derived from the same optimal weighting group.

We have clarified this in line 276 of the revised manuscript.

Line 319. Random selection from all combinations?

Reply: Yes, and we have clarified this in line 316 of the revised manuscript.

Line 331. not the right word here? "significant", or "much"?

Reply: Thanks, and we have verified this sentence.

Line 335. does not make sense to me. Do you mean "whether all ensemble members contribute to the performance of the combination"

Reply: Yes, and we have made a clear declaration in line 332 of the revised manuscript.

Line 381. Especially when using lumped models, which cannot represent the rainfall and loss variability that tends to be higher in arid areas.

Reply: Thanks for the supplement explanation. We have added this in the revised manuscript in line 378.

Line 428. This gives limited insight into where and why the performances were better. At least, the effect of catchment area should be explored too.

Reply: Thanks for the suggestion. We have analyzed the relationship between the combination performance and catchment area, as shown in figure R1. The result indicates that there is no obvious relationship between two of them. Thus, this resut was not shown in the revised manuscript.



Figure R1. The relationship between the NSE value and catchment area. The green/red markers represent the combination performed better/worse than the best individual member.



Figure 1. Spatial distribution of the outlets and total annual precipitation (Pr, mm) for 383 catchments in China.



Figure 2. Characteristics of the catchments over different regions. The red line in the boxplots represents the median value, the ends of the boxes represent the 25th and 75th percentiles, the whiskers represent the values at the 5th and 95th percentiles, and outliers are not shown.



Figure 3. NSE, NSE(ln), NSE(sqrt), PBias, and four PBiasFSV values for 16 ensemble members (model/objective function pairs). The boxplots indicate the spread of performance values of the evaluation metrics over 383 catchments in the calibration and validation periods.



Figure 4. The median value of NSE, NSE(ln), NSE(sqrt), absolute of PBias and four PBiasFSV values in the validation period for the catchments over the four sub-regions. The four hydrological models GR4J, HMETS, SIMHYD and XAJ are denoted by A, B, C and D, respectively. The four objective functions NSE, NSE(ln), NSE(sqrt), and PBias are denoted by a, b, c and d, respectively.



Figure 5. NSE, NSE(ln), NSE(sqrt), PBias, and four PBiasFSV values over 383 catchments for nine multi-model ensemble techniques with combinations of the 16 ensemble members in the validation period.



Figure 6. The median value of NSE, NSE(ln), NSE(sqrt), and absolute values of PBias four PBiasFSV over 383 catchments in the validation period based on different combinations in terms of ensemble members. The four hydrological models GR4J, HMETS, SIMHYD and XAJ are denoted by A, B, C and D, respectively. The four objective functions NSE, NSE(ln), NSE(sqrt), and PBias are denoted by a, b, c and d, respectively.



Figure 7. The relationship between the ensemble size and the performance metrics (NSE, NSE(ln), NSE(sqrt), absolute values of PBias and four PBiasFSV) over 383 catchments in the validation period. The light-colored envelopes: the 0.05 and 0.95 interquartile range values. The dark-colored envelopes: the 0.25 and 0.75 interquartile



range values. The red lines are the median values.

Figure 8. Frequency of individual members is selected in the best combination scheme in terms of different

evaluation metrics (NSE, NSE(ln), NSE(sqrt), absolute values of PBias and four PBiasFSV). The four hydrological models GR4J, HMETS, SIMHYD and XAJ are denoted by A, B, C and D, respectively. The four objective functions NSE, NSE(ln), NSE(sqrt), and PBias are denoted by a, b, c and d, respectively.



Figure 9. Cumulative distributions of NSE, NSE(ln), NSE(sqrt), absolute values of PBias and four PBiasFSV over

the 383 catchments in the validation period.



Figure 10. Geographic distribution of the NSE value of (a) the best individual member and (b) the combination over the 383 catchments in the validation period. Comparison of the best individual and GRC averaging method (c) on

geographic distribution and (d) related to annual precipitation. The green/red markers present GRC produced results

better/worse than the best individual member.

ID	Model	Number of	Characteristics of the model	References
		parameters		
А	GR4J	6	The effective rainfall is partitioned as a 10:90 split	Edijatno et al.
			representing direct runoff and delayed runoff, a nonlinear	(1999); Perrin
			production reservoir with two-unit hydrographs, a routing	et al. (2003)
			reservoir	
В	HMETS	21	Generation of hypodermic flow and groundwater flow with	Martel et al.
			two linear reservoirs, a routing module with two unit	(2017)
			hydrographs, a snowmelt module, an evapotranspiration	
			calculation module	
С	SIMHYD	11	Two linear reservoirs for the calculation of interflow and	Chiew et al.
			base-flow, a nonlinear routing reservoir, an	(2002)
			evapotranspiration calculation module	
D	XAJ	17	Linear reservoirs for surface flow routing, two recession	Zhao (1992);
			coefficients for interflow and groundwater flow routing,	Zhao et al.
			three-layer evapotranspiration system	(1980)

Table 1. Structures of the four lumped conceptual rainfall-runoff models

Table 2. Performance metrics for the evaluation of different phases of the hydrograph.

Performance metric	Sensitive hydrograph phase						
NSE	Peak and discharge dynamic	-∞ ~ 1					
NSE(ln)	Low-flow and discharge dynamic	$-\infty \sim 1$					
NSE(sqrt)	Discharge dynamic	0 ~ 1					
PBias	Overall water balance	$-\infty \sim \infty$					
PBiasFSV-5	Tendencies of overestimation and underestimation for FDC very high-						
	segment volume	$-\infty \sim \infty$					
PBiasFSV-20	Tendencies of overestimation and underestimation for FDC high-	$-\infty \sim \infty$					

	segment volume	
DDiesESV mid	Tendencies of overestimation and underestimation for FDC mid-	-00 ~ 00
	segment volume	
PBiasFSV-low	Tendencies of overestimation and underestimation for FDC very low-	-00 ~ 00
	segment volume	

Table 3. Basic characteristics of the nine multi-model averaging techniques used in this study

Combination method	Acronym	Method description	References		
Equal Weights	EWA	Unweighted average	Shamseldin et al.		
Averaging			(1997)		
Akaike's					
Information		Mean of the logarithm of the member variances			
Criterion	AICA	added a penalty equalling to double the number of	Akaike (1974)		
Averaging		calibrated parameters			
		Mean of the logarithm of the member variances			
Bayes Information		added a penalty equalling to the number of			
Criterion	BICA	calibrated parameters times the logarithm of the	Schwarz (1978)		
Averaging		number of time steps			
Bates and Granger		-	Bates and Granger		
Averaging	BGA	(1969)			
Granger	GRA	Based on ordinary least squares (OLS) algorithm	Granger and		

Ramanathan A			Ramanathan (1984)	
Granger	Weights based on ordinary least squares (OLS)		Granger and	
Ramanathan-B		algorithm and constrained its sum to unity	Ramanathan (1984)	
Granger	GRC	Based on ordinary least squares (OLS) algorithm	Granger and	
Ramanathan-C	one	and bias-corrected the results	Ramanathan (1984)	
Bayesian Model	BMA	Determining weights by probability distribution	Neuman (2003)	
Averaging	DIVITY	functions (PDFs)		
		Based on ordinary least squares (OLS) algorithm		
Multi-model	MMSE	and using the logic of bias reduction with respect	Krishnamurti et al.	
Super Ensemble	MINIGL	to individual member models along with variance	(2000)	
		reduction in simulation		

Table 4. The frequency (%) of individual members obtaining the best score for the performance metrics in the

validation period.

	NOF		NSE(sqrt)	PBias	PBiasFSV			
Model member	NSE	NSE(In)			5	20	mid	low
GR4J-NSE	17.2	0	0.8	11.2	13.8	7.8	2.9	3.9
GR4J-NSE(ln)	0.8	9.7	0.8	2.1	6.8	3.7	7.6	12.8
GR4J-NSE(sqrt)	5.5	1.3	16.4	3.7	5.7	3.7	10.4	4.4
GR4J-PBias	0.3	0	0	15.4	1.6	6	3.1	2.1
HMETS-NSE	20.1	0	1.6	11.5	12.5	11	4.4	4.2
HMETS-NSE(ln)	0.5	18.8	1.8	2.9	2.1	4.2	9.1	7.6
HMETS-NSE(sqrt)	4.4	3.1	17.8	4.7	4.4	11.7	8.4	3.1

HMETS-PBias	0	0	0	7	6.5	8.4	3.1	5
SIMHYD-NSE	7	0	1.8	4.4	1.6	9.7	4.7	5.2
SIMHYD-NSE(ln)	0.5	17.5	2.1	0.3	0.5	1.6	5.7	13.6
SIMHYD-NSE(sqrt)	2.3	2.3	7.8	1.8	0.8	1.6	7.3	8.9
SIMHYD-PBias	0	0	0	7	12.8	1.8	4.2	1
XAJ-NSE	26.6	2.1	5.2	7.3	9.7	13.3	5.7	3.4
XAJ-NSE(ln)	0.3	23.5	1.3	2.1	7.3	2.6	7.6	13.8
XAJ-NSE(sqrt)	13.6	21.7	42.6	2.6	2.3	8.1	12	7.8
XAJ-PBias	0.8	0	0	15.9	11.5	5	3.7	3.1

Table 5. Comparison of the multi-model combination and the best individual member for each of the 383 catchments in the validation period. Here, H4-NSE, H4-NSE(ln), H4-NSE(sqrt) and H4-PBias donate four hydrological models calibrated with a specified objective function, and H4C4 donates four hydrological models calibrated with four calibration strategies.

Acronym	NSE	NSE(ln)	NSE(sqrt)	PBias	PBiasFSV			
					5	20	mid	low
H4-NSE	70	11.2	45.2	10.7	14.1	13.8	4.4	8.4
H4-NSE(ln)	32.4	18.3	35.2	11.2	10.4	13.1	4.2	5.7
H4-NSE(sqrt)	60.1	17.8	56.4	11.7	13.3	12.5	7	6
H4-PBias	1.8	1	1.6	7.3	3.1	7.8	5	7.6
H4C4	71	17	55.4	12.3	20.4	13.6	8.4	8.4

Highlights:

- Four hydrological models calibrated with four objective functions are compared.
- The Granger Ramanathan average variant C (GRC) method performs the best.
- Using more than nine ensemble members does not further improve performance.
- Combinations of models and objective functions are better than the single model and objective.
- Averaging outperforms the ensemble members except in low-flow simulations.

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