Global Stable Isotope Dataset for Surface Water

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Abstract: Hydrogen and oxygen-stable isotopes are widely used as tracers of the water cycle, and surface water is an integral part of the water cycle. Compared with other water bodies, surface water is more susceptible to different natural and anthropogenic factors, and an accurate understanding of surface water changes is of great significance in ensuring regional water security, maintaining ecological balance, and promoting sustainable economic and social development. 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. For this reason, we have compiled and analyzed the stable hydrogen and oxygen isotope data in surface water from 22,389 sampling stations worldwide from 1956 to 2023, with 102,511 data records. The results found: (1) global surface water stable isotopes are gradually depleted from the equator to the poles and from the coast to the interior. However, there are significant differences in the spatial and temporal distributions of surface water isotopes in different regions. (2) The variation of stable isotopes in surface water is controlled by geographic location, topographic conditions, and meteorological factors (especially temperature), and its heterogeneity is considerable. The global stable isotope dataset of surface water provides vital information for an in-depth understanding of the water cycle and climate change. It can provide essential data references for global water resource management and researches. The Global Surface Water Stable Isotope

30   Dataset is available at https://doi.org/10.17632/fs7rwp7fpr.2 (Zhu, 2024).

31   **Keywords:** Stable isotopes; Surface Water; Global Dataset

32   **1.Introduction**

33   Water resources are an essential material basis for human survival and indispensable for

34   maintaining sustainable local socio-economic development, preserving ecological health, and

35   maintaining ecosystem stability (Immerzeel et al., 2020; Mehta et al., 2024). Due to human

36   activity and climate change, global hydrological systems have changed in recent decades,

37   increasing ecological vulnerability and sensitivity to climate change (Chahine, 1992; Liu et al.,

38   2021; Satoh et al., 2022). Hydrogen and oxygen isotopes, as a kind of stable isotopes widely

39   present in the water column (Reckerth et al., 2017; Sprenger et al., 2016), are an important method

40   for conducting water cycle studies and have an essential indicative role in the study of the water

41   cycle (Aggarwal et al., 2007; Joussaume et al., 1984; Vystavna et al., 2021). However, due to

42   restrictions imposed by their conditions in various regions of the world, there are a number of

43   difficulties and constraints in the gathering, integrating, and analysing of current stable isotope

44   data for surface water (Chen et al., 2020; Penna et al., 2018).

45   Since 1960, the Global Network of Isotopes in Precipitation (GNIP) was created by the

46   International Atomic Energy Agency (IAEA) and the World Meteorological Organization (WMO),

47   with the aim of constructing a worldwide monitoring network focusing on the in-depth study of

48   hydrogen and oxygen isotopes in precipitation (Aggarwal et al., 2012). Compared to global stable

49   isotope monitoring of precipitation, global surface water monitoring is lagging behind. In 2002,

50   the IAEA started building the Global Network of Isotopes in Rivers (GNIR), which aims to study

51   the interactions between surface water and groundwater using stable isotopes in runoff and to

52   identify the effects of climate change on river runoff and the effects of human activity on riverine

53   variability (Halder et al., 2015). Many academics worldwide have studied the stable isotope

54   composition of surface water, Scholars around the world for surface water stable isotope research

55   has achieved many results, a researcher using the U.S. river water stable isotope data, mapped the

56   isotope distribution of U.S. river water, and use the model to analyze the U.S. river water isotope

57   changes (Bowen et al., 2011; Dutton et al., 2005). In addition, the stable isotope composition of

58   surface water is affected by a variety of hydrological processes such as precipitation, evaporation,

59 surface runoff, etc., and can therefore provide valuable information on water cycle processes,

60 water resource management, and the impacts of climate change (Bowen et al., 2019; Darling, 2004;

61 Schulte et al., 2011). The source, flow, accumulation, and change rule of surface water can be

62 thoroughly understood by analysing and interpreting stable isotope data, which can offer a

63 scientific foundation for water resource management, water resource assessment, and ecological

64 and environmental protection (Dudley et al., 2022). In addition, surface water, as a "link" between

65 groundwater and precipitation (Cooley et al., 2021), offers fresh scientific perspectives on a

66 variety of hydrogeological phenomena, including the hydrogeologic evolution of the basin

67 (Bershaw et al., 2016), groundwater-surfac water interactions(Autio et al., 2023), groundwater

68 recharge (Jameel et al., 2023), and precipitation processes (Reckerth et al., 2017).

69   The establishment of a global stable isotope dataset for surface water is of great significance

70 in the current context of global climate change and water scarcity. The dataset will help integrate

71 and utilize surface water stable isotope data from various regions, improve the accessibility and

72 usability of stable isotope data, and provide more abundant and reliable data support for

73 researchers to carry out global-scale hydrological and environmental studies. In addition, based on

74 the global surface water stable isotope dataset, the analysis of the driving force of meteorological

75 factors on the global surface water stable isotope changes can provide a data basis for research on

76 water resources assessment, climate change adaptation, and optimization of agricultural irrigation.

77 In this work, we present the first global surface water stable isotope dataset, comprising measured,

78 website, and references data. Our goals are as follows: (1) to compile and gather surface water

79 stable isotope data globally; (2) to construct a global surface water stable isotope dataset, and to

80 promote the application of global surface water stable isotope dataset in the hydrological,

81 meteorological, ecological, and other fields.

82 **2. Data and methods**

83 **2.1 Compositions of the dataset**

84   The Dataset consists of three main elements: website data (GNIR,

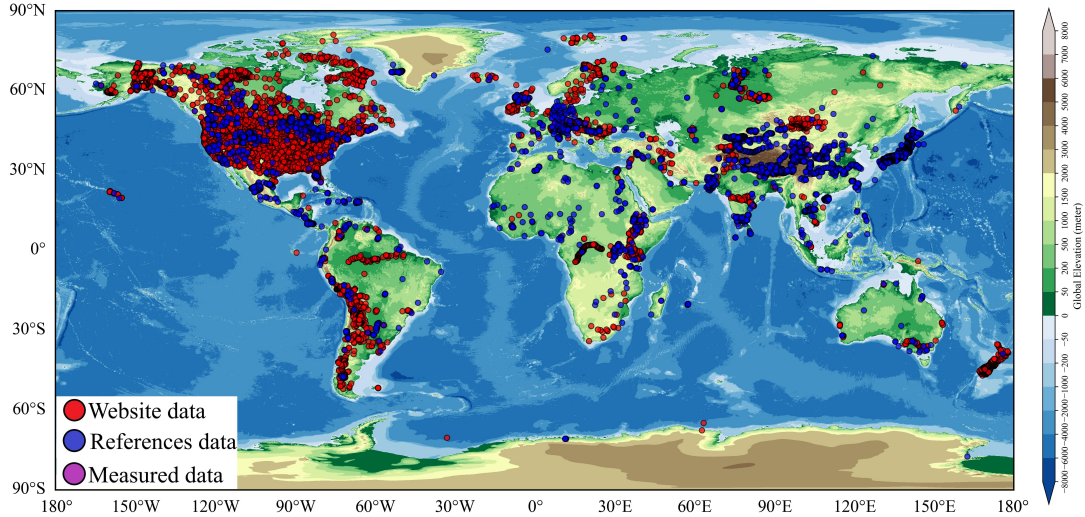
85 http://nucleus.iaea.org/wiser/explore, water isotopes website,

86 http://wateriso.utah.edu/waterisotopes), measured data and references data. The dataset

87 encompasses 22,432 surface water sampling sites across seven continents (Fig.1). Since 2015, an

88   ecohydrological observation system has been implemented in the Shiyang River Basin in the arid

89   zone of Northwest China to systematically gather surface water stable isotope data (Fig. S1),

90   serving as the primary source of measured data.

91

92   **Figure 1** Distribution of sample sites in the global stable isotope dataset for surface water.

93   Measured data: Surface water sampling sites are chosen whenever feasible at places where

94   the water is moving quickly because stagnant water is frequently impacted by pollution and

95   evaporation. After the sampling bottle was rinsed three times prior to sampling using water from

96   the sampling site, the bottle was placed below the surface of the water with the mouth facing up

97   and filled to a position approximately three-quarters of the bottle's volume. Following the

98   completion of the water sample collection process, the bottles are promptly sealed tightly, their

99   mouths are taped with waterproof tape, and labels bearing the name of the sampling location, the

100   sampling date, and additional information are affixed to the bottles. Every collected water sample

101   was kept in a refrigerator to be frozen in order to avoid data errors caused by evaporation.

102   References data: We added more information to the database by searching for the terms

103   "isotope," "surface water," and "river" in published papers on Web-of-Science. We chose scholarly

104   articles containing isotope data in textual, tabular, and graphical formats as the primary source of

105   data to enhance the precision of our data. The aforementioned papers explicitly identified the

106   water body type as "surface water." Alongside isotope data, we gathered spatial and temporal

107   informations, including the latitude and longitude of the sampling sites and the exact time of

108   sampling.

109   Moreover, the meteorological data utilized in this study were sourced from the NCEP-

110   NCAR reanalysis dataset (https://psl.noaa.gov/data/gridded/data.ncep.reanalysis.html) and the

111   CRUTS v. 4.07 dataset (https://crudata.uea.ac.uk/cru/data). The data utilized for the global

112   climate division are derived from Köppen's global climate classification (Peel et al., 2007)

113   (Fig. S2).

114 2.2 Data processing

115 2.2.1 Experiment

116   Prior to the experiment commencing, removing the samples to be analysed from the

117 refrigerator and transferring them to standard 1.5 mL glass sample bottles once they had melted in

118 the room. A filter with a pore size of 0.45 μm and a diameter of 13 mm was then applied to

119 eliminate any contaminants, such as silt and dust, that may have been carried in with the samples

120 during the transfer. All water samples were analyzed for stable isotope values using a liquid water

121 isotope analyzer (DLT-100, Los Gatos Research, USA). During the determination process, each

122 water sample was measured six consecutive times. To prevent residual contamination from

123 affecting the results, the first two measurements were discarded, and the stable isotope value was

124 calculated as the average of the last four measurements. The test results obtained are expressed as

125 thousandths deviation from the Vienna Standard Mean Ocean Water (V-SMOW):

$$\delta_{\text{sample}}(‰) = [(\frac{R_s}{R_v}) - 1] \times 1000$$

126   Here, R_s represents the ratio of $^{18}O/^{16}O$ or $^2H/^1H$ in the collected sample, and R_v is the ratio of

127 $^{18}O/^{16}O$ or $^2H/^1H$ in the Vienna standard sample. The analytical accuracy for δ^2H and $\delta^{18}O$ is

128 ±0.6‰ and ±0.2‰, respectively.

129 2.2.2 Data quality

130   Since the collected data included various problems such as missing values, outliers and

131 obvious duplicate entries as well as sampling date gaps and missing or incorrect latitude and

132 longitude information. Therefore, the collected raw data were pre-processed and data screened to

133 eliminate erroneous data.

134   In addition, We use the Liquid Water Isotope Analyzer (LWIA) post-analysis software to

135 examine the measured raw isotope data. LGR recommends our customized Post-Processing

136 Software to analyze the data. This software uploads the data files, performs all required

137 normalization and processing, and saves the processed data as readable TXT files. In addition, the

LWIA 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. Additionally, all isotope data were thoroughly examined to ensure each entry included clear "longitude," "latitude," "sampling time," and "isotope" data. Outliers and duplicates were removed (Fig. 2).

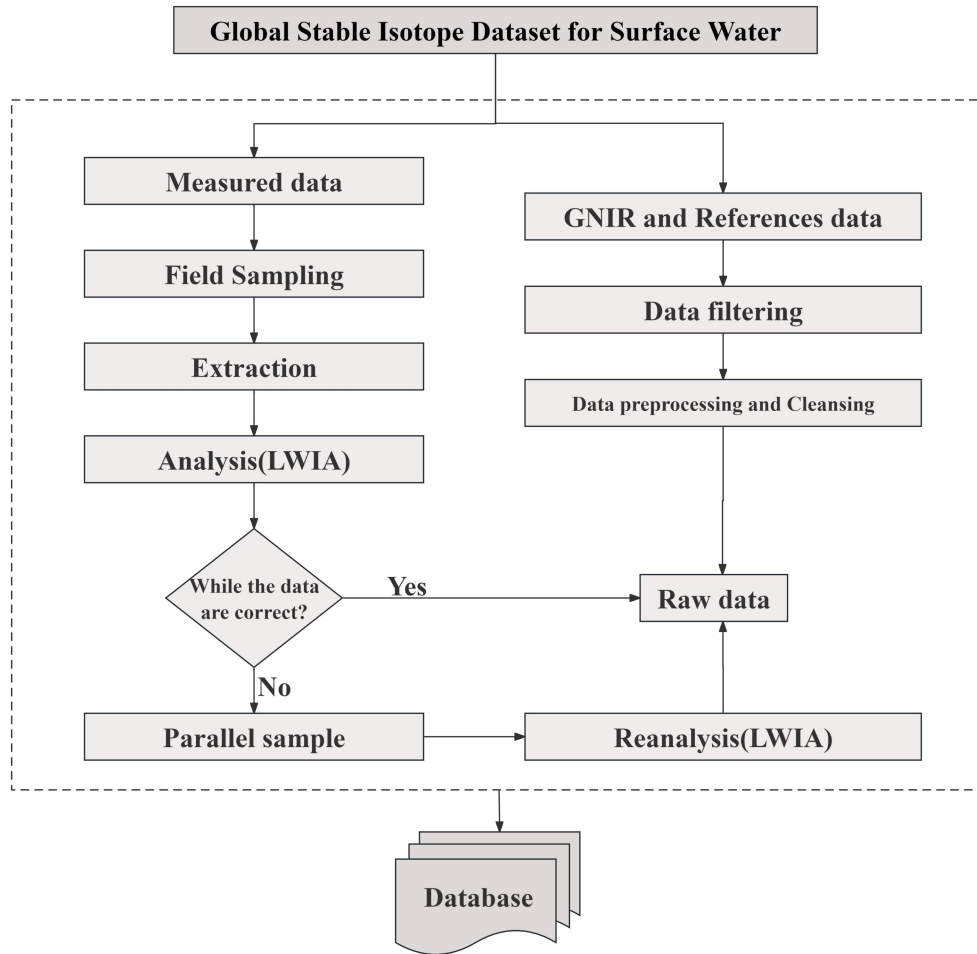



Figure 2 Flow of data processing and construction of global surface water stable isotope dataset.

2.3 Methods

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 δ^2H and $\delta^{18}O$ across different climatic regions (Vystavna et al., 2021). Furthermore, the Random Forest (RF) model can assess the importance of variables. In this study, we employed the RF model to evaluate the impact of various meteorological factors on the stable isotopes of surface water globally. The RF algorithm

153 integrates multiple decision trees to generate a cumulative effect. It predicts regression outcomes

154 based on the average results of these randomized decision trees, employing bootstrapping to

155 minimize the risk of overfitting (Breiman, 2001; Hu et al., 2017). Both root mean square error

156 (RMSE) and mean absolute error (MAE) were utilized to estimate the model's error (Kartal, 2024).

157 The detailed calculation process for RMSE and MAE is described in Text S1 in the Supporting

158 Information.

159 **3. Results and discussions**

160 **3.1 Volume, geographic distribution and temporal coverage of datasets**

161 As shown in Fig. 3, a total of 102,561 measurements of stable isotopes of hydrogen and

162 oxygen in surface water were collected for this dataset. This includes 79,525 website data,

163 1040measured data, and 21,946 references data. Most of GNIR data are primarily concentrated in

164 a few regions, such as the United States and Eastern Europe, and are sparsely distributed globally.

165 To expand our dataset, we incorporated data from published literature. This expanded dataset now

166 covers nearly the entire world with a relatively even distribution, including regions traditionally

167 difficult to access data from, such as Greenland, Antarctica, western Australia, and high-altitude

168 mountainous areas (Fig. 1). In terms of time range, the dataset covers the period from 1956 to

169 2023, and most of the data are distributed since 1990, which also suggests that the dataset can

170 better characterize the global distribution of stable isotopes in surface water over the past decades.

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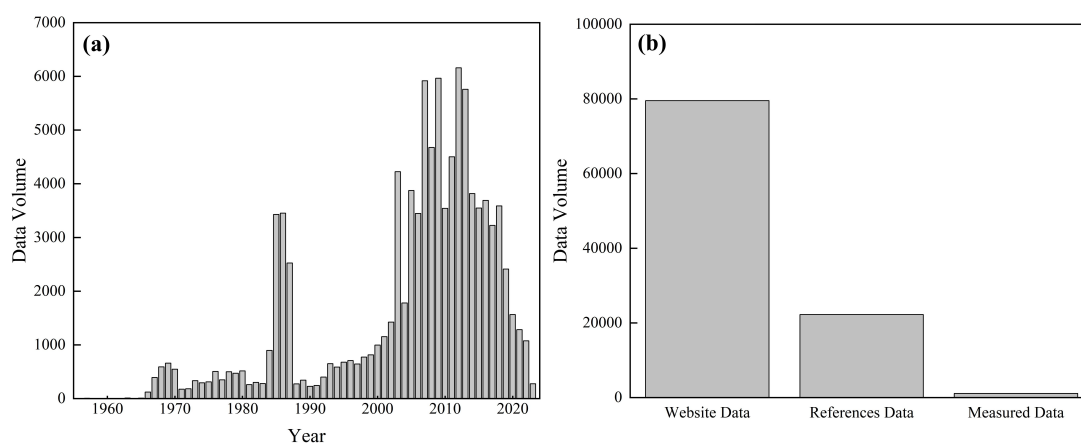
172 **Figure 3** Distribution of global surface water stable isotope dataset. (a) time series distribution; (b)

173 category distribution.

174 **3.2 Spatial and temporal variations of stable isotopes in global surface waters**

175 The variation of δ^2H ranged from -252.48‰ to 79.01‰, and $\delta^{18}O$ ranged from -26.30‰ to

176 15.41‰ over the whole dataset. On a seasonal scale, global surface water stable isotopes typically

177 exhibit pronounced variations, characterized by higher values in summer and lower values in

178 winter (Fig.4). To better observe these variations across different regions, we classified the globe

179 into five climatic zones—tropical, temperate, arid, continental, and polar, based on the "Köppen

180 climate zones" classification. Across the six climatic zones, stable isotopes of surface water

181 exhibit seasonal variations with higher values in summer and lower values in winter, except in

182 polar climatic zones. The most pronounced variations occur in arid zones, underscoring the

183 influence of meteorological factors on stable isotopes of surface water.

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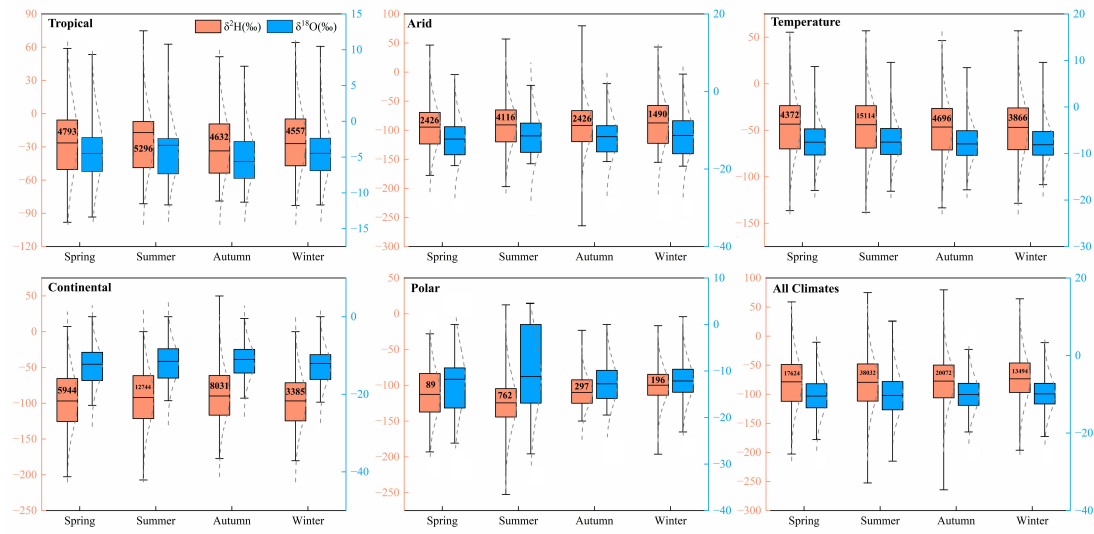
185 **Figure 4** Seasonal variation of δ^2H and $\delta^{18}O$ in surface water in different climatic zones (Numbers

186 indicates amount of stable isotope data).

187   Meanwhile, to better describe the spatial distribution of stable isotopes in global surface

188 water, we conducted interpolation to map their spatial distribution globally (Fig. 5). Generally, δ^2H

189 and $\delta^{18}O$ exhibit a consistent trend of gradually decreasing values from equatorial regions to high

190 latitudes and from coastal regions to inland areas of continents such as Eurasia and North America.

191 This trend is especially pronounced in high-latitude and high-altitude regions, where the values are

192 significantly lower. However, some areas do not exhibit a clear pattern in the distribution of δ^2H

193 and $\delta^{18}O$ values. This irregularity primarily results from the complex factors influencing runoff

194 generation and water flow concentration processes in various regions. Additionally, the presence

195 of open water bodies, such as lakes and reservoirs, exacerbates this irregular distribution

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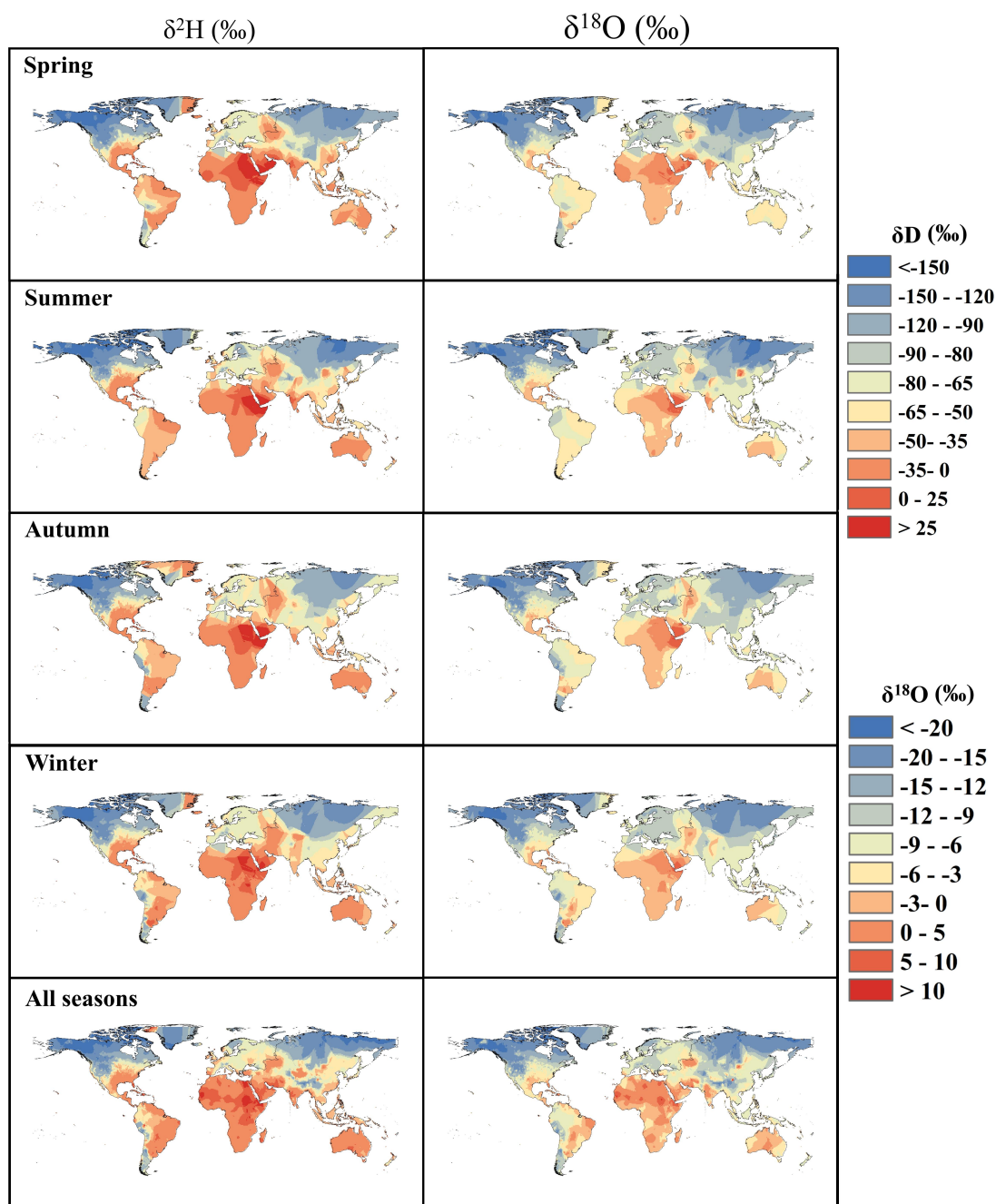
Figure 5 Spatial distribution of global surface water δ^2H and $\delta^{18}O$ in different seasons (Unweighted data, using kriging grid methods).

To better understand the relationship between surface water and precipitation, we compared the spatial interpolation results of surface water isotopes with those of global precipitation isotopes. We found that the isotope distribution in surface water is largely consistent with the isotope distribution in precipitation across most areas (Fig. S3). This consistency primarily arises because surface water is predominantly recharged by precipitation. Moreover, the spatial variation in the isotopic composition of surface water serves as a valuable indicator of its recharge

relationship with groundwater and precipitation (Kendall and Coplen, 2001). This is particularly

evident in the tropics and at high altitudes, where precipitation serves as the primary source of

surface water recharge. In these regions, the spatial distributions of surface water isotopes and

precipitation isotopes exhibit a high degree of similarity (Fig. S3).

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

Here, we fit δ^2H and $\delta18O$ to surface waters in six climatic zones, the results indicated a

strong correlation between δ^2H and $\delta^{18}O$ across six various climate zones (Fig. 6). The relationship

between δ^2H and $\delta^{18}O$ for global surface water is $\delta^2H = 7.92\delta^{18}O + 7.80$ ($R^2 = 0.98$), which is

closer to the intercept and slope of the global meteoric water line (GMWL: $\delta^2H = 8\delta^{18}O + 10$), and

this confirms once again that the source of recharge of global surface water is precipitation.

However, the fitted lines of δ^2H and $\delta^{18}O$ for surface water were significantly different in different

climatic zones (Fig. 6), and the fitted lines of δ^2H and $\delta^{18}O$ exhibited the lowest intercept and

slope under arid climate ($\delta^2H = 7.50 \delta^{18}O + 3.30$, $R^2 = 0.98$), which also suggests that under arid

climate, the surface water experienced significant evapotranspiration, which led to the isotopic

enrichment of surface water, δ^2H and $\delta^{18}O$ values were higher compared to other climatic zones.

In the coldest polar climate zone, the fitted line of δ^2H and $\delta^{18}O$ is $\delta^2H=5.57\delta^{18}O+17.18$ ($R^2=0.95$),

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 δ^2H and $\delta^{18}O$ compared to the other climate

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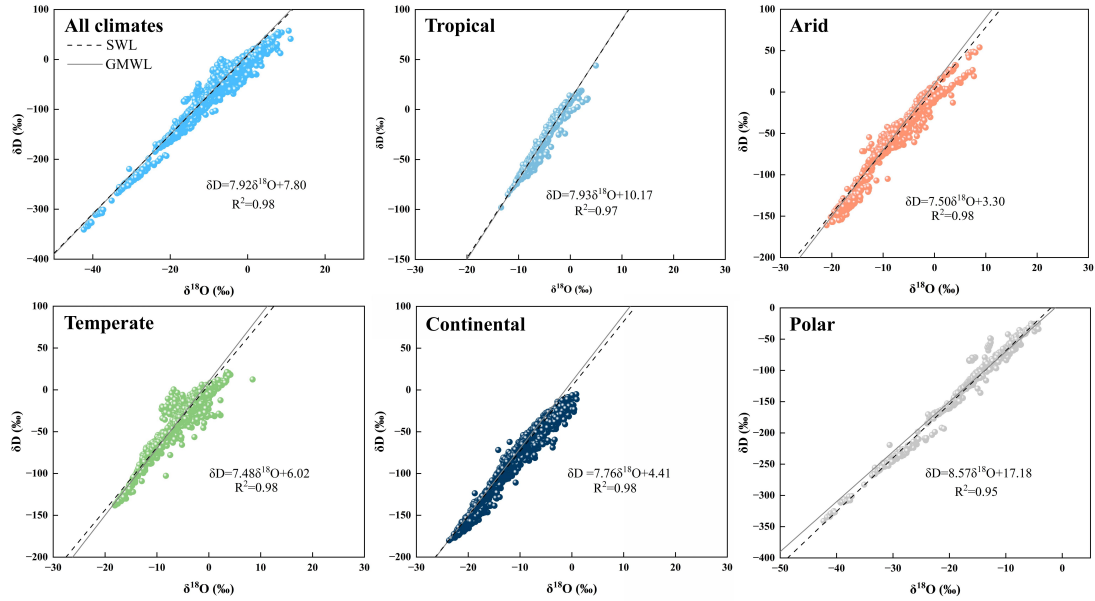
Figure 6 Relationship between δ^2H and $\delta^{18}O$ in different climatic zones.

3.4 Controlling factors for stable isotopes in surface water

For precipitation stable isotopes, there is a significant "latitude effect" and "continent effect (Dansgaard, 1964)," this pattern of variation is also observed in the stable isotopes of surface water, characterized by a gradual decrease in stable isotope values from low to high latitudes and from coastal to arid inland areas. However, in low-latitude regions near the equator, where surface water is primarily recharged by precipitation and climatic factors do not vary significantly along latitude, there is no significant spatial variation in the stable isotopes of surface water.

Additionally, numerous studies have demonstrated that the stable isotope composition of surface water is predominantly influenced by climatic factors (Araguás-Araguás et al., 1998; Dansgaard, 1964; Wang et al., 2017). To assess the importance of various meteorological variables on the stable isotopes of surface water globally, we employed a RF model. The RF regression analysis fitted to the stable isotopes of surface water indicated a strong model fit for both the training and test sets. This suggests that variables such as temperature, precipitation, potential evapotranspiration, vapor pressure, wind speed, and relative humidity possess significant explanatory power for the stable isotopes of surface water (Fig. 7). The validation results of the RF model demonstrate excellent prediction performance for both $\delta^{18}O$ and δ^2H, with $\delta^{18}O$ showing better prediction accuracy than δ^2H, as indicated by smaller RMSE and MAE values (Table S1). Among the six meteorological factors considered, temperature exerts the strongest influence on surface water stable isotopes. Potential evapotranspiration also exhibits a strong

247   controlling effect, suggesting that temperature and evapotranspiration are the primary factors

248   governing changes in global surface water stable isotopes. Additionally, relative humidity and

249   wind speed demonstrate high explanatory power for variations in surface water stable isotopes.

250   Previous studies have indicated that wind speed and relative humidity significantly influence

251   evaporation from water bodies (Gallart et al., 2024; Skrzypek et al., 2015), which can

252   subsequently impact surface water stable isotopes. While vapor pressure and precipitation offer

253   weaker explanations for variations in surface water stable isotopes, these factors can largely be

254   attributed to the residence time of surface water and the local hydrological cycle. The residence

255   time of surface water and the characteristics of the local hydrological cycle vary significantly

256   across different regions. Large open water bodies typically have longer residence times and slower

257   hydrological cycles, resulting in a more enriched isotopic composition of surface water (Feng et

258   al., 2016). In contrast, water bodies with faster hydrological cycles, such as rivers, may exhibit

259   different isotopic compositions (Ala-aho et al., 2018). However, interpreting these patterns on a

260   large scale requires further investigation and validation.
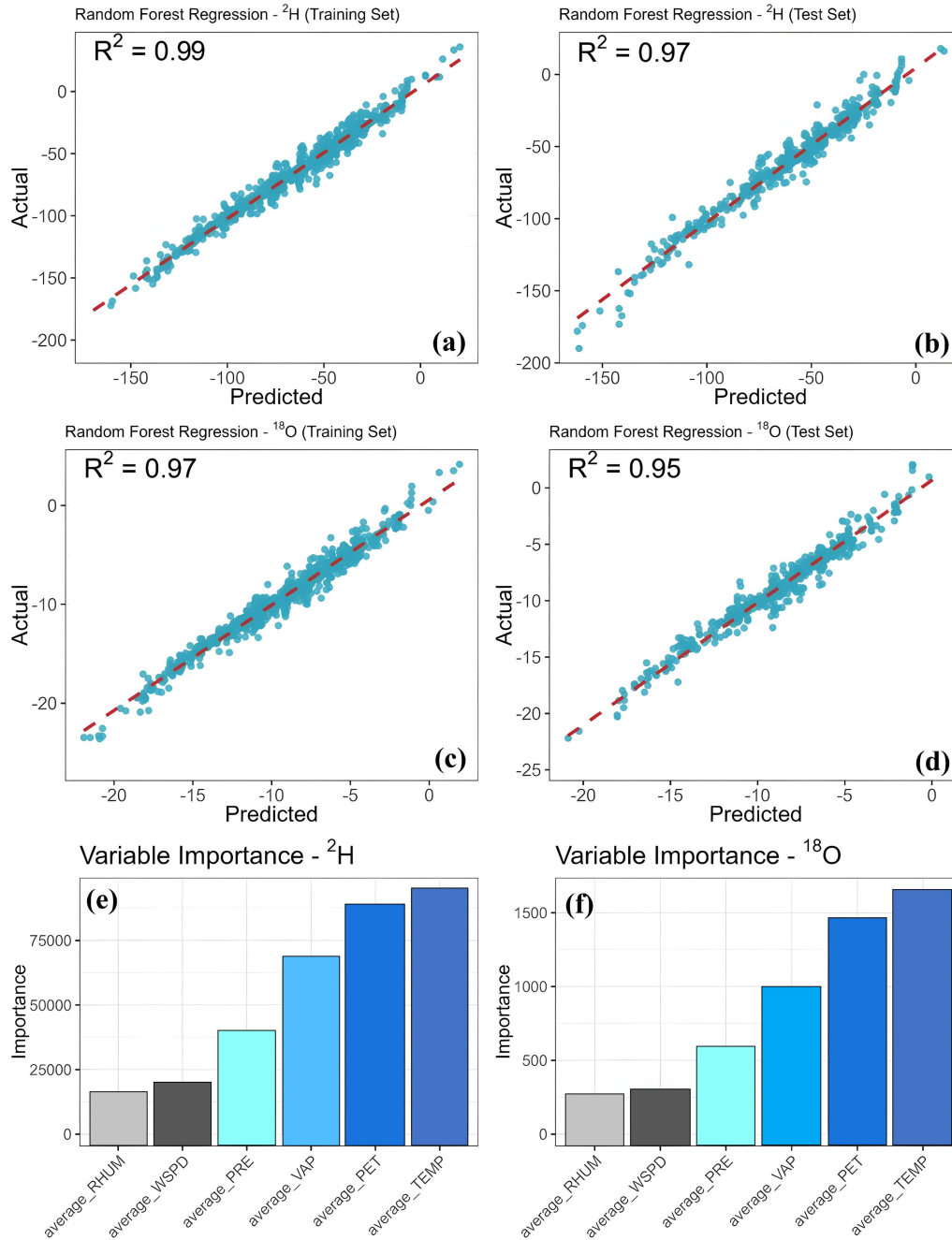
Figure 7 The relationship between δ2H and δ^{18}O and meteorological factors was analyzed using RF model. (a) δ^{2}H regression results for the training set. (b) δ^{2}H regression results of the test set. (c) δ^{18}O regression results of the training set. (d) δ^{18}O regression results of the test set. (e) Effect of meteorological factors on δ^{2}H. (f) Effect of meteorological factors on δ^{18}O.

Simultaneously, for lakes, reservoirs, and other large open water bodies, the controls on surface water stable isotopes can be more complex. Studies have demonstrated that global stable isotope variations in lakes result from the combined effects of solar radiation, evapotranspiration, catchment area size, and other factors (Vystavna et al., 2021). These controls vary across different

270 regions, contributing to diverse stable isotopic compositions in surface waters worldwide. For

271 instance, in arid zones, solar radiation primarily controls stable isotopic variations in lakes,

272 whereas in temperate climatic zones, evaporation and transpiration play a dominant role.

273 Consequently, the controlling factors for surface water stable isotopes vary significantly across

274 different regions. However, overarching patterns suggest that geographic and meteorological

275 factors collectively govern the stable isotopic changes in surface water within a region.

276 **3.5 Challenges and limitations in the construction of surface water isotope**

277 **datasets and future research directions**

278 At present, due to the limitations of sampling techniques and methods, there may be

279 significant differences in sampling methods and frequencies across various geological

280 environments and hydrogeological conditions. These differences can affect the comparison and

281 analysis of the data. Constructing a comprehensive isotope dataset for surface water requires

282 careful consideration of spatial and temporal coverage to ensure data accuracy and comparability

283 (Ankor et al., 2019). However, due to cost, labor, and equipment constraints, as well as the harsh

284 natural conditions in sampling areas, it is challenging to achieve continuous observation of

285 different watersheds over long time series. This limitation results in some incompleteness of the

286 data in terms of spatial and temporal scales (Penna et al., 2014). In addition, the accuracy of

287 current stable isotope data has yet to be harmonized due to issues such as sample preservation,

288 analytical techniques, and instrumental accuracy. These challenges may lead to problems in the

289 comparability and overall reliability of the data.

290 In the future, establishing harmonized standards for data collection, storage, and sharing will

291 be essential for creating a global isotope database for surface water. Additionally, integrating data

292 from different sources, times, and locations will be necessary to develop a more comprehensive

293 global isotope database for surface water (Chen et al., 2024). With advances in artificial

294 intelligence, there is a growing trend towards integrating isotope data with hydrologic modeling

295 (Gierz et al., 2017; Nelson et al., 2021). This integration promises to enhance our understanding of

296 hydrologic processes and improve water resource management practices. Furthermore, it

297 facilitates improvements in the spatial and temporal coverage of data, offering more robust

298 insights into water dynamics and interactions within ecosystems. Meanwhile, within the context of

299 global change, climate change, and isotopes are becoming increasingly integrated and

interdisciplinary. In the longer term, there is potential to develop a comprehensive understanding and application of isotope datasets for surface water. This development will rely on integrating expertise from disciplines such as geology, hydrology, meteorology, and others, fostering a holistic approach to studying and managing water resources in a changing climate.

4. Data availability

The Global Surface Water Stable Isotope Dataset is now publicly available and the data can be found at 10.17632/fs7rwp7fpr.2 (Zhu, 2024).

5. Conclusion

The global surface water stable isotope dataset provides crucial information for advancing our understanding of the water cycle, climate change, and environmental monitoring. In this study, we established a global surface water stable isotope dataset by combining measured data and reference data from existing station data. This approach enriched the dataset and enabled comprehensive analysis across different regions and climatic zones. The results reveal pronounced spatial and temporal variations in the stable isotope composition of global surface water, with significant differences observed in the isotopic composition of surface water across different climates. The variations in global surface water isotopes are influenced by a combination of geographic and meteorological factors, with temperature and evapotranspiration among the climatic factors exhibiting strong explanatory power for the isotopic composition of surface water. Observations of stable isotopes in global surface water play a crucial role in enhancing our understanding of the global water cycle, climate change, and water resource management. They provide essential data support for interdisciplinary research, helping to uncover connections between hydrological processes, climate variability, and environmental changes worldwide. Although we have enriched this dataset as much as possible, there are still regions with sparse data, such as Siberia and Eastern Europe. In the future, efforts should focus on strengthening observations in these challenging areas where data availability is limited. Improving the resolution of global surface water stable isotope data can be achieved by integrating interdisciplinary approaches and leveraging artificial intelligence methods. This approach will help fill data gaps, enhance accuracy, and provide more comprehensive insights into global water dynamics and environmental changes.

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Conflict of Interest Statement

The authors declare no conflicts of interest.

Author contributions statement

Guofeng Zhu and Rui Li: Writing-Original draft preparation. Siyu Lu and Longhu Chen: Data curation. Xiaoyu Qi: Writing-Reviewing and Editing. Gaojia Meng and Yuhao Wang: Methodology. Wenmin Li: Investigation. Zhijie Zheng, Jiangwei Yang and Yani Gun: Software

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