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The estimation of young water fraction based on isotopic signals: challenges and recommendations

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Young water fraction (*Fyw*) is defined as the fraction of water in a stream with a transit time of less than 2–3months. *Fyw* is a metric used to quantify the proportion of precipitation input converted into the runoff in the form of fast flow, which provides new insights for characterizing the mechanisms of water storage and release, understanding the time-scale of ecohydrological processes and indicating water-related risks. However, *Fyw* has been advanced for a relatively short time, and the research on its applicability conditions and main drivers is still ongoing. Studies estimating *Fyw* are still very few and this index has not been reported in many landscapes and climate backgrounds, limiting its further application in hydrological studies. On the basis of summarizing the progresses of *Fyw* in previous studies, this paper provides a preliminary analysis of the potential uncertainties in the *Fyw* estimation, which can be due to temporal trends in the isotopic composition of precipitation, uneven sampling interval of stream water, and complex hydrological systems. Finally, this paper provides some recommendations for the optimization of the sampling design and the methods used for the *Fyw* estimation.

KEYWORDS

young water fraction, isotope tracers, sources of uncertainty, water-related risks, further studies

Introduction

The rate of water transport in catchments regulates processes such as biogeochemical cycling, pollutant transport, and chemical weathering. The time water takes to travel through a catchment, from inputting as precipitation to reaching the outlet, is an important indicator to characterize the catchment hydrology and determine the sensitivity of the catchment to pollutants (Sprenger et al., 2019). Since the migration, transformation, and phase change of water are accompanied by the transport, mixing, and fractionation of hydrogen and oxygen stable isotopes (i.e., ^{18}O and ^{2}H), these isotopes are widely used to perform hydrological and meteorological analyses at different scales, such as the identification of water vapor sources and transport patterns, the quantification of the contribution of end members to runoff, and the evaluation of water interactions and estimation of evaporation losses (e.g., Chen et al., 2015;

Eissa et al., 2016, 2018; Zuecco et al., 2019; Laonamsai et al., 2021, 2022; Wang et al., 2022). During the process of runoff generation in rainfall-dominated catchments, the isotopic signal in precipitation is usually dampened when it is transmitted to river water, due to the buffering effect of the catchment and its mixing with groundwater and soil water with relatively constant isotopic signals. Based on the regularities of isotope fluctuation decay during the conversion from precipitation into river water, mean transit time (*MTT*), mean residence time and damping ratio can be estimated to evaluate the water age and water transport rate (McGuire and McDonnell, 2006; Bansah and Ali, 2019; Sprenger et al., 2019; Benettin et al., 2022). Such metrics have been widely applied to analyze the catchment behaviors in many regions across the world.

Recently, Kirchner (2016) found that the distribution function of water transit time in a catchment is often not static in space, especially for those landscapes characterized by strong spatial heterogeneity, and great uncertainty is likely to exist in the estimation of *MTT*, because of the aggregation bias. Consequently, Kirchner (2016) developed the concept of a substitutive metric, the young water fraction (*Fyw*), which is defined as the runoff component that is younger than 3 months in the water flowing through the catchment outlet. *Fyw* is negligibly affected by the aggregation bias (with an error usually less than 2%, Kirchner (2016)), and thus it can be used to effectively investigate the hydrological processes and the response of a catchment to climate change and human activities (e.g., groundwater abstraction, contaminant transport, or land use changes), and to evaluate hydrogeological and environmental risks related to water storage and release mechanisms in catchments. The estimation of *Fyw* is based on the aggregate parameter model, with precipitation as the input and runoff at the outlet as the output (shown in Figure 1). The isotopic signal of the output water is considered as the convolution of the isotopic fluctuation function (set as a sine function) of the input water and the transit time distribution function (set as a Gamma function). Using the Fourier transform method, the shape and scale coefficients of the Gamma distribution function can be determined, and then *Fyw* can be obtained by integration. Through a numerical simulation experiment, Kirchner (2016) found that *Fyw* can be approximated using the isotopic amplitude ratio between stream water and precipitation obtained by sine function fitting. This simple method is known as "amplitude ratio method" and has become the most commonly used method to estimate the *Fyw*. In the fitting of the sine function, the precipitation amount and the discharge are commonly used as weights for the observed isotopic compositions of precipitation and stream water (e.g., von Freyberg et al., 2018; Gallart et al., 2020a). To estimate *Fyw*, isotopic time series of input and output water, are required to be longer than a year. Typically, higher *Fyw* is associated with shorter flow paths, implying that surface water and groundwater in the catchment are more susceptible to pollutant contamination, while lower *Fyw* is associated with longer flow paths and slower recharge rates. Therefore, this metric could benefit the understanding of water recharge mechanisms, as well as of the exchange and transfer of pollutants, and is thus of practical importance for the management of water-related risks.

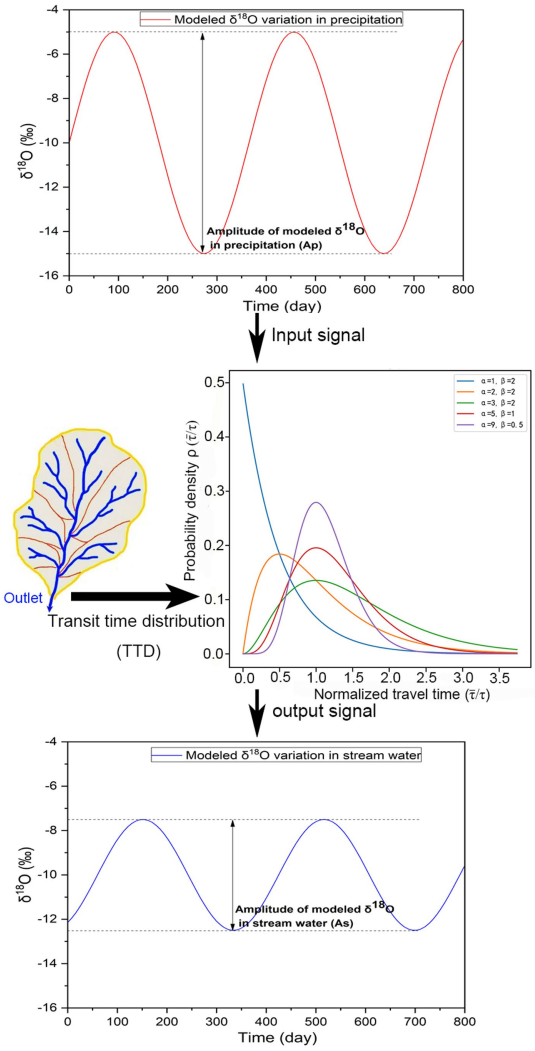

FIGURE 1
Conceptual scheme showing the *Fyw* estimation based on the lumped parameter model.

Jasechko et al. (2016) collected isotopic data from more than 60,000 precipitation samples from 459 meteorological stations and 10,000 river water samples from 254 rivers worldwide, and they estimated the *Fyw* based on the amplitude ratio method. Jasechko et al. (2016) found that the arithmetic mean value of *Fyw* in rivers worldwide is 26%, the amount weighted mean value is 34% and the median value is 21%, providing a reference for studies on *Fyw* in different geographic regions, at different spatial scales, and under different climatic backgrounds. Since then, the *Fyw* estimation has been determined in different study areas. For example, *Fyw* was found to be positively correlated with vegetation coverage and proportion of swamp, negatively correlated with the watershed area and elevation, but not significantly correlated with average runoff coefficient in Tibetan Plateau catchments (Song et al., 2017). Higher *Fyw* are typically associated with wetter climates, soils with lower permeability, and higher precipitation intensity in Swiss catchments (von Freyberg et al., 2018). Wilusz et al. (2017) reported that an increase in *Fyw* may result from increased precipitation amount in the Plynlimon region of Wales. In the Alpine area, the increase of snowpack duration promotes the emptying of groundwater storage in winter, thus decreasing the *Fyw*, while the snowpack with short duration is generally associated with the increased rapid flow path, resulting in increased *Fyw* (Gentile et al., 2022).

In previous studies, the interference of environmental and systematic factors, such as sampling frequency, evaporation and snowmelt, on the accuracy of *Fyw* estimates have been preliminarily explored (e.g., Ceperley et al., 2020; Gallart et al., 2020a). However, the source of uncertainties and the extent of application of this metric have not been fully explored, which limits its development as a practical indicator for catchment properties. The goal of this paper is to summarize the potential sources of uncertainty and possible limitations of *Fyw*, in the aspects of both hydro-meteorological conditions and data quality. Furthermore, in this perspective paper we provide some methodological recommendations aimed to reduce the uncertainty in *Fyw* estimation.

Uncertainty in the complexity of isotopic composition of precipitation and stream water

The theoretical basis of the *Fyw* estimation is the attenuation of isotope amplitude during the mixing process between precipitation, with a clear seasonal isotope periodicity, and water sources (e.g., shallow and deep groundwater, soil water), with an isotopic composition less time variable compared to precipitation. In the *Fyw* estimation, the lumped parameter model is based on the premise that precipitation is the only initial water source in the hydrologic system and phase shift in the path of water migration is not considered. Under this hypothesis, the influences of precipitation input in multiple forms (e.g., snowmelt and ice melt) and natural and anthropogenic processes on the composition and periodicity of isotopes in stream water are generally overlooked. For instance, based on data from three Alpine catchments, Ceperley et al. (2020) showed the limitations of isotopic periodicity in snowmelt-dominated catchments, and proposed an optimized method for the *Fyw* estimation in high altitude areas, considering the influence of lag release of water caused by the seasonal snowmelt. However, the uncertainty brought by melt water should be further explored in other mountainous catchments with different size and elevations, as well as with different contributions of melt water to stream runoff. In addition, previous research (i.e., Ceperley et al., 2020; Gentile et al., 2022) showed that there is a lack of studies providing *Fyw*, as well as transit times estimations in glacierized catchments; in these catchments *Fyw* can be larger than *Fyw* determined for snowmelt-dominated catchments due to fast flow paths and a less permeable bedrock (Schmieder et al., 2019; Zuecco et al., 2019).

In precipitation, the isotopic variations caused by sublimation of snow and ice, water-vapor exchange and sub-cloud secondary evaporation may lead to uncertainty in the sine-wave fitting, whose impacts also need to be evaluated in the *Fyw* estimation. Previous studies also showed that processes such as evaporation and scheduling of reservoirs may interfere the isotopic periodicity in stream water inherited from rainfall (Reckerth et al., 2017; Xia et al., 2021). Therefore, in catchments with complex flow systems or those heavily influenced by human activities, the uncertainty of the *Fyw* estimation based on the current estimation methods may be large. Therefore, to estimate *Fyw* is necessary to develop a more flexible approach, considering the isotopic variation associated with phase behavior changes.

Effects of trends in the isotopic composition of precipitation and stream water

Previous studies have confirmed that although *Fyw* is dependent on catchment properties, the accuracy of its estimation results is also confounded by systematic factors such as weighting methods, sampling frequency and selection of calculation periods (von Freyberg et al., 2018; Stockinger et al., 2019; Gallart et al., 2020a). Under the influence of climate change, the global temperature increase is widespread, leading to an enrichment trend in isotopic composition in precipitation at longer time scales. Wang and Chen (2020) reported the trend variations in temperature, precipitation, and $\delta^{18}O$ in precipitation based on data from stations of the global network of isotopes in precipitation (GNIP) with long-term records. Wang and Chen (2020) found that among 98 selected stations around the world, about 2/3 (65 stations) showed a significant upward trend of $\delta^{18}O$ in precipitation. Such a trend may also be transmitted to the isotopes in the river water and cause the amplitudes obtained from the sinusoidal function fit to not reflect the actual seasonal fluctuations of the isotopes in the water. The commonly-used amplitude ratio method for the *Fyw* estimation is based on the assumption that the isotopes in the waters vary seasonally following a fixed sinusoidal curve. However, in actual catchments, the isotope signals do not vary in a constant pattern. Fitting multi-year isotope records using sine waves will oversimplify the shape of the interannual isotope signal. The interannual differences in the amplitudes of isotopic fluctuations and the effects of isotopic trends at longer time scales on the periodicity are not considered, which are possible sources for inaccurate *Fyw* estimates.

Impact of the sampling approach of stream water

As the *Fyw* estimation is based on comparison of periodicity between precipitation and stream water, the extent that the captured isotopic records can reflect the actual variability is important. Gallart et al. (2020a) found that the accuracy of estimated *Fyw* is greatly dependent on the sampling frequency of stream water. Weekly-resolution sampling could not reflect the isotopic variation under high flows, thus resulting in an underestimation of *Fyw* in their catchment. Stockinger et al. (2019) pointed out that a 1-year isotopic time series is not long enough for an accurate *Fyw* estimation, and the selection of the fitting period may lead to a marked uncertainty. However, as the *Fyw* has been proposed for a relatively short time, in many studies, the time series of isotopic data, used to estimate the *Fyw*, was originally collected for the investigation of hydrological processes occurring at short timescales. Furthermore, in isotope-based studies, it is common to increase the sampling frequency of stream water in the rainy season with concentrated precipitation and high flows. Previous studies have shown that flows are positively correlated with *Fyw* (von Freyberg et al., 2018; Gallart et al., 2020b). Therefore, isotopic data collected mainly at the event timescale (i.e., during high flows) may lead to an overestimation of *Fyw*, as the proportion of high-flow condition in the "isotope discharge" (i.e., the observed flow accompanied with isotope collection), which is involved in sine-wave fitting, exceeds that of the low flow records. Additionally, it is difficult to guarantee long-term and periodic stream water sampling, and the isotope datasets of river water with irregular sampling frequency and data gaps are common in many study areas, due to different research objectives and limitations in logistics conditions (e.g., Ceperley et al., 2020). In previous studies focusing on *Fyw*, the influence of such widespread heterogeneous datasets on the estimation uncertainty has not been determined yet.

Concluding remarks and future perspectives

Although research on *Fyw* based on isotopic signals has received much attention during the past few years and has been continuously promoted, there is still a lack of comparative understanding on *Fyw* under different landscapes and climate conditions. The knowledge about the influencing factors of this metric and the sources of uncertainty in the processes and results of its estimation is still very limited. Factors, such as temporal isotopic trends under changing climate, commonly-used irregular sampling schemes for isotope hydrology, complex recharge sources and evaporation conditions, have potential impacts on the accuracy of *Fyw* estimation. In future studies, more effort to explore the error sources and to develop optimization methods for *Fyw* estimation should be made. For example, future research should conduct *Fyw* estimations in areas with potential isotopic complexity (e.g., where there is a complex isotopic signal of melt waters or enhanced evaporation in the water sources), develop detrending models to reduce (or lower down) the impact of an existing trend on the isotopic periodicity, implement a sampling approach consistent with the full flow record during the observation period (i.e., able to capture all flows, without a bias toward low or high flows). To develop and test better methodological approaches for *Fyw* estimation, researchers should consider using long-term isotopic datasets (> 5–10 years) and datasets collected at very high temporal resolutions (e.g., von Freyberg et al., 2017). Combining *Fyw* estimation and transit times modeling across more catchments should help to better understand the drivers of *Fyw* and its sources of uncertainty, as well as to develop specific recommendations for the application of this metric. By deepening the understanding of *Fyw* and by reducing the uncertainty in its estimation, this metric could be applied more effectively to improve our comprehension of runoff generation and tracer transport in a variety of catchments.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

CX: formal analysis, methodology, and writing-original draft, GZ, KC, and LL: writing -review & editing and ZZ: writing-original draft. JL: formal analysis and writing -review & editing. All authors contributed to the article and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

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