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Revision notes: We would like to thank the editor and reviewers for the valuable and comments. which were very helpful for the further improvement of the manuscript. We have looked through each comment the editor and reviewers raised and responded and incorporate it in the revised manuscript. The following is the detailed response:

### **Reviewer #1:**

The manuscript entitled "Global Surface Water Stable Isotope Dataset" effectively compiles stable isotope data from surface waters around the world, a first and unique dataset that is important for advancing hydrology and meteorology research. Based on my many years of work in the field of isotope hydrology, I believe this is a fundamental and important piece of work. This work will inevitably greatly promote the global sharing of data in the field of isotope hydrology and facilitate the coordinated observation of global surface water isotopes.

A sincere suggestion: the authors should consider inviting more international colleagues to participate in similar global studies. In fact, I have been following the achievements of the author's research group in recent years (which are very outstanding). I believe that globally collaborative research would be very beneficial for the authors to increase the impact of their articles, and would also better promote data sharing and global coordinated observation.

After a thorough review of the data,I am convinced that the quality control measures for the stable isotope data are rigorous and I wholeheartedly support its publication, but the authors still need to address the following questions before publication,I feel that such an excellent paper deserves better expression.

Response: Thank you for your support and recognition of the importance of your comments in improving the quality of our manuscript. Based on your suggestions, we have thoroughly reviewed and revised the content of the manuscript, removing non-essential repetition and making the content more concise and clear.

### Major comments:

1. The introduction is well written. However, the author needs to add some research progress on stable isotope datasets for surface water and how they compare.

Response: Thanks to your suggestion, we have added relevant research advances to the introduction, which is revised below:

Many academics worldwide have studied the stable isotope composition of surface water, Scholars around the world for surface water stable isotope research has achieved many results, a researcher using the U.S. river water stable isotope data, mapped the isotope distribution of U.S. river water, and use the model to analyze the U.S. river water isotope changes (Bowen et al., 2011; Dutton et al., 2005).

- Bowen, G.J., Kennedy, C.D., Liu, Z., Stalker, J., 2011. Water balance model for mean annual hydrogen and oxygen isotope distributions in surface waters of the contiguous United States. J. Geophys. Res. 116, G04011. https://doi.org/10.1029/2010JG001581
- Dutton, A., Wilkinson, B.H., Welker, J.M., Bowen, G.J., Lohmann, K.C., 2005.
  Spatial distribution and seasonal variation in18 O/16 O of modern precipitation and river water across the conterminous USA. Hydrological Processes 19, 4121 4146. https://doi.org/10.1002/hyp.5876

2. Section 3.3 The predictors used here are not independent, e.g. evapotranspiration is influenced by parameters such as temperature and wind speed. Does this possible interdependence affect the results and conclusions?

Response: Random forest regression models can improve the accuracy and robustness of predictions by constructing multiple decision trees and averaging their results. In addition, random forest regression models are commonly used for prediction and classification. In this study, we used a random forest regression model to assess the importance of key meteorological variables on precipitation stable isotopes. Therefore, multicollinearity between variables is not a serious problem. A better practice for random forest regression models is to directly assess model performance and variable contributions through cross-validation and feature importance assessment (Vystavna et al., 2021).

From the smaller Root Mean Square Error (RMSE) and Mean Absolute Error (MAE), it can be seen that  $\delta^{18}$ O has a better prediction performance, while  $\delta^{2}$ H has higher RMSE and MAE values (Table S1). This is mainly due to the larger numerical range and volume of  $\delta^{2}$ H, on the other hand, these values are located in a reasonable range according to the existing studies on the prediction of stable isotopes in surface water. Therefore, we can consider the assessment of the importance of meteorological variables used in this study for the assessment of stable isotopes in surface water as reasonable and accurate.

| Variant           | RMSE  | MAE   |
|-------------------|-------|-------|
| $\delta^2 H$      | 12.87 | 10.02 |
| δ <sup>18</sup> Ο | 3.23  | 0.89  |

 Table S1 Random Forest Model Assessment Indicators

Vystavna, Y., Harjung, A., Monteiro, L.R., Matiatos, I., Wassenaar, L.I., 2021. Stable isotopes in global lakes integrate catchment and climatic controls on evaporation. Nat Commun 12, 7224. https://doi.org/10.1038/s41467-021-27569-x

# 3. Section 3.4 This section should highlight the applicability of the surface water stable isotope dataset, comparing it to current research and emphasizing the scientific value of the data.

Response: Thank you for your suggestions, and we have made significant adjustments to this paragraph based on the suggestions of two reviewers. We have shifted the focus to a discussion of the correlation between the surface water isotopes  $\delta^2$ H and  $\delta^{18}$ O, which helps us to better understand the role of stable isotopes in surface water as indicators of climate change. Below is the revised content:

### Global surface water $\delta^2 H$ and $\delta^{18} O$ correlations

Here, we fit  $\delta^2$ H and  $\delta$ 18O to surface waters in six climatic zones, the results indicated a strong correlation between  $\delta^2$ H and  $\delta^{18}$ O across six various climate zones (Fig. 6). The relationship between  $\delta^2$ H and  $\delta^{18}$ O for global surface water is  $\delta^2$ H = 7.92 $\delta^{18}$ O + 7.80 (R<sup>2</sup> = 0.98), which is closer to the intercept and slope of the global

meteoric water line (GMWL:  $\delta^2 H = 8\delta^{18}O + 10$ ), and this confirms once again that the source of recharge of global surface water is precipitation. However, the fitted lines of  $\delta^2 H$  and  $\delta^{18}O$  for surface water were significantly different in different climatic zones (Fig. 6), and the fitted lines of  $\delta^2 H$  and  $\delta^{18}O$  exhibited the lowest intercept and slope under arid climate ( $\delta^2 H = 7.50 \ \delta^{18}O + 3.30$ ,  $R^2 = 0.98$ ), which also suggests that under arid climate, the surface water experienced significant evapotranspiration, which led to the isotopic enrichment of surface water,  $\delta^2 H$  and  $\delta^{18}O$  values were higher compared to other climatic zones. In the coldest polar climate zone, the fitted line of  $\delta^2 H$  and  $\delta^{18}O$  is  $\delta^2 H = 5.57\delta^{18}O + 17.18$  (R<sup>2</sup>=0.95), and the higher slope and intercept indicate that under the influence of the cold climate, the surface water undergoes little evaporation, and the presence of surface water may be in the form of snow and ice, resulting in significantly lower values of  $\delta^2 H$  and  $\delta^{18}O$  compared to the other climate zones.



Figure 6 Relationship between  $\delta^2$ H and  $\delta^{18}$ O in different climatic zones.

### 4. Section 3.4 Recognize any limitations in your study that may affect the interpretation of the results.

Response: Thanks to your suggestion, we have revised section 3.4, which is shown in the previous section.

5. Some references in the manuscript are outdated, please replace them.

Response: Thanks to your suggestions, we have updated the older references in the manuscript.

### **Specific comments**:

1. I apologize that I did not clearly find the location distribution of the actual points in Figure 1, the author should add this information in the text or in an additional file.

Response: Thanks to your suggestion, we have added a geographic map of the actual points in the Supporting information. Below are the revised details::

Since 2015, an ecohydrological observation system has been implemented in the Shiyang River Basin in the arid zone of Northwest China to systematically gather surface water stable isotope data (Fig. S1), serving as the primary source of measured data.



Figure S1 Distribution of sampling sites in the Shiyang River Basin.

## 2. Why did you choose two meteorological datasets, the NCEP-NCAR reanalysis dataset and the CRUTS v.4.07 dataset? Are they different in any way ?

Response: CRU is one of the most widely used climate datasets currently produced by the NERC Centres for Atmospheric Science (UK) (NCAS), but the only meteorological variables included in CRUTS v.4.07 are (Precipitation rate) PRE, (Potential evapo-transpiration) PET, and (Mean 2m temperature) TEMP, while vapour pressure (VAP), wind speed (WSPD), and relative humidity (RHUM) data are obtained from the NCEP-NCAR reanalysis data were obtained.

#### 3. Line126: What is LIMA and is it the same as LWIA in Figure 2?

Response: We apologize for the vague description of the Figure 2, the correct expression should be LWIA.

4. Line 134: The full name of ANOVA should be shown in its entirety the first time, and then the abbreviation is used in the later text, similar situation please ask the authors to solve it together.

Response: Thanks to your suggestion, we have filled in the full name of ANOVA here. Here are the details with modifications:

Based on previous studies, a one-way analysis of variance (ANOVA) was used to determine the significance (p < 0.05 at a 95% confidence level) of the slopes and intercepts of the linear regression fits for surface water stable isotopes  $\delta^2$ H and  $\delta$ 180 across different climatic regions.

5. Line123: Here it is  ${}^{1}\text{H}/{}^{2}\text{H}$  at the beginning and  $\delta D$  later, are these two statements the same? Please harmonize the statements.

Response: These two mean the same thing, but for the sake of harmonization, we have modified the whole text and the representation is now  $\delta^2$ H.

#### 6. Line142: What is the calculation method of RMSE and MAE?

Response: Both root mean square error (RMSE) and mean absolute error (MAE) were utilized to estimate the model's error (Kartal, 2024). The RMSE and MAE are calculated as follows:

| $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \left M_{i} - P_{i}\right ^{2}}$ | (1) |
|--|-----|
| $MAE = \frac{1}{n} \sum_{i=1}^{n} \left  M_i - P_i \right ^2$            | (2) |

where M and P are the measured and predicted values and n denotes the number of samples in the validation set.

Kartal, V., 2024. Machine learning-based streamflow forecasting using CMIP6 scenarios: Assessing performance and improving hydrological projections and

climate change. Hydrological Processes 38, e15204. https://doi.org/10.1002/hyp.15204

### 7. Line146: 102862 should be written as 102,862, and other figures in the text should be written the same way.

Response: Thanks to your suggestion, we have revised all the figures in the text to make them more understandable to the reader. Here are the details with modifications:

As shown in Fig. 3, a total of 102,561 measurements of stable isotopes of hydrogen and oxygen in surface water were collected for this dataset. This includes 79,525 website data, 1040 measured data, and 21,946 references data.

### 8. The information in Figure 4 is vague and needs to be reformatted to improve the resolution.

Response: Thanks to your suggestion, we have now increased the resolution of Figure 4 and here is the revised Figure 4:



Figure 4 Seasonal variation of  $\delta^2$ H and  $\delta^{18}$ O in surface water in different climatic zones (Numbers indicates amount of stable isotope data).

### 9. According to Figure 1, the authors collected data for Antarctica, but this part is missing from the spatial distribution.

Response: We do not spatially interpolate  $\delta^2$ H and  $\delta^{18}$ O in Antarctica here because the number of sampling points in Antarctica is too small and spread out for spatial differencing, which would lead to large errors.

10. Line 171: "The most pronounced variations occur in arid zones, underscoring the influence of climatic factors on stable isotopes of surface water." Are the potential causes of such pronounced variations observed in arid zones explored ?

Response: Since the goal of our study is to suggest a global surface water stable isotope dataset, surface water stable isotopes are most affected by meteorological factors according to the results of our Random Forest Model imputation, and many current studies have demonstrated that surface water stable isotopes are most affected by temperature and evapotranspiration in arid zones.

References:

- Gui, J., Li, Z., Feng, Q., Cui, Q., Xue, J., 2023. Contribution of cryosphere to runoff in the transition zone between the Tibetan Plateau and arid region based on environmental isotopes. Hydrol. Earth Syst. Sci. 27, 97–122. https://doi.org/10.5194/hess-27-97-2023
- Hamidi, M.D., Gröcke, D.R., Kumar Joshi, S., Christopher Greenwell, H., 2023. Investigating groundwater recharge using hydrogen and oxygen stable isotopes in Kabul city, a semi-arid region. Journal of Hydrology 626, 130187. https://doi.org/10.1016/j.jhydrol.2023.130187
- Vystavna, Y., Harjung, A., Monteiro, L.R., Matiatos, I., Wassenaar, L.I., 2021. Stable isotopes in global lakes integrate catchment and climatic controls on evaporation. Nat Commun 12, 7224. https://doi.org/10.1038/s41467-021-27569-x

11. Line 185-194: Interpolation was performed here to map changes in spatial distribution, what interpolation method was used? This should have been explained earlier.

Response: Thank you for your suggestion, here we use the Kriging method for global simplified interpolation, because the global surface water data involves different water bodies such as rivers, reservoirs (lakes), and Kriging interpolation takes into account the spatial correlation nature of the described objects in the process of data gridded, so that the interpolation results are more scientific and close to the actual situation. The modified content is as follows:



Figure 5 Spatial distribution of global surface water  $\delta^2 H$  and  $\delta^{18}O$  in different seasons (Unweighted data, using kriging grid methods).

### 12. Figure 5 needs to be redone to improve resolution.

Response: Thanks to your suggestion, we have modified Figure 5 as follows:



Figure 5 Spatial distribution of global surface water  $\delta^2 H$  and  $\delta^{18}O$  in different seasons (Unweighted data, using kriging grid methods).

### 13. What is meant by SWL in figure 7, which should be explained in the text ?

Response: Thanks to your suggestion, we have modified Figure 7 and its now named Figure 6:



Figure 6 Relationship between  $\delta^2 H$  and  $\delta^{18}O$  in different climatic zones.

### **Reviewer #2:**

Li et al. have collected the isotopic dataset of surface water around the world via website, field observation, and reference data, which is important for understanding the hydrological processes, water resource management. Although this study analyzed these data from different aspects such as spatial and temporal scales, the relationships across different climatic zones, some analyses are too tedious and redundant. The detailed comments are listed as follows.

Response: Thank you for your valuable comments and suggestions on our manuscript. Based on your comments and suggestions, we have thoroughly revised the manuscript, including the introduction, methods, results, and discussion sections. We have also improved the English grammar of the manuscript and the quality of the manuscript has been greatly improved.

1. Line 18-19, analysis, this sentence of "global surface water isotopes' spatial and temporal distribution could......" is hard to understand. Please reshape it.

Response: We have now revised to read as follows:

The spatial and temporal distribution of global surface water stable isotope data is extremely uneven on a global scale due to factors such as observation conditions and instrumental analysis.

### 2. Line 29, research-researches.

Response: We have corrected the error here. The revised formulation is as follows:

It can provide essential data references for global water resource management and researches.

3. Line 41-42,"due to restrictions imposed by their conditions in various regions of the world,..." this part of sentence is very vague. Should listed in details on the conditions referring to?

Response: We have now revised to read as follows:

However, there are a number of challenges and limitations in the collection, processing and analysis of current stable isotope data for surface water due to limitations such as geographic location and sample collection in different parts of the

### globe.

4. Figure 2, the chart figure is too ambiguous for data processing. For example, data filtering, how you do it? From your published data, some wrong data are listed. How can explain the dashed circle data like a line. Hence, these published data should be thoroughly checked it and it is true from reference data.

Response: Thank you for your suggestion, due to an oversight on our part, the last version of the dataset had incorrect data. We have now checked the entire dataset again to make sure it is appropriate. Here is a link to the latest version of the dataset.

Zhu, Guofeng (2024), "Global Stable Isotope Dataset for Surface Water", Mendeley Data, V2, doi: 10.17632/fs7rwp7fpr.2

### 5. Line 49, the word of "slowly" is improper in describing the status of network.

Response: We have modified the content here. The revised content is as follows:

Compared to global stable isotope monitoring of precipitation, global surface water monitoring is lagging behind.

6. Line 243, the subtitle 3.4 is too long. I can not well catch your description on this section. It seems like a literature review and many contents are irrelevant and vague. Hence, this section should be reshaped and make it more concise.

Response: We have re-described this section to make it more concise. Here is the revised content:

### Global surface water $\delta^2 H$ and $\delta^{18} O$ correlations

Here, we fit  $\delta^2$ H and  $\delta^{18}$ O to surface waters in six climatic zones, the results indicated a strong correlation between  $\delta^2$ H and  $\delta^{18}$ O across six various climate zones (Fig. 6). The relationship between  $\delta^2$ H and  $\delta^{18}$ O for global surface water is  $\delta^2$ H = 7.92 $\delta^{18}$ O + 7.80 (R<sup>2</sup> = 0.98), which is closer to the intercept and slope of the global meteoric water line (GMWL:  $\delta^2$ H =  $8\delta^{18}$ O + 10), and this confirms once again that the source of recharge of global surface water is precipitation. However, the fitted lines of  $\delta^2$ H and  $\delta^{18}$ O for surface water were significantly different in different climatic zones (Fig. 6), and the fitted lines of  $\delta^2$ H and  $\delta^{18}$ O exhibited the lowest intercept and slope under arid climate ( $\delta^2$ H = 7.50  $\delta^{18}$ O + 3.30, R<sup>2</sup> = 0.98), which also suggests that under arid climate, the surface water experienced significant evapotranspiration, which led

to the isotopic enrichment of surface water ,  $\delta^2$ H and  $\delta^{18}$ O values were higher compared to other climatic zones. In the coldest polar climate zone, the fitted line of  $\delta^2$ H and  $\delta^{18}$ O is  $\delta^2$ H=5.57 $\delta^{18}$ O+17.18 (R<sup>2</sup>=0.95), and the higher slope and intercept indicate that under the influence of the cold climate, the surface water undergoes little evaporation, and the presence of surface water may be in the form of snow and ice, resulting in significantly lower values of  $\delta^2$ H and  $\delta^{18}$ O compared to the other climate zones.



Figure 6 Relationship between  $\delta^2$ H and  $\delta^{18}$ O in different climatic zones.

#### 7. Line 81 composition of the dataset-compositions of dataset.

Response: Thanks to your suggestion, We have modified the content here. The revised content is as follows:

2.1 Compositions of the dataset

8. Line 126, I can not well understand the LIMA method. How do you use this method to test raw data and ensure the data accuracy. Hence, the study should be explained it more detailed.

Response: We apologize for the vague description of the sentence, which we have now revised to read as follows:

We use the Liquid Water Isotope Analyzer (LWIA) post-analysis software to examine the measured raw isotope data. LGR recommends our customized Post-Processing Software to analyze the data. This software uploads the data files, performs all required normalization and processing, and saves the processed data as readable TXT files. In addition, the LGR software automatically checks for instrumental fault indications, provides a selection of data filters, displays a variety of graphical displays, and can be configured by the user. With LWIA, we can know which raw data values of the sample are wrong and need to be tested again, and we can see the reasons for the data errors .

### 9. Line 113-121, I can not well catch the author's expressions. This part is the laboratory measurements for samplers. why you state this in the manuscript.

Response: Field sampling and experimental analyses of water bodies are an important basis for stable isotope data, and our dataset contains a large amount of measured data. Therefore, we explain the sample processing and experimental analyses in this section to facilitate the reader's understanding of the process of sampling and experimental analyses of water stable isotopes.

10. Figure 2, the manuscript should be listed in detail to how do the data filtering and the reasons. For example, what motivate the data filtering for the GNIR and references data.

Response: We have detailed the reasons for data filtering below.

Since the collected data included various problems such as missing values, outliers and obvious duplicate entries as well as sampling date gaps and missing or incorrect latitude and longitude information. Therefore, the collected raw data were pre-processed and data screened to eliminate erroneous data.

11. Line 133, the section of methods. This study focus on the global surface water data. Why the authors have analyzed the impact of various factors on the isotopes from Random forest model Moreover, the motivation of this question is not well explained in the Introduction section.

Response: Thank you for your suggestion, here we chose the random forest model to analyze the effects of multiple meteorological factors on surface water stable isotopes. This is because existing studies have found that surface water stable isotope data are largely controlled by meteorological factors, making it particularly important to resolve the relationship between surface water surface water stable isotope datasets and climatic factors.

Random Forest as a powerful machine learning algorithm has significant advantages in feature importance assessment. Feature importance assessment is a self-contained tool of Random Forest, and the advantage of this approach is that it is able to handle high-dimensional data and has a good tolerance for missing values and outliers of features. In addition, Random Forest is also very resistant to overfitting because it reduces the overfitting problem that may exist in a single model by integrating multiple models. Another distinguishing feature of Random Forest is its ability to assess the importance of features, which helps in understanding which features in the data have the greatest impact on the prediction results.

In addition, we emphasized in the introduction the importance of analyzing the influence of meteorological factors on global stable isotope changes in surface water. The following is the revised content:

The establishment of a global stable isotope dataset for surface water is of great significance in the current context of global climate change and water scarcity. The dataset will help integrate and utilize surface water stable isotope data from various regions, improve the accessibility and usability of stable isotope data, and provide more abundant and reliable data support for researchers to carry out global-scale hydrological and environmental studies. In addition, based on the global surface water stable isotope dataset, the analysis of the driving force of meteorological factors on the global surface water stable isotope changes can provide a data basis for research on water resources assessment, climate change adaptation, and optimization of agricultural irrigation.

### 12. Line 155, what means for the word "onwards".

Response: We apologize for the vague description of the sentence, which we have now revised to read as follows:

In terms of time range, the dataset covers the period from 1956 to 2023, and most of the data are distributed since 1990, which also suggests that the dataset can better characterize the global distribution of stable isotopes in surface water over the past decades. 13. Line 164. This sentence gives the seasonal variations of isotopic data. However, I DON not know this relevant information on this seasonal data including the number, location, and so on. Hence, this manuscript should include this statistical seasonal data from your website, references, and measured data. Are the current data belonged to seasonal data?

Response: Thanks to your suggestion, we have now modified Figure 4, and the total amount of data as well as the distribution of the data can now be visualized through the box-and-line plot, which is shown in the modified Figure 4 below.



Figure 4 Seasonal variation of  $\delta^2$ H and  $\delta^{18}$ O in surface water in different climatic zones (Numbers indicates amount of stable isotope data).

14. Line 24-256, the sentence can be removed from the manuscript. It makes the manuscript like a review manuscript. I suggest that the manuscript can be cut the similar expressions like references overlay.

Response: Thank you for your suggestion, we have removed the inappropriate statement.