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### RESEARCH ARTICLE

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#### Key Points:

- We designed 288 experiments from multiparameterization schemes of six physical processes to assess parameterization uncertainty of Noah‐MP
- Dominant physical processes for energy and water fluxes simulations over 10 regions in China were identified with sensitivity scores • Best scheme combinations for
- corresponding simulations were selected with multiple comparisons of the parameterization schemes

[Supporting Information:](http://dx.doi.org/10.1029/2019WR024814)

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## Assessment and Reduction of the Physical Parameterization Uncertainty for **Assessment and Reduction of<br>Parameterization Uncertainty<br>Noah-MP Land Surface Model Noah-MP Land Surface Model**<br>Yanjun Gan<sup>1[,](https://orcid.org/0000-0003-2573-3828)2</sup> **D**, Xin-Zhong Liang<sup>3,4</sup> **D**, Oingyun Duan<sup>5</sup> **D**, Fei Chen<sup>1,6</sup> **D**, Jianduo Li<sup>1</sup> **D**,

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Abstract The community Noah land surface model with multiparameterization options (Noah-MP) provides a plethora of model configurations with varying complexity for land surface modeling. The practical application of this model requires a basic understanding of the relative abilities of its various parameterization configurations in representing spatiotemporal variability and hydrologic connectivity. We designed an ensemble of 288 experiments from multiparameterization schemes of six physical processes to assess and reduce the structural uncertainty for land surface modeling over 10 hydrologic regions in China for the period 2001–2010. The observed latent heat (LH) was well reproduced by the ensemble. Meanwhile, most experiments underestimated sensible heat (SH) throughout the year and overestimated the cold season but underestimated the warm season terrestrial water storage anomaly (TWSA). The sensitive processes and best-performing schemes varied not only with regions but also among variables. The LH and SH were most sensitive to runoff-groundwater (RUN), surface heat exchange coefficient (SFC), and radiation transfer (RAD). The TWSA was dominated by RUN and RAD while largely influenced by soil moisture factor for stomatal resistance (BTR) and frozen soil permeability (INF) over some limited regions. By contrast, supercooled liquid water (FRZ) had little influence on all variables. Our optimization for individual variables produced high mean Taylor skill scores that ranged from 0.95–0.99 for LH, 0.82–0.99 for SH, and 0.63–0.95 for TWSA depending on regions. The simultaneous optimization made trade‐off among the three variables, which improved TWSA performance at the cost of reducing the skill for LH and SH over a few regions.

#### 1. Introduction

Land surface models (LSMs) play an important role in numerical weather prediction and climate projection, as they control the water, energy, and nutrient exchanges between the land surface and atmosphere (Dickinson et al., 2006; Gan et al., 2015; Liang et al., 2012; Pitman, 2003). They have evolved from simple bucket models representing water and energy balances (Manabe, 1969) to complex models representing an increasing number of interactions and feedbacks between physical, chemical, and biological processes (Bonan et al., 2011; Chen & Dudhia, 2001; Choi et al., 2013; Choi & Liang, 2010; Dai et al., 2003; Dickinson et al., 1986; Liang et al., 1994; Oleson et al., 2008; Sellers et al., 1997). The diversity of land surface modeling approaches motivates the development of unified modeling frameworks that provide multiple schemes for the same processes, such as the Noah land surface model with multiparameterization options (Noah‐MP; Niu et al., 2011; Yang et al., 2011), Joint UK Land Environment Simulator (JULES; Best et al., 2011; Clark et al., 2011), and Structure for Unifying Multiple Modeling Alternatives (SUMMA; Clark et al., 2015a, 2015b). Among them, Noah‐MP has received increasing attention due to its large improvement of the widely used baseline model Noah (Chen & Dudhia, 2001; Ek et al., 2003) and its coupling to the community Weather Research and Forecasting (WRF) model (Barlage et al., 2015), WRF‐Hydro model (Gochis et al., 2013), and National Water Model (NWM; Cosgrove et al., 2017).

The flexibility in the selection of different schemes under the same modeling framework accommodates a plethora of physics configurations with varying complexity. The total number of combinations of alternative schemes for the 10 processes of the original Noah‐MP is up to 4,608 (Gayler et al., 2014) and this number has been increasing due to the incorporation of new schemes for even more physical processes in the latest version. Noah‐MP has been evaluated at global scales (Yang, Niu, et al., 2011), regional scales (Cai et al., 2014; Chen et al., 2015; Ma et al., 2017; Niu et al., 2011; Park & Park, 2016; Xia et al., 2017; Zheng & Yang, 2016), basin scales (Cai et al., 2014; Cuntz et al., 2016; Mendoza et al., 2015), and site scales (Arsenault et al., 2018; Cai et al., 2016; Gao et al., 2015; Pilotto et al., 2015; Zhang et al., 2016; Zheng et al., 2015). However, most researchers used a single, subjective set of scheme combination mainly based on their own experience or previous studies. In reality, a scheme combination that performs in one situation may not be appropriate for another due to the substantial spatial and temporal heterogeneities in surface soil and vegetation characteristics and their associated physical processes (Clark et al., 2011; Gayler et al., 2014; Mendoza et al., 2015).

A systematic and rigorous intercomparison of the multiple parameterizations would help to identify the dominant processes and appropriate configurations for representing varying hydroclimate, soil, and vegetation conditions (Bai et al., 2009; Best et al., 2015; Henderson‐Sellers et al., 1993). This would further help to (1) reinforce our understanding of model behavior across different regions (Ma et al., 2017), (2) provide guidance for improving model physics (Wang et al., 2018), (3) conduct multiparameterization ensemble prediction (Zheng & Yang, 2016), and (4) perform parameter sensitivity analysis and optimization (Arsenault et al., 2018; Duan et al., 2017; Gan et al., 2014). Nevertheless, the intercomparison work is not only constrained by the computational cost of a large number of scheme combinations, but also with great uncertainty owing to the interactions among different processes.

Previous studies on Noah‐MP parameterization intercomparison were limited to a few sites, a few scheme combinations, or short‐term simulations due to the otherwise high computational cost of model simulations. Moreover, most research focused on the sensitivities of physical processes, whereas few tried to optimize the combinations of parameterization schemes. Besides, a systematic intercomparison of the Noah‐MP parameterization schemes across different hydrologic regions over the continental China domain has not been made. For example, Yang, Niu et al. (2011) conducted 36 ensemble experiments to explore the influences of soil moisture factor for stomatal resistance, runoff and groundwater, leaf dynamics, and stomatal resistance in simulating land surface fluxes over global 50 largest river basins for the period 1983–2006. They concluded that runoff and groundwater are predominant over the other processes in controlling globally averaged soil moisture and evapotranspiration and their relationship. Afterward, Hong et al. (2014) employed the microgenetic algorithm (Krishnakumar, 1990) to identify the best scheme combinations of Noah‐MP for evapotranspiration and runoff simulation over the Han River basin in South Korea for the period 2001–2003. They found that radiation transfer, surface exchange coefficient, and runoff and groundwater are the most important processes, but the scheme sets chosen to produce the most accurate simulations are very different between evapotranspiration and runoff. Gayler et al. (2014) designed 720 ensemble experiments to identify the most responsive processes for water and energy fluxes simulations during the 2009 vegetation period at two agricultural field sites with different soil and hydroclimate conditions in Southwest Germany. The authors observed that the way Noah‐MP responds to the alternative scheme options is quite different among output variables and research sites. Zhang et al. (2016) conducted 1,152 ensemble experiments for sensible and latent heat simulation in 2008 at the Dali site in Southwest China. They reported that stomatal resistance, soil moisture factor for stomatal resistance, runoff and groundwater, and surface exchange coefficient are the most important factors.

The main purpose of this paper is to assess and reduce the uncertainties associated with the physical parameterizations of Noah‐MP in simulating land surface fluxes over 10 large hydrologic regions in China with varying hydroclimate, soil, and vegetation conditions. We accomplish this by directly comparing the performances among different parameterization schemes and objectively analyzing their differences with statistical methods. Section 2 describes the Noah‐MP model, evaluation data, and analysis approach. Section 3 presents the results and discussion. Section 4 concludes our main findings.



### 2. Model Description, Evaluation Data, and Analysis Approach 2. Model Des<mark>cription</mark>, Evaluation Data, a<br>2.1. Noah‐MP Physical Parameterization Options

Noah‐MP is a new‐generation LSM enhanced from the Noah model through the incorporation of improved physics and multiple parameterization options for different land‐atmosphere interaction processes. The major advances in model physics and related theories can be found in Niu et al. (2011) and Yang et al. (2011). We adopted the Noah‐MP v1.6 and selected the control configuration for the following six processes as suggested by Yang, Niu et al. (2011), and Ma et al. (2017): (1) dynamic vegetation (Dickinson et al., 1998; Yang & Niu, 2003), (2) Ball‐Berry type canopy stomatal resistance scheme (Ball et al., 1987), (3) Canadian Land Surface Scheme (CLASS) ground snow surface albedo (Verseghy, 1991), (4) Jordan's scheme (Jordan, 1991) for partitioning precipitation into rainfall and snowfall, (5) Noah‐type lower boundary condition of soil temperature, and (6) semiimplicit snow/soil temperature time scheme. Table 1 lists the alternative parameterization options for other six processes to generate 288 scheme combinations for subsequent analyses. A brief description of the differences among these options follows:

- 1. Soil moisture factor  $\beta$  for stomatal resistance (BTR) has three schemes. The notable difference is that the CLM type (Oleson et al., 2004) shows a sharper and narrower range of variation with soil moisture than the Noah type (Chen & Dudhia, 2001) does, and the SSiB type (Xue et al., 1991) is even steeper than the CLM type.
- 2. Runoff and groundwater (RUN) have four schemes. The SIMGM and SIMTOP are based on TOPMODEL (i.e., TOPography‐based hydrological MODEL) to parameterize both surface and subsurface runoff as functions of water table depth, with a simple groundwater model for the former (Niu et al., 2007) and an equilibrium water table for the latter (Niu et al., 2005). The Schaake96 and BATS use free drainage concept for subsurface runoff, with an infiltration-excess-based surface runoff model for the former (Schaake et al., 1996) and a fourth‐power function of the top 2‐m soil wetness for the latter (Yang & Dickinson, 1996).
- 3. Surface heat exchange coefficient (SFC) has two schemes. The M‐O treats the effect of the roughness lengths with the zero-displacement height  $d_0$  (Brutsaert, 1982) while Chen97 accounts for the difference between roughness lengths for heat and momentum (Chen et al., 1997).
- 4. Frozen soil permeability (INF) has two schemes in the parameterization of soil hydraulic properties. NY06 defines the soil permeability using soil moisture (Niu & Yang, 2006) while Koren99 uses only the liquid water volume (Koren et al., 1999).
- 5. Supercooled liquid water (FRZ) in frozen soil has two schemes for the freezing-point depression equation. NY06 takes a more general form (Niu & Yang, 2006), while Koren99 takes a variant form with an extra term that accounts for the increased interface between soil particles and liquid water (Koren et al., 1999).
- 6. Radiation transfer (RAD) has three schemes to treat the canopy gap with regard to subgrid distributions of vegetation. Scheme 1 parameterizes gap probability as a function of solar zenith angle and the 3‐<sup>D</sup> structure of the vegetation canopy, scheme 2 assumes the gap probability to be zero, and scheme 3 sets the gap probability to one minus the green vegetation fraction (Niu & Yang, 2004).

#### 2.2. Model Input and Setup

The static input data for Noah‐MP were derived from various sources: (1) global multiresolution terrain elevation data 2010 (GMTED2010) 30‐s topography height, (2) United States Geological Survey (USGS) <sup>30</sup>‐s land use, (3) Food and Agriculture Organization (FAO) 30‐s soil texture, and (4) National Environmental Satellite, Data, and Information Service (NESDIS) 0.144‐degree monthly 5‐year climatological albedo and green vegetation fraction. We remapped these data onto the model grid using the Weather Research and Forecasting (WRF) model Preprocessing System (WPS) version 3.9.1 (Wang et al., 2017). The soil column was divided into four layers with thicknesses of 0.1, 0.3, 0.6, and 1.0 m from the top to the bottom.

We used the 3-hourly,  $0.1^{\circ} \times 0.1^{\circ}$  China Meteorological Forcing Dataset (CMFD) developed at the Institute of Tibetan Plateau Research, Chinese Academy of Sciences (He & Yang, 2011; Yang et al., 2010) to drive the Noah-MP. This data set includes the forcing fields of surface pressure, 2-m air temperature and specific humidity, 10‐m wind speed, downward shortwave radiation, downward longwave radiation, and

#### Table 1





Note. CLM = Community Land Model; SSiB = Simplified Simple Biosphere Model; BATS = Biosphere‐Atmosphere Transfer Scheme.

precipitation for the period 1979–2013. CMFD has been widely employed for land surface modeling over China (Chen et al., 2011; Leng et al., 2015; Liu & Xie, 2013; Xue et al., 2013; Zheng et al., 2017).

Our study area was over the entire China land, centered at  $35.0^{\circ}$ N and  $105.0^{\circ}$ E with 700 latitudinal  $\times$  400 longitudinal grids at an equal 0.1° spacing. Figure 1 illustrates the distributions of elevation, vegetation, and soil conditions, as well as the aridity index, which is defined as the ratio of mean annual precipitation to potential evapotranspiration. Table 2 summarizes the distinct characteristics of the 10 hydrologic regions of China.

To minimize the impact of uncertain initial condition on model performance in an efficient way, a two‐stage spin‐up was performed to provide different initial conditions for each of the 288 ensemble experiments. First, the 30‐year forcing data from 1 January 1981 to 1 January 2011 was cycled 3 times to drive Noah‐MP with the physical options as the EXP6 in Yang, Niu et al. (2011), and then the 20‐year forcing from 1 January 1981 to 1 January 2001 was applied in each of the 288 experiments to get equilibrium states. By using the final states of these spin-up experiments as initial conditions, 288 ensemble experiments were then integrated, respectively, for another 10-year period from 1 January 2001 to 31 December 2010, results of which were aggregated to monthly for subsequent analyses. All simulations for the spin‐up and ensemble experiments were run at a 1‐hr time interval.

#### 2.3. Evaluation Data and Metric

We used surface sensible heat (SH) and latent heat (LH) monthly data from the FLUXNET model tree ensemble (MTE) products by Max Planck Institute for Biogeochemistry, available on the global 0.5° grid for the period 1982–2011 (Jung et al., 2010, 2011). These products have been widely employed to evaluate land‐atmosphere energy exchanges for LSMs (Bonan et al., 2011; Ma et al., 2017; Xia et al., 2016a; Xia et al., 2016b) and climate models (Anav et al., 2013; Lawrence et al., 2012).

We also used terrestrial water storage anomaly (TWSA) monthly data from the Gravity Recovery and Climate Experiment (GRACE) satellite retrieval products, available on the global 1° grid for the period 2002–2017 (Landerer & Swenson, 2012; Tapley et al., 2004). There are three products from different processing centers, and we adopted their arithmetic mean to reduce measurement errors (Sakumura et al., 2014). This error reduction, however, comes with some signal loss, and hence we applied a gain factor to minimize the loss (Landerer & Swenson, 2012). GRACE data have been widely employed to understand the water cycle for large-scale hydrologic modeling (see a review by Güntner, 2008).

We interpolated the observational products onto our model grid by bilinear interpolation. They were used as the reference for model evaluation. In particular, we adopted Taylor skill score (Taylor, 2001) to quantify the differences between model simulations and observations:



Figure 1. The distributions of (a) elevation, (b) aridity index, (c) vegetation, and (d) soil conditions over 10 hydrologic regions of China.

$$
T = \frac{2(1+R)}{(\hat{\sigma} + 1/\hat{\sigma})^2} \tag{1}
$$

where R is the correlation coefficient and  $\hat{\sigma}$  is the ratio of simulated to observed standard deviation. The Taylor skill score ranges from zero to unity, and a higher score indicates a more accurate simulation.

For simultaneous optimization of SH, LH, and TWSA, we aggregated Taylor skill scores into a weighted mean as

$$
\overline{T} = \sum_{k=1}^{3} w_k T_k \tag{2}
$$

To improve the overall model performance, we assigned larger weights to the variables that were poorly simulated or with lower skill scores

$$
w_k = \frac{1 - T_k^{\max}}{\sum_{k=1}^3 (1 - T_k^{\max})}
$$
(3)

where  $T_k^{\max}$  is the maximum Taylor skill score of all ensemble experiments for the kth evaluation variable 3  $1.$ 

and 
$$
\sum_{k=1}^{\infty} w_k =
$$

#### 2.4. Analysis Approach

To objectively examine the differences among the large ensemble of model physical parameterization configurations, a sensitivity score is required. Assume that there are m physical processes (i.e., experimental factors, here  $m = 6$ ) with each process having a different number of parameterization schemes (i.e., treatments). The mean objective function value (i.e., treatment mean) of the jth scheme  $(j = 1, 2, \dots)$  of the









ith process  $(i = 1, 2, \cdots, m)$  can be represented by  $\overline{Y}_j^{(i)}$ . We defined an index to quantify the sensitivity of these physical processes as

$$
S_i = \frac{\Delta \overline{Y}^{(i)}}{\max\left\{\Delta \overline{Y}^{(1)}, \Delta \overline{Y}^{(2)}, \cdots, \Delta \overline{Y}^{(m)}\right\}}
$$
(4)

where  $\Delta\overline{Y}^{(i)}=\overline{Y}^{(i)}_{\max}-\overline{Y}^{(i)}_{\min}$  is the difference between the largest and the smallest treatment means of the *i*th process.

To test differences in all possible pairs of means, multiple comparison procedures are often used (Bretz et al., 2010). Suppose that a physical process A has a parameterization schemes (e.g., the physical process RUN has four parameterization schemes) and  $\overline{Y}_1, \overline{Y}_2, \dots, \overline{Y}_a$  are the mean objective function values (i.e., treatment means) of corresponding schemes (i.e., treatments). We adopted the test procedure of Tukey (1949), which has been highly recommended for its computational simplicity and statistical features (Benjamini, 2010). It makes use of the distribution of the studentized range statistic

$$
q = \frac{\overline{Y}_{\text{max}} - \overline{Y}_{\text{min}}}{\sqrt{\frac{MS_E}{n}}} = \frac{\overline{Y}_{\text{max}} - \overline{Y}_{\text{min}}}{\sqrt{\frac{SS_E}{n(N-a)}}}
$$
(5)

where  $\overline{Y}_{\text{max}}$  is the largest treatment mean,  $\overline{Y}_{\text{min}}$  is the smallest treatment mean, *n* is the sample size of each treatment, N is the total sample size of all treatments,  $MS_E$  is the mean square error,  $SS_E = \sum_{i=1}^{a}$  $_{p=1}$  $\sum_{i=1}^{n}$  $q=1$ 

 $(Y_{p,q}-\overline{Y}_p)^2$  is the sum of the square error, and  $N-a$  is the degree of freedom associated with  $MS_E$ . Tukey's test declares that the two means are significantly different at the significance level  $\alpha$  $(0 \leq \alpha \leq 1)$  if

$$
|\overline{Y}_k - \overline{Y}_l| > q_\alpha(a, N - a) \sqrt{\frac{MS_E}{n}}
$$
\n(6)

where  $q_{\alpha}(a, N-a)$  can be obtained from the critical value table of the studentized range distribution.

Tukey's test is based on the assumptions that the samples are mutually independent and normally distributed with equal variances. We checked the normality by Kolmogorov‐Smirnov test (Massey, 1951) and the homogeneity by Levene's test (Levene, 1960). When these two assumptions were violated, we applied the transformation of Box and Cox (1964) to normalize the data with constant variance. We set  $\alpha$  to 0.05 and therefore distinguished the categories of the parameterization schemes by Tukey's test at 95% confidence level.

#### 3. Results and Discussion

#### 3.1. Evaluation of the Ensemble Experiments

We evaluated SH, LH, and TWSA from the 288 experiments against observations. The Noah‐MP‐simulated terrestrial water storage consists of canopy‐intercepted water, snow water equivalent, total soil water depth, and groundwater storage (Ma et al., 2017). These components shall be evaluated separately to identify the specific sources of model deficiencies (Xia et al., 2017). However, we focused on comparing total TWSA due to the lack of high-quality observations for individual components in China. Following Xia et al. (2016b), Xia et al. (2017), and Ma et al. (2017), we excluded the water storage in lakes and rivers, which are not modeled in Noah‐MP. We then calculated monthly TWSA relative to the same baseline time‐average (i.e., 2004–2009) as GRACE‐derived TWSA for the period 2003–2010. Finally, we used the same regional mask at the model spatial resolution to derive regional averages of the observed and simulated monthly SH, LH, and TWSA over all the hydrologic regions.

Figure 2 shows the multiyear mean annual cycle of spatially averaged SH, LH, and TWSA for the ensemble experiments and observations over 10 hydrologic regions. The boxplots present the uncertainty ranges by five statistics (i.e., the minimum, first quartile, median, third quartile, and the maximum) of the ensemble experiments. The ensemble experiments basically captured the annual cycle of observations with relatively wide uncertainty ranges in the warm season. This indicates that the performance differences of the selected schemes are more distinct in the warm season.

The seasonal variability of SH was largest over region 10, followed by regions 1–4, medium over regions 5 and 9, and smallest over regions 6–8. This decreasing trend from cold, arid to hot, humid regions is consistent with the finding of Zhou and Huang (2014), and it is attributable to the impacts of the land-air temperature difference and surface wind speed. Most experiments underestimated SH in all seasons over all hydrologic regions. The most obvious underestimation occurred over the most humid regions 6–8 in all seasons and over other regions in the warm rainy season. Pilotto et al. (2015) also found that the underestimation of SH is more significant in the rainy season than in the dry season due to the larger cold bias of soil temperature. Ma et al. (2017) found that Noah‐MP underestimates SH throughout the year over most arid regions and greatly underestimates SH in the early growing season over the humid regions. They demonstrated that the underestimation can be alleviated by using a leaf area index climatology prescribed for each land use type.

The seasonal variability of LH was largest over regions 1–3 and 5–8, medium over regions 4 and 9, and smallest over region 10. This decreasing trend from humid to arid regions shows strong latitudinal gradients corresponding to climate patterns in China and is in line with the findings of Yao et al. (2013) and Ma et al. (2019). The ensemble range of LH generally contained observations in most seasons but underestimated LH in winter over all hydrologic regions. This is likely related to the model's failure to reproduce direct root water uptake from the saturated zone, which is a dominant process controlling evapotranspiration of the phreatophytes (Wang et al., 2018; Zheng et al., 2015). In addition, LH underestimation can also be detected in summer over regions 1–3 and 5 and in spring and early summer over regions 7, 8, and 10.



Figure 2. Multiyear mean annual cycle of spatially averaged (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions, where box plots are results simulated by 288 ensemble experiments and red circles are observations.

It could be attributed to the dry biases of soil liquid water content in the topsoil (Gao et al., 2015). By contrast, LH was overestimated in summer over regions 6–9. This LH overestimation compensates the concurrent large SH underestimation.

The seasonal variability of TWSA was largest over regions 8 and 9, followed by regions 5–7, medium over regions 1–4, and smallest over region 10. The regional differences agree well with the spatial patterns of precipitation, which are mainly determined by the East Asian monsoon system and the topographic effects (Zhai et al., 2005). Additionally, regional characteristics such as topography, soil, and vegetation conditions also influence TWSA by partitioning water storage in soil and river systems. The ensemble experiments overestimated TWSA in the cold season but underestimated it in the warm season over most regions. One exception was for the regions 2, 3, and 5, where TWSA was underestimated in the cold season but overestimated in the warm season. The large uncertainty ranges for overestimation or underestimation of TWSA are mainly

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Figure 3. Taylor skill score for (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions simulated by 288 ensemble experiments. Orange bars are Taylor skill scores larger than the ensemble mean, while blue bars are those smaller than the ensemble mean.

due to the variability of different scheme combinations in simulating soil moisture, runoff, and groundwater. Besides, snow water equivalent is an important water storage term for the cold regions of China. It not only influences the estimates of terrestrial water storage but also affects total runoff and soil moisture via snowmelt (Xia et al., 2017). The large uncertainty ranges in the cold season for the cold regions may be related to the variability of different scheme combinations for the simulation of snowpack-snowmelt and soil freezethaw processes, which are controlled by ground heat flux (Yang, Niu, et al., 2011).

#### 3.2. Uncertainty Analysis of the Ensemble Experiments

Figure 3 compares the performances of the ensemble experiments over 10 hydrologic regions using Taylor skill score. The SH scores ranged between 0.55 and 0.99, with the mean decreasing from 0.97 over regions 4 and 10, 0.90–0.92 over regions 1–3 and 9, to 0.81–0.85 over regions 5–8. The LH scores ranged between 0.81 and 0.99, with the mean of 0.95–0.98 over all regions, except for a reduction to 0.93 over region 8. Thus, the ensemble can well reproduce observed SH and LH variations over all regions. By contrast, TWSA had worse scores, ranging between 0.27 and 0.96, with the mean decreasing from 0.90 over region 1, 0.80–0.84 over regions 2, 5, 7, and 8, 0.55–0.71 over regions 3, 4, 9, and 10, to 0.43 over region 6.

Figure 4 compares Taylor skill scores among different parameterization schemes for each of the six processes. The SH scores exhibited similar behaviors in the SFC process over regions 1–6 and 9, where M‐<sup>O</sup>

100



Figure 4. The relationship between parameterization scheme and Taylor skill score for (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions simulated by 288 ensemble experiments, where numbers with different colors represent parameterization schemes and dashed lines are the mean Taylor skill scores of all ensemble experiments. BTR = soil moisture factor for stomatal resistance; RUN = runoff-groundwater; SFC = surface heat exchange coefficient; INF = frozen soil permeability; FRZ = supercooled liquid water; RAD = radiation transfer.

scheme performed better than Chen97 scheme. Conversely, Chen97 outperformed M-O over regions 7, 8, and 10. Since M-O using zero-displacement height produces greater SH than Chen97 (Yang, Niu, et al., 2011), it can partly alleviate underestimation, and conversely, Chen97 can reduce overestimation. The SH scores over regions 1–6 also depended on the RAD process, where setting gap to (1–fveg) generally outperformed f(3D, cosz) and zero. This is reasonable since the RAD process controls the radiation transfer through the vegetation canopy with regard to subgrid distributions of vegetation (Niu et al., 2011). The (1−fveg) scheme yields the largest undercanopy solar radiation, while the zero scheme gives the smallest. Moreover, substantial SH score differences existed between the parameterization schemes of the RUN process over regions 1, 4–6, and 8–10, where the best schemes varied a lot with regions. Among the four schemes, SIMTOP produces the wettest soil and greatest evapotranspiration while BATS produces the driest soil and smallest evapotranspiration (Yang, Niu, et al., 2011).

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For LH simulation, substantial score differences occurred among the four schemes in the RUN process, where BATS performed the best over regions 4, 6, 7, 9, and 10 but worst over other regions by underestimation. Therefore, the RUN process influences the partitioning of available energy into SH and LH through soil moisture (Xia et al., 2014). The RAD process dominated the model performance over regions 1–5, where setting gap to (1−fveg) outperformed the other two schemes over region 4 but performed worse over the other four regions. Regions with smaller green vegetation fraction have a larger between‐canopy gap, exposing more understory vegetation or snow surface to solar radiation and thus producing larger LH by (1−fveg) scheme. Substantial differences were also simulated over regions 4 and 6–10 by the SFC process, where Chen97 outperformed M‐O. This occurred because M‐O produces smaller LH to balance larger SH by using zero‐displacement height (Yang, Niu, et al., 2011). Furthermore, large differences were produced over regions 2–6, 9, and 10 by the INF process, where Koren99 outperformed NY06. The NY06 produces higher permeability in frozen soil and thus more soil water and less surface runoff than Koren99 (Niu & Yang, 2006). Therefore, the INF process influences LH simulation through soil moisture over the regions with frozen soil.

The TWSA score differences were similar over all regions between the schemes in the INF process, where NY06 was generally better than Koren99. The INF process also influenced the water storage, where NY06 reduced TWSA overestimation in the cold season. Substantial score differences were identified over all regions with the RUN process, where BATS performed the best over regions 2 and 7 whereas the worst over other regions. The RUN process directly influences the partitioning of water storage into the soil and river systems (Zheng et al., 2017). Moreover, substantial differences were observed in the SFC process over region 9 where Chen97 outperformed M‐O, and in the RAD process over regions 1, 3–5, and 8 where setting gap to (1−fveg) performed worse than the other two schemes. Chen97 produces more LH and thus less soil moisture than M‐O, whereas (1−fveg) produces more LH and thus less soil moisture than the other two schemes. Hence, the SFC and RAD processes indirectly affect TWSA through LH.

#### 3.3. Sensitivity Analysis of the Physical Processes

Figure 5 compares the sensitivity scores, based on the average Taylor skill score over all experiments using the same scheme, for SH, LH, and TWSA over 10 hydrologic regions. The sensitivity categories of the physical processes agreed fairly well with the performance differences of the parameterization schemes as identified in Figure 4. However, the sensitivity scores can also identify the insensitive or sensitive processes that are hard to be distinguished by direct comparison of the scheme performances. For instance, the INF process has two schemes that produced significant differences for SH and LH over region 4 (Figure 4) but was insensitive as compared to other processes (Figure 5). This is because only a few experiments using NY06 resulted in worse performance than all others using Koren99, and their performance differences were statistically insignificant. Overall, the number of sensitive processes varied from one to three over different regions, and the FRZ process was insensitive over all regions since its two schemes exhibited nonsignificant performance difference.

For SH simulation, the RUN, SFC, and RAD processes dominated skill score differences, whereas the BTR, INF, and FRZ processes had little influence. SFC was the most sensitive process except for regions 5 and 8, where, respectively, RAD and RUN took over. This agrees with Yang, Niu et al. (2011) in that SFC is the most important factor for SH. The importance of SFC in controlling the total surface energy flux to the atmosphere (i.e., SH and LH) has been shown by many other studies (Chen & Zhang, 2009; Gao et al., 2015; Niu et al., 2011).

For LH simulation, the RUN, SFC, and RAD processes dominated skill score differences over most regions, except that the BTR process also had pronounced influence over regions 1 and 4. On the other hand, the influences of the INF and FRZ processes were negligible. Our result is in general accordance with Hong et al. (2014), who found the sensitivity order for evapotranspiration simulation as RAD > SFC > RUN >  $BTR > INF > F R Z$ .

For TWSA simulation, the RUN and RAD processes dominated skill score differences over almost all regions, whereas the SFC and FRZ processes had little influence. Meanwhile, BTR was sensitive over region 2 and INF was sensitive over regions 1 and 2. Our result is similar to Hong et al. (2014), who found the sensitivity order for runoff simulation as RUN > SFC > RAD > INF > BTR > FRZ. The difference is that



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Figure 5. Sensitivity scores of different physical processes for (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions simulated by 288 ensemble experiments. BTR = soil moisture factor for stomatal resistance; RUN = runoff-groundwater; SFC = surface heat exchange coefficient;  $INF = frozen soil permeability; FRZ = supercooled liquid water; RAD = radiation transfer.$ 

we found SFC to be less sensitive than RAD over almost all regions, while INF was more sensitive than RAD over the regions with frozen soil (regions 1, 2, and 10).

#### 3.4. Combinatorial Optimization of the Parameterization Schemes

Based on the scheme categories from multiple comparisons (supporting information Figures S1–S4), we selected the best schemes for optimization of SH, LH, and TWSA independently and simultaneously in each of the 10 hydrologic regions (Table 3). Although the best schemes so selected were generally consistent with those from direct performance comparison (Figure 4), multiple comparisons provide a clearer way of distinguishing parameterization schemes. The best schemes varied with regions of characteristic hydroclimate, soil, and vegetation conditions. Depending on regions, the number of best experiments varied from <sup>2</sup>–96 for SH, 2–36 for LH, 4–64 for TWSA, and 2–16 for their simultaneous optimization. The best schemes also varied with variables, especially in the most sensitive processes. For instance, the best RUN schemes were Schaake96 and BATS for SH but SIMGM and SIMTOP for LH over region 1. Thus, optimizing a



Table 3

Best Schemes Based on the Multiple Comparisons of Different Physical Processes for Different Regions and Variables



Note. SH = sensible heat; LH = latent heat; TWSA = terrestrial water storage anomaly; BTR = soil moisture factor for stomatal resistance; RUN = runoff-groundwater; SFC = surface heat exchange coefficient; INF = frozen soil permeability; FRZ = supercooled liquid water; RAD = radiation transfer.

> single variable can sometimes degrade the skill in simulating other variables (Hong et al., 2014). Overall, the best schemes for the simultaneous optimization of SH, LH, and TWSA were more consistent with those for the independent optimization of TWSA because a larger weight was assigned to TWSA than SH and LH. However, the best schemes for SH and LH were also so identified for simultaneous optimization of the three variables even though they were not optimal for TWSA, that is, the Noah scheme in the BTR process over regions 6, the SIMTOP scheme in the RUN process over region 8, and the NY06 scheme in the INF process over regions 8. On the other hand, the worst schemes for SH and/or LH were not identified as the best schemes for simultaneous optimization even if they were optimal for TWSA, that is, the Chen97 scheme in the SFC process over region 5, the M‐O scheme in the SFC process over region 8, the NY06 scheme in the INF process over region 5, and the f(3D, cosz) scheme in the RAD process over regions 1, 3, and 8. The outcome can be explained by the fact that the performance differences between those and other schemes of the same process were relatively less obvious for TWSA than for SH and/or LH.



Figure 6. Taylor diagrams of the best experiments for the simulation of sensible heat (first column, a, d, g, and j), latent heat (second column, b, e, h, and k), and terrestrial water storage anomaly (third column, c, f, i, and l) based on independent optimization of sensible heat (first row, a--c), latent heat (second row, d--f), and terrestrial water storage anomaly (third row, g--i) and simultaneous optimization of all three variables (fourth row, j--l). Gray solid lines represent the Taylor skill score contours. SH = sensible heat; LH = latent heat; TWSA = terrestrial water storage anomaly.

AGU<br>100



Figure 7. Multiyear mean annual cycle of spatially averaged (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions, where gray bands are results simulated by 288 ensemble experiments, blue bands are results simulated by the best experiments of independent optimization, green bands are results simulated by the best experiments of simultaneous optimization, and red circles are observations.

Figure 6 presents the Taylor diagrams of the simulations by the best parameterization scheme combinations (i.e., best experiments) based on independent SH, LH, and TWSA optimization and their simultaneous optimization as shown in Table 3. The best experiments always had larger Taylor skill scores for LH than SH and TWSA, regardless which optimization was used. The independent optimization of one variable reduced the scores of other variables. For example, the SH optimization (Figure 6a) reduced the scores for LH (Figure 6b) and TWSA (Figure 6c) when comparing with LH optimization (Figure 6e) and TWSA optimization (Figure 6i), respectively. The simultaneous optimization allowed tradeoffs among all variables and produced overall more reasonable results (Figures 6j–6l), although it inevitably reduced the scores over some regions for some variables. The score reduction was much obvious for SH over regions 3, 6, and 9 (comparing Figure 6a with Figure 6j), for LH over regions 4, 9, and 10 (comparing Figure 6e with Figure 6k), and for TWSA over region 8 (comparing Figure 6i with Figure 6l).



Figure 8. Mean Taylor skill scores for (a) sensible heat, (b) latent heat, and (c) terrestrial water storage anomaly over 10 hydrologic regions, where red lines are results simulated by 288 ensemble experiments, blue lines are results simulated by the best experiments of independent optimization, and green lines are results simulated by the best experiments of simultaneous optimization.

#### 3.5. Comparison Between the Ensemble and Best Experiments

Figure 7 compares multiyear mean annual cycles of SH, LH, and TWSA averaged over each of the 10 hydrologic regions from all 288 experiments (i.e., ensemble experiments) and those using the best parameterization scheme combinations (i.e., best experiments) based on independent and simultaneous optimizations. The uncertainty ranges of the best experiments were much narrower and closer to observations than those of the ensemble experiments. The result based on the simultaneous optimization agreed better with that from TWSA‐independent optimization giving its larger weight than SH and LH. The optimized Noah‐MP can better capture the overall water and energy cycles, including both timing and magnitude. Nonetheless, there were still large SH underestimations over the most humid regions 6–8, which are related to cold soil temperature biases (Pilotto et al., 2015) and so unable to be reduced through the optimization of the existing parameterizations. Meanwhile, the relatively large LH bias over the highly irrigated cropland region 5 is likely due to the use of leaf dynamics in Noah‐MP, which may capture crop growth under rainfed but not irrigated conditions (Cai, Yang, David, et al., 2014).

Figure 8 compares the mean Taylor skill scores of SH, LH, and TWSA for ensemble experiments and best experiments based on independent and simultaneous optimizations. The score gain was the largest from TWSA optimization, about 0.2 (46%) over region 6, 0.16–0.18 (24–32%) over regions 3, 9, and 10, 0.07–0.12 (10–15%) over regions 4, 5, 7, and 8, and 0.05 (6%) over regions 1 and 2. The gain from SH optimization was about 0.06–0.1 (7–12%) over regions 5–7, 0.05 (5%) over regions 1–3 and 9, and less than 0.02 (3%) over other regions. Although the gain from LH optimization was not significant (less than 0.03 or 3%), its score was already larger than SH and TWSA. The score from simultaneous optimization agreed well with that from TWSA optimization over all regions. Because of the tradeoff, the simultaneous optimization reduced the SH score respectively by 0.16 (18%), 0.14 (17%), and 0.07 (7%) over regions 3, 6, and 9, reduced the LH score respectively by  $0.02 \ (2\%)$ ,  $0.02 \ (1\%)$ , and  $0.04 \ (4\%)$  over regions 4, 9, and 10, and reduced the TWSA score by 0.03 (4%) over region 8.

The low discrepancy of SH and LH from observations implies that the surface energy budget was well reproduced by the best parameterization combinations. The relatively large TWSA discrepancy is attributable to model biases in soil moisture, groundwater, and snow water equivalent. These biases are likely related to the model assumption of evenly distributed soil texture (Wang et al., 2018), which could be improved by considering vertical heterogeneity in soil layers (Gao et al., 2015) and more so by incorporating three‐dimensional subgrid variability (Choi et al., 2007). The Noah-MP's disagreement with GRACE observations may be partly due to its lack of lake water storage (Ma et al., 2017). In addition, Noah‐MP simulates only the natural part of TWSA without considering anthropogenic impacts such as irrigation and reservoir regulation, which were detected by GRACE (Cai, Yang, David, et al., 2014; Ma et al., 2017). Furthermore, GRACE data contain measurement, aliasing, and signal leakage errors that can also lead to the disagreement (Güntner, 2008; Seo et al., 2006). Obviously, the overall performance of any LSM, as evaluated standalone, is highly dependent on the quality of the forcing data, especially precipitation and radiation, which play an essential role in surface flux exchanges through impacts on topsoil temperature and moisture (Gao et al., 2015). The model discrepancies from the observational reference may, therefore, be a result of the uncertainties in the reference itself as well as the errors in the forcing data, which also account for the nonclosure of the surface water and energy budgets. For example, the FLUXNET MTE products have an underestimated interannual variability because some explanatory variables that used to train the MTE were assumed static over years (Jung et al., 2011). Nonetheless, some parameterization schemes and/or parameters have considerable impacts on model performance and can be tuned to better represent the regional hydroclimatic regimes and watershed properties (Gan et al., 2014, 2018). Our analysis above has further demonstrated how to identify sensitive processes and best parameterizations for a specific LSM.

#### 4. Summary and Conclusions

We conducted sensitivity and uncertainty analyses on the community LSM, Noah-MP, to identify the most responsive processes and the best parameterization combinations for simulating SH, LH, and TWSA over 10 hydrologic regions in China. For this, we designed and conducted an ensemble of 288 parameterization experiments, combining six physical processes (BTR, RUN, SFC, INF, FRZ, and RAD) each with multiple alternative schemes. We used Taylor skill score to quantify the model performance. The ensemble generally captured the observed seasonal variability of surface energy and water budgets. The model simulated LH realistically, with scores ranging from 0.81–0.99 among regions, underestimated SH systematically, with scores between 0.55 and 0.99, and overestimated (underestimated) TWSA in the cold (warm) season over most regions, with scores reduced to 0.27–0.96. Direct comparison of these scores allows us to detect significant performance differences among alternative parameterization schemes in terms of specific processes.

However, performance differences among various schemes across multiple processes were difficult to be distinguished by direct comparison. Sensitivity scores based on the difference between the largest and smallest mean Taylor skill scores were able to identify the relative degrees of sensitivity across all physical processes. We found that the process sensitivities were region-specific because the performances of different parameterization schemes were depended on regional characteristics such as hydroclimate, soil, and vegetation conditions. In particular, the RUN, SFC, and RAD processes were most sensitive for SH and LH over almost all regions. By contrast, the TWSA was dominated by the RUN and RAD processes while largely influenced by the BTR and INF processes over some limited regions. On the other hand, the FRZ process was relatively insensitive over all regions for all variables.

We further used Tukey's test to identify the best parameterization schemes by multiple comparisons of the mean Taylor skill scores for different schemes of the same process. The independent optimization of individual variables improved the mean scores by 0.6–12.1% for SH, 0.1–3.1% for LH, and 5.4–45.5% for TWSA, comparing with those of ensemble experiments. No single scheme combination performed well over all regions or all variables. The best scheme combination from one region may perform poorly in other regions, and improving the skill for one variable may reduce the score for other variables. As such, the simultaneous optimization made tradeoffs among all variables, which generally reduced the skill enhancement from independent optimization, but still improved the overall model performance over the ensemble. The score gains were <sup>−</sup>12.1–9.5% for SH, <sup>−</sup>2.6–3.0% for LH, and 5.6–45.5% for TWSA, comparing with those of the ensemble mean.

Although the sensitive physical processes and the best parameterization schemes varied with regions and variables, our systematic analyses allow us to recommend the best Noah‐MP configurations for simulating surface water and energy fluxes over China as follows—process (scheme): RUN(4), SFC(1), RAD(3), INF(2), BTR(1), FRZ(2) for SH; RUN(3), SFC(2), RAD(2), INF(2), BTR(1, 2, 3), FRZ(2) for LH; RUN(2), SFC(2), RAD(2), INF(1), BTR(3), FRZ(2) for TWSA; and RUN(2), SFC(2), RAD(2), INF(1), BTR(3), FRZ(2) for their joint.

Caution must be taken for our conclusion and recommendation above. The best configurations may not be good at modeling extremes such as drought and flood, since our emphasis was placed on seasonal rather than interannual variability of the land surface fluxes. We have focused on the model structural uncertainty that arises from alternative parameterization schemes of the selected physical processes, which is only one of the many sources of uncertainty in LSMs (Nearing et al., 2016). We have not tuned specific parameters in these schemes but taken their default values, which are not universal. Some key parameters should be tuned to improve each scheme's performance, especially considering regional surface characteristics (Cuntz et al., 2016; Mendoza et al., 2015). Besides, data uncertainties from the forcing conditions (Xia et al., 2005), soil

textures (Zheng & Yang, 2016), and vegetation variations (Li et al., 2018) can affect model skill scores. Data sets from different sources need to be evaluated and compared to increase our confidence in model simulations. Some significant physics such as subgrid variability (Choi et al., 2007), crop dynamics (Bonan & Doney, 2018), and lake dynamics (MacKay et al., 2009) are still missing in Noah‐MP. Future improvement may include these physics to account for lateral flow, rhizosphere effect, dynamic crop growth, surface water storage, and human‐induced water use. Nonetheless, our study offers not only a systematic approach for model structural sensitivity and uncertainty analyses but also an optimized set of physics configurations from the existing parameterizations, facilitating further model improvement.

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observation‐based monthly sensible heat and latent heat products are available at [https://www.bgc](https://www.bgc-jena.mpg.de/geodb/projects/Home.php)‐jena.mpg.de/ [geodb/projects/Home.php](https://www.bgc-jena.mpg.de/geodb/projects/Home.php), and the global GRACE‐derived terrestrial water storage anomaly products are available at [http://grace.jpl.nasa.gov.](http://grace.jpl.nasa.gov)

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