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Tracing isotopic fingerprints: Unveiling the impact of noodle formulation and cooking water on the isotopic signatures of wheat-derived noodles

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ABSTRACT

This study examines how variations in δ^2H and $\delta^{18}O$ values of cooking water affect the isotopic fingerprint of noodles with different gluten-to-starch formulations, aiming to enhance the current understanding of isotopic changes during food processing and their implications for food authenticity. Eight differently formulated noodles were boiled using waters with six distinct isotopic compositions ranging from of −160‰ to +50‰ for δ^2H and from −22.9‰ to +99.9‰ for $\delta^{18}O$, respectively. Linear regression analysis revealed that formulation and water isotopic composition significantly affected the δ^2H in cooked noodles ($p < 0.05$), with model R^2 values ranging from 0.66 to 0.94. Additionally, the δ^2H values of noodles changed with the isotopic signatures of the cooking water. On the contrary, $\delta^{18}O$ in the noodles remained stable despite boiling processing and was also not changing due to the water's isotopic signature. Since consistent effects of formulation and cooking water isotopic signature was observed, an equation for determining the exchange factor (*f(H)ex*) between noodles and cooking water was developed. The fraction of hydrogen atoms in different noodles for exchange was highest at 19.3% in noodles with the formulation of 45:55(gluten-to-starch) and the lowest at 11.1% in noodles with 100% gluten. The findings prove that cooking water systematically alters the isotopic signatures of noodles, underscoring the necessity of considering this type of effect in food authentication and traceability practices.

1. Introduction

Food authentication is crucial for maintaining supply chain integrity, ensuring that food products are authentic, accurately labelled, and compliant with geographic and botanical origins. Various analytical techniques have been applied to investigate and confirm the compositional authenticity of food products (Danezis et al., 2016; Frigerio et al., 2024). Notably, stable isotope ratios analysis (SIRA) has become a prominent method for determining the geographical and botanical origins of food components, exploiting the distinctive isotopic signatures shaped by environmental influences (Li et al., 2023; Liu et al., 2023).

Wheat (*Triticum aestivum* L.) is a crucial global staple crop, providing essential nutrition and energy to humans (Pandey et al., 2020). As international trade expands, interest in the geographical origin and quality of wheat products has grown among consumers and stakeholders (Gupta et al., 2023; Sung et al., 2023). Research has shown that stable isotopes, particularly δ^2H and $\delta^{18}O$, can reveal climatic conditions and water sources during plant growth (Camin et al., 2017; Durante et al., 2016; Li et al., 2018; Zeng et al., 2024). These isotopes reflect a synthesis of environmental, physiological, and biochemical factors, offering significant potential for enhancing food traceability and establishing product authenticity (Laursen et al., 2016). However, a significant gap exists in understanding the impact of post-harvest processing, especially cooking, on these isotopic signatures. The prevailing literature predominantly focused on unprocessed agricultural commodities, overlooking the potential modifications induced by culinary preparation.

Recent advances in isotopic chemistry have highlighted the sensitivity of stable isotopes, hydrogen (δ^2H) and oxygen ($\delta^{18}O$), to food

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processing techniques, such as boiling, which can significantly alter their ratios in wheat-derived products (Yang et al., 2024). Some studies have demonstrated that hydrogen and oxygen isotopes undergo fractionation primarily during evaporation and condensation, producing distinctive isotopic signatures in boiled food (Gibson et al., 2016; Kendall and Caldwell, 1998; Zhou et al., 2015). Focusing on wheat, wheat grains primarily consist of starch and proteins, which interact differently with water during the milling and subsequent processes (Pandey et al., 2020). Previous studies also suggested that isotopic fractionation would occur during these processes as these macromolecules exchange hydrogen and oxygen atoms with vapour or water (Chesson et al., 2009; Kelly et al., 2009; Péron et al., 2018). Meanwhile, the formation of the three-dimensional starch-gluten networks involves interactions between starch, glutenin, and gliadin proteins, linked by different hydrogen bonding, which can lead to isotope ratio exchanges when exposed to water under heating (Lambrecht et al., 2018; Schuler et al., 2022). However, the mechanism of hydrogen and oxygen isotope alteration during processing like boiling has yet to be elucidated. For the underlying explanation of the changes in δ^2H and $\delta^{18}O$ in wheat-processed products, the current investigation seeks to bridge this knowledge gap by innovatively examining the influence of the isotopic composition of cooking water on the isotopic distribution in wheat-derived products with varying formulations during their cooking process.

The experimental design involved eight formulations of gluten-to-starch ratios in noodles, which were cooked using waters with markedly different δ^2H and $\delta^{18}O$ values. It is hypothesized that varying isotopic compositions of the cooking water would significantly influence the isotopic signatures of the noodles due to the isotope exchange that occurs during the boiling process. Hence, the study aims to 1) determine the effects of noodle formulation, the isotopic composition of cooking water, and their combined impact on the isotopic fingerprints (δ^2H and $\delta^{18}O$) of the cooked noodles; and to 2) quantify and predict the isotopic exchangeability between cooking water and wheat noodles (a prevalent wheat-derived product) during boiling. The findings from this study are expected to substantially enrich the scientific understanding of how boiling processing modifies the isotopic fingerprints of wheat products. By incorporating isotopic analysis into the assessment of processed foods, the current research provides a theoretical basis for comprehensive food authentication practices that consider both the raw and processed states, improving the isotopic analysis application for food authentication.

2. Method and materials

2.1. Experimental design and sampling

For noodle production, wheat gluten powder and wheat starch powder, purchased from the Lotus Health Group Company in Zhou Kou, Henan Province, China, were used. Eight different formulations of gluten-to-starch powder (0:100, 15:85, 30:70, 45:55, 55:45, 70:30, 85:15, and 100:0 (w:w)) were prepared. Each formulation weighed a total of 1000 g, with gluten and starch portions adjusted accordingly. The blended flour samples were mixed by hand shaking in a sealed bag for 3 min. This mixing process was repeated three times for each formulation to ensure consistency.

2.2. Noodles preparation

Extruded noodles were produced using a pilot-scale, co-rotating, intermeshing twin-screw extruder (DSE-25, Brabender, Duisburg, Germany). The operational settings included a 25 mm screw diameter, a 20:1 screw length-to-diameter ratio, and 3 mm circular dies, with the extrusion process conducted at room temperature (25 °C). The moisture content of the material inside the extruder was maintained at 35% during extrusion. Once the extruder reached a steady state, the noodles were collected, cut into 20 cm lengths on a tin plate, and packaged in polyethylene bags. The packaged noodles were stored in a freezer at −18 °C for further analysis.

2.3. Preparation of cooking water with different hydrogen/oxygen abundance

Six batches of water with different hydrogen isotopic abundances (HA-HF) and six with different oxygen isotopic abundance (OA-OF) were prepared as follows.

Tibet bottle drinking water (purchased from Tibet Plateau Natural Water Co., LTD) was selected and labelled as HA water ($\delta^2H = -160.0 \pm 1.9‰$). Deionized water from the laboratory made by Beijing groundwater was selected as HC water ($\delta^2H = -78.8 \pm 1.6‰$). HA water and HC water were mixed at a ratio of 1:1 to obtain HB water ($\delta^2H = -124.8 \pm 0.6‰$). Deuterium water ($D_2O$) (purchased from Shanghai Macklin Biochemical Co., Ltd) was mixed with HC to obtain the highest hydrogen abundance water (HF water, $\delta^2H = +49.8 \pm 1.8‰$). HC and HF water were mixed at ratios of 1:2 and 2:1 to obtain HD ($\delta^2H = -33.5 \pm 1.1‰$) and HE ($\delta^2H = 12.8 \pm 0.8‰$) water, respectively.

Tibet bottle drinking water (purchased from Tibet Plateau Natural Water Co., LTD) was selected and labelled as OA water ($\delta^{18}O = -22.9 \pm 0.5‰$). Deionized water made by Beijing groundwater was selected as OB water ($\delta^{18}O = -10.8‰ \pm 0.5‰$). Heavy oxygen water ($H_2^{18}O$) (purchased from Shanghai Macklin Biochemical Co., Ltd) was mixed with HB to obtain the highest oxygen abundance water (OF water, $\delta^{18}O = 99.96 \pm 0.9‰$). OB mixed with OF at the ratios of 2:1, 1:1, 1:2 to obtain OC ($\delta^{18}O = 29.7 \pm 0.3‰$), OD ($\delta^{18}O = 48.7 \pm 0.2‰$), OF ($\delta^{18}O = 60.3 \pm 0.4‰$) water, respectively.

2.4. Boiling treatments

The boiling process was performed as described by Yang et al. (2024) previously. Briefly, thawed noodle samples (100g, 20 cm in length) were placed in a 22 cm diameter stainless-steel pot with 1000 mL of cooking water. The pot was heated on an induction cooker at 1500W. The cooking process was conducted according to the noodles' optimum cooking time, measured according to AACC-I Approved Method 60-50 with slight modifications. Each boiling treatment for the same formulation was performed in triplicates. After the noodles were completely cooked, they were freeze-dried in a freeze-dryer (CHRIST, Osterode, Germany) under a vacuum of 0.1 mbar and a temperature of −50 °C. The dried noodle samples were ground into a fine powder. The sample powder was sealed in bags and stored in a chamber until further analysis.

2.5. Stable isotope analysis

The δ^2H and $\delta^{18}O$ in each sample were measured using a comparative equilibration method (Kelly et al., 2009). Samples and reference standards (1 ± 0.2 mg) were placed in silver capsules (6 mm × 4 mm), which were folded to seal the sample and eliminate air. These were then equilibrated under laboratory conditions for at least 5 days before analysis. Isotope ratios were measured with an IsoPrime100 mass spectrometer (IsoPrime100, Isoprime, Manchester, UK), with a cracking temperature of 1450 °C, helium flow rate of 120 mL/min, and reference gas pressure of 1200 mbar. The stable isotope ratios are expressed in the delta (δ) notation and calculated against the Vienna Standard Mean Ocean Water (V- SMOW), which was calculated based on Equation (1):

$$\delta\ (‰) = ((R_{sample}) / (R_{standard} - 1)) \times 1000 \quad (1)$$

Where δ (‰) is the value of δ^2H and $\delta^{18}O$, while R is the ratio of $^2H/^1H$ or $^{18}O/^{16}O$.

A multi-point calibration was conducted using USGS54 (Canadian lodgepole pine), and USGS55 (Mexican ziricote), USGS56 (South African red ivorywood). The $\delta^2H_{VSMOW\text{-}SLAP}$ of USGS54, USGS55 and USGS56

were −150.4 ± 1.1‰, −28.2 ± 1.7‰, −44.0 ± 1.8‰, respectively. The $\delta^{18}O_{VSMOW\text{-}SLAP}$ of USGS54, USGS55 and USGS56 were +17.79 ± 0.15‰, +19.12 ± 0.07 ‰, +27.2 ± 0.03‰ respectively. In the analysis sequence, two standard samples for calibration were interspersed after every 10 samples. In the analysis, two calibration standards were included after every 10 samples. Each sample was measured in triplicate, and the average of the three measurements was used. The laboratory's analytical precision was less than 1‰ for δ^2H and 0.2‰ for $\delta^{18}O$ across the replicates.

2.6. Data analysis

The data underwent initial assessment for normal distribution and homoscedasticity using the Shapiro-Wilk test (Shapiro and Wilk, 1965). Following this, Turkey's honesty significant difference (HSD) test was conducted to evaluate the significance of δ^2H and $\delta^{18}O$ between each differently formulated noodle sample with different water treatments, applying a 5%, 1%, and 1‰ probability level, respectively. To further evaluate the interaction effects of the formulation and cooking water abundance, two linear regression models were applied for δ^2H and $\delta^{18}O$, comparing the effects of cooking with different coefficients for each noodle batch. Statistical analyses were conducted using SPSS 22.0 software (SPSS Inc., Chicago, USA) and Origin 2021b (Origin Lab Corporation, Northampton, MA, USA).

3. Results and discussion

3.1. Stable isotope distributions in cooked noodles grouped according to the formulations

The stable hydrogen and oxygen isotopic ratios (δ^2H and $\delta^{18}O$) in cooked noodles, grouped according to the formulations, are presented in Fig. 1, Tables 1 and 2. These results demonstrate significant variations in isotopic distributions across different noodle formulations, regardless of the isotopic composition of the cooking water.

Fig. 1A illustrates the distribution of δ^2H values in the cooked noodles, which are grouped based on formulation. Noodles from the initial formulation (0:100 gluten-to-starch ratio) exhibited δ^2H values ranging from −57.2 ± 0.1‰ in HA water to −27.1 ± 0.2‰ in HF water (Fig. 1A and Table 1). The δ^2H significantly decreased with increased gluten content, as evidenced by the 100:0 formulation exhibiting a more depleted δ^2H range from −86.5 ± 0.1‰ in HA to −63.3 ± 0.2‰ in HF (Table 1). This indicates that the δ^2H values in noodles were negatively correlated with the increase in gluten proportion. Similarly, for $\delta^{18}O$ (Fig. 1B and Table 2), the 0:100 formulation showed minimal variation across treatments, maintaining values around 26.5 ± 0.2‰. However, as the gluten-to-starch ratio increased to 100:0, there was a marked isotopic enrichment, with values ranging from 32.7 ± 0.3‰ in OA to 33.6 ± 0.2‰ in OF (Table 2). This pattern underscores a clear influence of noodle composition (based on formulation) on isotopic variations during cooking.

Previous studies have established a range of global δ^2H values in wheat, which can be influenced by botanical and environmental factors (Laursen et al., 2016; Rashmi et al., 2017; Wadood et al., 2019). The results of the current study suggest that the isotopic composition of noodles also depends significantly on their gluten-to-starch ratio, a factor not extensively covered in existing literature. Meanwhile, in C_3-plants, the relative ^2H abundance of organic compounds were in the following sequence (ranging from most to least abundance): amino acid > organic acid > carbohydrates > bulk materials > protein) (Dahal and Schmit, 2018). The isotopic fractionation observed can be attributed to metabolic pathways during biosynthesis, where starch enrichment correlates with ^2H content (Yakir and DeNiro, 1990). This aligns with theories proposing that increased starch levels under photoheterotrophic conditions enhance isotopic signatures due to metabolic activities in the chloroplast, impacting the reductive pentose phosphate pathway.

3.2. Effect of different water isotope compositions on the stable isotope of eight formulated noodles

The δ^2H and $\delta^{18}O$ of eight different wheat noodle formulations (0:100, 15:85, 30:70, 45:55, 55:45, 70:30, 85:15, and 100:0) were evaluated after boiling in water with varying isotopic compositions (HA-HF). The results are presented in Figs. 2 and 3, respectively.

Fig. 2 shows a clear trend of increasing δ^2H with increasing isotopic abundance of water, with significant differences indicated by the letters in all panels (A-H). This suggest that a strong influence of the water abundance on the cooked noodles' δ^2H value and the isotope exchange may occur between noodles and the cooking water. Each formulation exhibits a distinct range of δ^2H. Notably, the δ^2H in panels C (formulation of 30:70), D (formulation of 45:55) and E (formulation of 55:45) ranged from approximately-70‰ to −30‰, −80‰ to-40‰, −90‰ to −40‰, respectively, showing a broader range than other formulations. This broader range indicates an even stronger impact of the water's isotopic composition on these noodles' δ^2H.

Fig. 3 explores the $\delta^{18}O$ values for the same noodle batches, cooked under different water isotopic conditions (OA-OF). The $\delta^{18}O$ values show a more stable trend compared to δ^2H, with significant differences primarily observed at higher isotopic compositions of the cooking water.

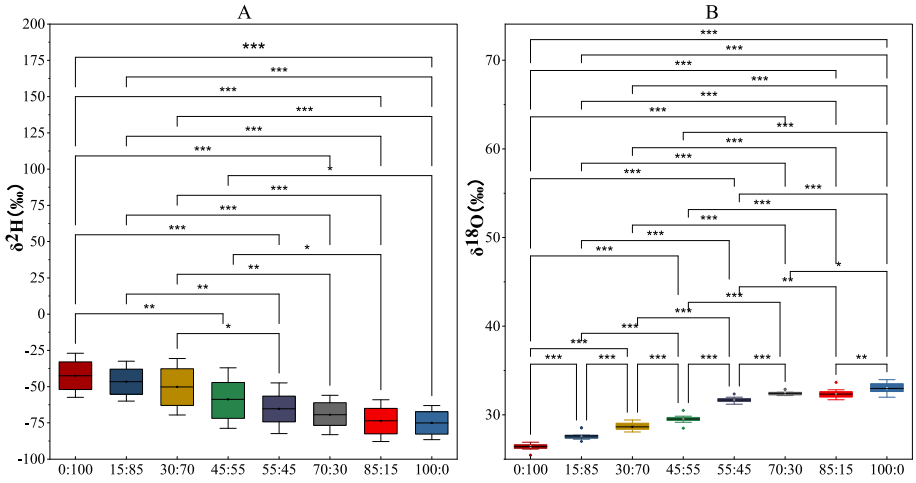

Fig. 1. Boxplot of δ^2H (A)and $\delta^{18}O$(B) wheat noodles considered together boiled in water with different abundances grouped according to the formulations. Significantly different mean values are indicated with different symbols based on Turkey's HSD test (*$p < 0.05$, **$p < 0.01$, ***$p < 0.001$).

Table 1
Stable hydrogen isotopic ratios (δ^2H) of eight differently formulated noodles boiled in water varying in isotopic abundance.

Gluten: Starch (w:w)	Uncooked noodles	Treatment (water abundance of hydrogen isotope)					
		HA (−160‰)	HB (−124.8‰)	HC (−78.8‰)	HD (−33.5‰)	HE (+12.8‰)	HF (+50.0‰)
0:100	−39.4 ± 0.7	−57.2 ± 0.1	−52.2 ± 0.2	−45.5 ± 2.1	−39.0 ± 0.6	−32.6 ± 0.3	−27.1 ± 0.2
15:85	−44.1 ± 0.1	−60.0 ± 0.0	−55.4 ± 0.2	−49.2 ± 0.7	−43.5 ± 0.5	−37.3 ± 0.6	−32.4 ± 0.0
30:70	−45.6 ± 1.4	−69.4 ± 0.1	−62.9 ± 0.3	−54.3 ± 0.5	−46.0 ± 0.3	−37.7 ± 0.1	−30.7 ± 0.1
45:55	−54.7 ± 0.1	−78.5 ± 0.3	−72.3 ± 0.4	−62.5 ± 0.8	−54.1 ± 0.8	−46.0 ± 1.1	−37.5 ± 0.5
55:45	−62.5 ± 1.3	−81.1 ± 1.3	−74.9 ± 0.6	−68.7 ± 1.0	−59.7 ± 0.1	−56.2 ± 0.3	−49.4 ± 2.0
70:30	−65.8 ± 0.2	−82.6 ± 0.5	−76.9 ± 0.2	−70.5 ± 1.6	−65.1 ± 0.3	−60.9 ± 0.3	−56.8 ± 0.8
85:15	−71.9 ± 1.0	−87.5 ± 0.4	−82.6 ± 0.2	−76.6 ± 0.5	−70.1 ± 0.7	−65.0 ± 0.3	−59.6 ± 0.6
100:0	−74.1 ± 0.2	−86.5 ± 0.1	−82.7 ± 0.2	−77.4 ± 1.3	−72.8 ± 0.0	−67.3 ± 0.3	−63.3 ± 0.2

Note: HA—HF indicated the cooking water with different hydrogen isotopic abundance.

Table 2
Stable oxygen isotopic ratios ($\delta^{18}O$) of eight differently formulated noodles boiled in water varying in isotopic abundance.

Gluten: Starch (w:w)	Uncooked noodles	Treatments (water abundance of oxygen isotope)					
		OA (−22.9‰)	OB (−10.8‰)	OC (29.7‰)	OD (47.8‰)	OE (60.8‰)	OF (99.9‰)
0:100	26.5 ± 0.3	26.2 ± 0.7	26.5 ± 0.1	26.4 ± 0.2	26.4 ± 0.2	26.6 ± 0.3	26.4 ± 0.2
15:85	27.7 ± 0.2	27.2 ± 0.1	27.4 ± 0.1	27.6 ± 0.1	27.6 ± 0.2	27.8 ± 0.3	28.0 ± 0.4
30:70	28.6 ± 0.7	28.3 ± 0.3	28.7 ± 0.4	28.7 ± 0.3	28.3 ± 0.2	29.1 ± 0.4	28.8 ± 0.4
45:55	29.3 ± 0.3	29.3 ± 0.0	29.2 ± 0.7	29.6 ± 0.1	29.6 ± 0.0	29.6 ± 0.2	29.8 ± 0.7
55:45	31.2 ± 0.7	31.4 ± 0.1	31.4 ± 0.2	31.5 ± 0.2	31.8 ± 0.1	31.8 ± 0.2	32.1 ± 0.3
70:30	32.4 ± 0.3	32.3 ± 0.1	32.2 ± 0.0	32.3 ± 0.1	32.5 ± 0.1	32.7 ± 0.2	32.7 ± 0.2
85:05	32.1 ± 0.5	31.8 ± 0.1	32.0 ± 0.0	32.3 ± 0.2	32.5 ± 0.1	32.8 ± 0.1	32.8 ± 0.0
100:0	32.7 ± 0.4	32.7 ± 0.3	33.2 ± 0.3	33.1 ± 0.2	33.4 ± 0.3	33.7 ± 0.2	33.6 ± 0.2

Note: OA—OF indicated the cooking water with different oxygen isotopic abundance.

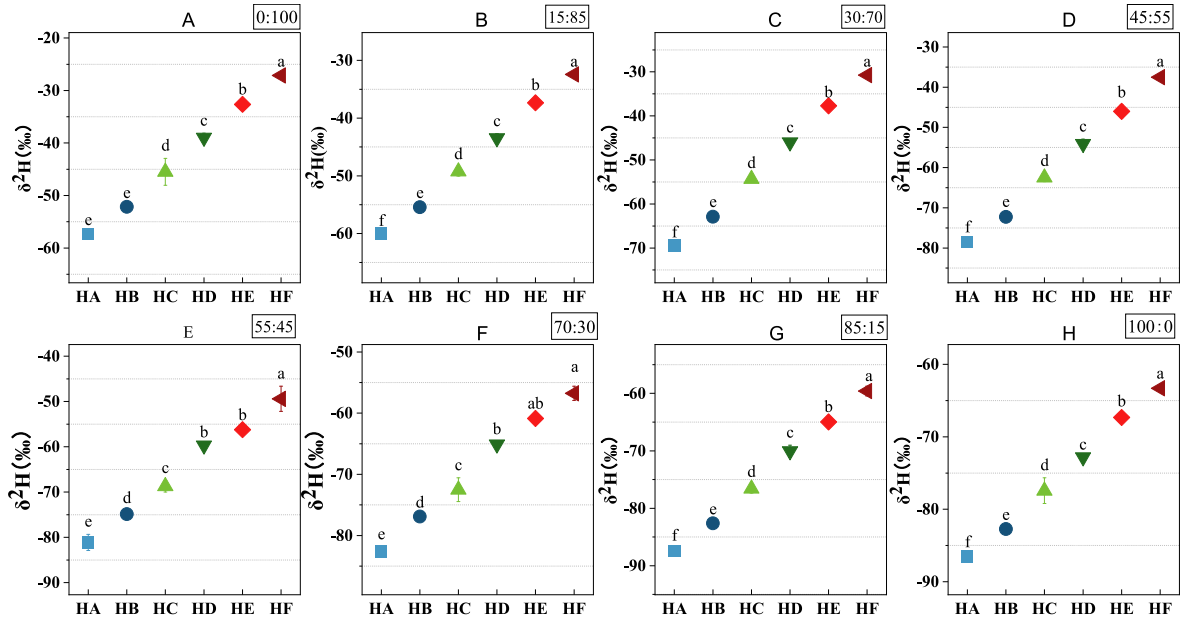

Fig. 2. Stable hydrogen isotopic ratios in eight differently formulated wheat noodles (A–H) boiled in water with increasing isotopic abundance (HA-HF). Significantly different mean values as indicated with different letters based on Turkey's HSD test ($p < 0.05$).

For example, when the noodle with 100% starch is cooked in OA water, the $\delta^{18}O$ value is around 26.2 ± 0.7‰, but it only slightly increases to approximately 26.4 ± 0.2‰ when cooked in OF water.

In summary, both δ^2H and $\delta^{18}O$ values in noodles are influenced by the isotopic composition of the cooking water. However, δ^2H exhibits a more pronounced response compared to $\delta^{18}O$. Different noodle formulations show distinct isotopic ranges, indicating that formulation composition also plays a critical role in isotopic uptake. The significant differences observed through Tukey's HSD test confirm the robustness of the isotopic variations due to noodle formulation and the isotopic composition of the water composition.

3.3. Effects of formulation, cooking water abundance and their interactions on δ^2H and $\delta^{18}O$ in noodles with different formulations

In this investigation, linear regression models were utilized to rigorously analyse the influence of formulation and cooking water on isotopic variations in noodles. The selection of linear regression was predicated on its demonstrated efficacy in modelling the quantitative relationships between independent variables (formulation and water abundance) and dependent variables (isotopic values of δ^2H and $\delta^{18}O$). This statistical methodology enables the prediction of isotopic alterations based on specified formulation and isotopic signatures of the

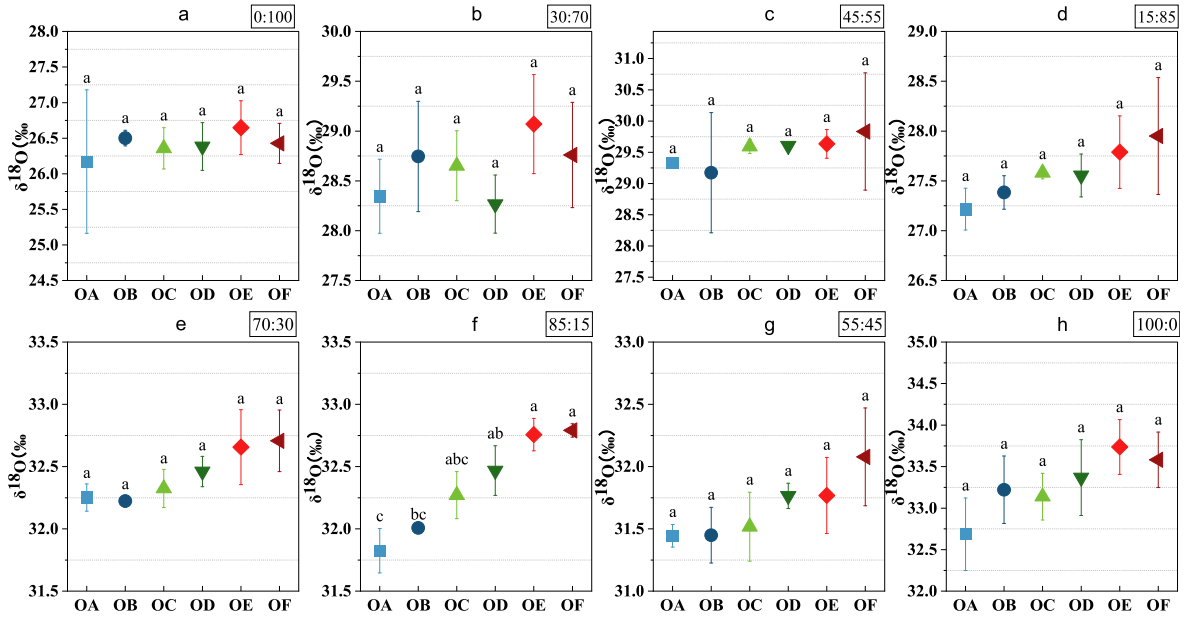

Fig. 3. Stable hydrogen isotopic ratios in eight differently formulated wheat noodles (a–h) boiled in water with increasing isotopic abundance (OA-OF). Significantly different mean values are indicated with different letters based on Turkey's HSD test ($p < 0.05$).

cooking water, facilitating the precise interpretation of the interactive effects of these variables. Due to the δ^2H in uncooked noodles ranging from −74.1‰ to −39.4‰, the water used in the current study could be divided into two categories: 1)δ^2H of water higher than all noodle samples and 2)δ^2H lower than all noodle samples. Thus, the combinations of the cooking waters' isotopic abundance were grouped into six ranges.

The first linear model (LM1) evaluated the correlation between δ^2H and formulation. In contrast, the second model (LM2) incorporated an additional coefficient for cooking (i.e., cooked vs uncooked values with no regard for water abundance). Table 3 summarizes the results for the different abundance of water utilized. R^2 represents the proportion of variance for δ^2H that is predictable from the independent variables (formulation and water abundance). The R^2 values of all water abundance combinations ranged from 0.66 to 0.94, indicating a good to excellent fit for the models across different water abundance ranges. A higher R^2 value in LM2 suggest that it might be a more refined or adjusted model than LM1. All p-values were <0.01, indicating that the models were statistically significant, affirming that changes in δ^2H are strongly associated with the tested variables. The Beta values indicates the average degree and direction of changes in δ^2H due to interactions between water abundance and formulation. δ^2H is highly responsive to cooking, reflecting significant shifts likely due to evaporation or hydrogen exchange processes. This aligns with findings from other studies, where cooking and water sources significantly impact δ^2H values due to the sensitivity of hydrogen isotopes to environmental conditions (Wadood et al., 2019; Yang et al., 2024).

Similarly, LM1 evaluated the correlation between $\delta^{18}O$ and formulation, and LM2 added a coefficient for the cooking status. Table 4 summarizes the results for the different abundance of water utilized. R^2 values of LM1 were generally low among all models, ranging from 0.11 to 0.37, suggesting a weaker fit compared to the models for δ^2H. Similar to LM1, the R^2 of LM2 was also low, suggesting that adding the cooking factor did not improve the explanatory power of the model. The lower R^2 values for $\delta^{18}O$ imply that the models, whether including heating or not, were less effective at explaining variations in $\delta^{18}O$, indicating its relative stability against processing factors like cooking. Significance levels of the models (p-values) were generally low but acceptable (mostly below 0.05). The Beta values showed minor variations between cooked and uncooked states. This suggests that $\delta^{18}O$ remains stable, showing minimal response to cooking. Gat (1996) explored $\delta^{18}O$ stability in water molecules within biological and environmental samples, finding that $\delta^{18}O$ remains relatively unaffected by temperature changes compared to δ^2H. This stability is due to the stronger bond in the oxygen-hydrogen pair, which is less susceptible to exchange reactions. The minimal changes in $\delta^{18}O$ with the inclusion of cooking in the regression model align with these findings, suggesting that $\delta^{18}O$ in the samples remained stable despite boiling processing. This stability makes $\delta^{18}O$ a reliable indicator for the original water source or geographical origin, less influenced by post-collection processes such as cooking.

The influence of water abundance seems to be more pronounced in δ^2H values than in $\delta^{18}O$. In δ^2H, different ranges of water abundance significantly affect the model fits and coefficients, possibly due to the isotopic signature of the water used in the formulation or cooking process. The consistency of the significant model performance across both isotopes suggests that the formulations themselves (ingredients, isotopic

Table 3
The results from the first (LM1) and second (LM2) linear models on the δ^2H, showing the R^2 value, a p-value of the model, the p-value of the cooked-uncooked coefficient, the Beta value, and the confidence intervals (CI), for six different cooking water abundance ranges.

Cooking water abundance combination	−160 to −78.8 ‰		−160 to −124.8‰		−124.8 to −78.8‰		−33.5 — +50 ‰		−33.5 – +12.8‰		+12.8 — +50 ‰	
	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2
Model R^2	0.81	0.86	0.66	0.93	0.81	0.92	0.83	0.88	0.92	0.94	0.81	0.89
p-Model	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Cooked-Uncooked p-value		<0.01		<0.01		<0.01		<0.01		<0.01		<0.01
Beta	−5.01	−11.8	−4.88	−15.41	−5.05	−8.94	−5.42	6.84	−5.33	3.93	−5.38	7.93
CI 2.5		−5.56		−17.67		−11.19		4.02		1.94		4.99
CI 97.5		−4.47		−13.15		−6.69		9.65		5.92		10.88

Table 4
The results from the first (LM1) and second (LM2) linear models on the $\delta^{18}O$, showing the R^2 value, a *p*-value of the model, the *p*-value of the heated-unheated coefficient, the Beta value, and the confidence intervals (CI), for six different water abundance ranges.

Cooking water abundance combination	−22.9 to −10.8 ‰		27.9–99.9‰		27.9–60.8‰		29.7–49.8 ‰		49.8–99.9‰		49.8–60.8‰		60.8–99.9‰	
	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2	LM1	LM2
Model R^2	0.11	0.11	0.37	0.37	0.26	0.26	0.12	0.12	0.27	0.27	0.13	0.14	0.14	0.15
P-Model	0.02	0.08	0.01	0.01	0.01	0.01	0.02	0.06	0.01	0.01	0.01	0.04	0.01	0.03
Cooked-Uncooked *p*-value		0.84		0.63		0.72		0.89		0.60		0.69		0.54
Beta	−0.32	−0. 13	−0.63	0.26	−0.52	0.21	−0.35	0.09	−0.54	0.32	−0.37	0.28	−0.39	0.43
CI 2.5	−0.04	1.23	−0.44	1.33	−0.30	1.39	−0.06	1.46	−0.32	1.52	−0.09	1.66	−0.10	1.83
CI 92.5	−0.60	−1.49	−0.81	−0.81	−0.75	0.97	−0.63	−1.29	−0.77	−0.88	−0.66	−1.11	−0.68	−0.97

composition) strongly correlate with δ^2H and $\delta^{18}O$ values. However, the impact of formulations may be obscured by cooking effects, especially for $\delta^{18}O$ where these processes did not yield significant differences. The results also indicate that the wheat isotopic signature will be unavoidably changed during cooking indicating the isotope exchange between the external cooking water and the macro-substance in noodles like protein, and starch occurred. Hence, a factor for the exchangeability of different wheat-contained products during boiling was required (see section 3.4).

3.4. Calculating the hydrogen isotope exchangeability between cooking water and noodles

According to the results of section 3.2 and section 3.3, the δ^2H in cooked noodles was highly correlated with the δ^2H in cooking water, indicating an exchange of hydrogen isotopes occurred between the external cooking water and hydrogen fractions in the noodles during boiling. Thus, a factor indicating the exchangeability of hydrogen isotopes between each noodle formulation and cooking water is needed.

For this investigation, noodles can be considered to have three parts of reservoirs (A, B and C) of hydrogen isotope. Reservoir A (absorbed water) indicates the absorbed water that can be removed during freeze-drying treatment. Reservoir B (exchangeable hydrogen) consists of the hydrogen that can be exchanged with water during cooking; this part of hydrogen cannot be removed. Reservoir C (non-exchangeable hydrogen) consists of hydrogen and oxygen cannot be exchanged. Based on the isotope mass balance, it can be assumed that the total isotopic composition of H atoms within the cooked noodles can be described as:

$$\delta^2H_{cooked\ noodles}=f\,(H)_{ex}\times\delta^2H_{noodles\text{-}ex}+(1-f(H)_{ex})\times\delta^2H_{cooked\ noodles\text{-}nex} \quad (2)$$

Where $f(H)_{ex}$ is a fraction of H atoms available for exchange, $\delta^2H_{cooked\ noodles\text{-}ex}$ is the isotopic composition of exchangeable H atoms within the samples. The $\delta^2H_{cooked\ noodles\text{-}ex}$ will vary, depending on the isotopic composition of the cooking water available for exchange ($\delta^2H_{cooking\ water}$) and the fractionation α_{ex} between H atoms in water and material, such that:

$$\alpha_{ex}=\delta^2H_{cooked\ noodles\text{-}ex}/\delta^2H_{cooking\ water} \quad (3)$$

We assumed that $f\,(H)_{ex}$ and $\delta^2H_{cook\ noodles\text{-}nex}$ is constant for noodles under exploration. We also explicitly assume that $\alpha_{ex}=1$, as per Bowen et al. (2005). This assumption is counter to most work on exchangeable H in complex biological materials, which assume α is constant throughout an experiment, without explicitly defining a value (Hobson et al., 1996; Schimmelmann et al., 1993). As a result, the following equation is obtained:

$$\delta^2H_{cooked\ noodle}=f\,(H)_{ex}\times\delta^2H_{cooking\ water}+(1-f\,(H)_{ex})\times\delta^2H_{cooked\ noodles\text{-}nex} \quad (4)$$

We calculated the $f\,(H)_{ex}$ within different noodles using the H isotopic composition of the cooked noodles cooked with two isotopically different waters (δ^2H_{w1} and δ^2H_{w2}). Writing Equation (2) for both waters and rearranging give the fraction of exchangeable hydrogen, $f\,(H)_{ex}$, as

$$f\,(H)_{ex}\,(\%)=(\delta^2H_{cooked\ noodle\ 1}-\delta^2H_{cooked\ noodle\ 2})\,/\,(\delta^2H_{w1}-\delta^2H_{w2})\times 100 \quad (5)$$

where $\delta^2H_{cook\ noodles}$ and $\delta^2H_{cook\ noodles\ 2}$ are the δ^2H of the cooked noodles that were boiled by waters w1 and w2. In the current study, the $f\,(H)_{ex}$ was calculated by two pairs of water: 1) HA and HF 2) HB and HC.

Using the two pairs of water, noodles' $f\,(H)_{ex}$ varied substantially with different formulations (Table 5). The results indicated that the $f\,(H)_{ex}$ differences range from 0.1% to 1.5% for the same formulation, depending on the formulation.

The consistency across different water pairs for noodles with a 0:100 starch ratio suggests a stable exchangeability fraction $f\,(H)_{ex}$ close to 14.2%. The slight variation (0.1%) indicates that the exchangeable ability is highly stable for high starch-content noodles. Similar to high starch content, noodles with a 100:0 gluten ratio also exhibit stable $f\,(H)_{ex}$ values around 11.0%–11.2%. Notably, for the 55:45 gluten-to-starch ratio, $f\,(H)_{ex}$ varies from 13.6% to 15.1% across different water pairs. This range (13.6–15.1%) shows a slightly higher variability compared to the extremes (pure starch or pure gluten), indicating that mid-range formulations might have less stable exchangeability fractions. For other formulations such as 15:85 and 85:15, $f\,(H)_{ex}$ values showed minor variations but remained relatively consistent, with differences generally within the 1% range. The variability observed in these intermediate formulations suggests that the interaction between starch and gluten impacts the hydrogen isotope exchange differently than pure components.

The stability of $f\,(H)_{ex}$ across different water pairs and formulations suggests that the hydrogen isotope exchangeability in noodles is largely reliable, with some expected variations due to the molecular interactions within the noodle matrix. The consistent $f\,(H)_{ex}$ values for pure starch and pure gluten noodles imply that the measurement method is robust for these simpler systems. However, the slightly higher variability in mid-range starch ratios suggests that these formulations have more complex interactions, possibly due to the balance of hydrogen bonds between starch and gluten. Compared with other studies, our findings align with Schmidt et al. (2005) who noted similar stability in hydrogen isotope exchangeability in plant tissues. The slight variability in mid-range formulations is also consistent with the observations by Sachse et al. (32) where mixed matrices showed more nuanced isotopic behaviours.

In Table 6, the predicted δ^2H in cooked noodles boiled with cooking water abundance of −78.8‰ and −35.5‰ to validate the model and coefficient is presented. On average, the difference between predicted and estimated values was 2‰, which did not exceed the overall analytical precision of +2‰. However, the difference varied with the change in gluten-to-starch ratios. Meanwhile, we admitted that in Equations (2) and (3), the uncertainty in the isotopic fractionation factor (α_{ex}) can introduce uncertainty into the calculation of $f\,(H)_{ex}$. We assume α is constant throughout the experiment, which is in line with many precious studies (Hobson et al., 1996; Schimmelmann et al., 1993).

Table 5
Calculated fractions (%) of hydrogen isotope exchangeability in each formulated noodle by using different pairs of cooking water.

Gluten: Starch (w:w)								
Pair of water	0:100	15:85	30:70	45:55	55:45	70:30	85:15	100:0
−160 and + 50‰	14.3	13.1	18.4	19.5	15.1	12.3	13.3	11.0
−124.8 and + 12.8‰	14.2	13.1	18.3	19.1	13.6	11.7	12.8	11.2
Average value	14.3	13.1	18.4	19.3	14.4	12.0	13.1	11.1

Table 6
The estimated and predicted δ^2H using the calculated fractions δ^2H for cooked noodles boiled in water with abundances of −78.8‰ and −33.5‰. The difference between measured and predicted values(E_i-P_i) is also given in the table.

Gluten: Starch (w:w)	Estimated 1 (−75.8‰)	Estimated 2 (−33.5‰)	Predicted 1 (−75.8‰)	Predicted 2 (−33.5‰)	Difference 1 (E_1-P_1)	Difference 2 (E_2-P_2)
0:100	−45.5 ± 2.1	−39.0 ± 0.6	−45.0	−38.8	−0.1	−0.1
15:85	−49.2 ± 0.7	−43.5 ± 0.5	−48.7	−43.0	−0.6	−0.5
30:70	−54.3 ± 0.5	−46.0 ± 0.3	−51.7	−43.7	−2.6	−2.3
45:55	−62.5 ± 0.8	−54.1 ± 0.8	−59.4	−51.0	−3.1	−3.1
55:45	−66.2 ± 1.0	−59.7 ± 0.1	−64.8	−58.6	−1.4	−1.1
70:30	−72.5 ± 1.6	−65.1 ± 0.3	−67.4	−62.2	−3.1	−2.9
85:15	−75.6 ± 0.5	−70.1 ± 0.7	−72.8	−67.1	−2.8	−2.9
100:0	−77.4 ± 1.3	−72.8 ± 0.0	−74.6	−69.8	−2.8	−3.0

However, others also used a calculated α value from experimental results (33), or used an assumed α value, ranging from 1.060 to 1.100 (Leyden et al., 2006; Schimmelmann et al., 1999; Wassenaar and Hobson, 2000, 2003). Although these simplified equations were supported in this comparative study, consideration of isotope fractionation between the exchangeable hydrogen and the water should not be overlooked in future studies (Bowen et al., 2005; Wassenaar and Hobson, 2000).

The results also indicate that $f\ (H)_{ex}$ values for noodles with 100% gluten were 11.0%–11.2%. In contrast, noodle samples containing (with starch content from 0 to 85%) had a larger fraction of exchangeable hydrogen atoms, ranging from 11.7% to 19.5‰. This higher exchangeability in starch-containing noodles suggests that the hydrogen atoms in starch are more available for exchange than those in gluten. The results align with the observations of Ehleringer et al. (2000) who reported significant hydrogen isotope exchange in plant tissues exposed to different water sources. The exchangeability fraction $f\ (H)_{ex}$ for plant leaves ranged from 0.10 to 0.20, similar to our findings for starch-rich noodles, suggesting a consistent pattern of exchangeable hydrogen in organic matrices.

Each organic molecule can be assigned a theoretical exchangeable hydrogen pool relative to its total hydrogen atoms based on the molecular model. Common biomolecules like starch, proteins, and simple carbohydrates exist in various molecular structures within environmental matrices(Schimmelmann et al., 2006; Smith and Ziegler, 1990). Carbohydrates with the empirical formula $(C_6H_{10}O_5)_n$, such as starch, contain 70% hydrogen atoms bound to carbon and 30% bound to oxygen in hydroxyl groups, resulting in a theoretical exchangeable hydrogen pool relative to total hydrogen atoms (α) value (α_{theo}) of 30%. For wheat starch, which comprised 25% amylose (α(1 → 4) bound glucose molecules) and 75% amylopectin (α(1 → 4) branched with α (1 → 6) bound glucose molecules) (Sakintuna et al., 2003) (Fig. S1, provided as Supplementary Material). These glucose polymers are known for their linear and helical structures, with weak crystalline regions and minimal intermolecular hydrogen bonding (Tester et al., 2004).

Proteins are composed of amino acids, and the analysed amino acid composition of wheat grains along with their theoretical α values is shown in Table S1 (provided as Supplementary Material) (Péron et al., 2018). Based on this, the theoretical contribution of amino acids to the exchangeable hydrogen in wheat gluten was calculated as $\alpha_{theo} = 37\%$ (Péron et al., 2018). However, intramolecular and inter-strand hydrogen bonds influence the conformation of the three-dimensional gluten network. Proteins consist of various polypeptides, with peptide bonds formed between carboxyl and amine groups (Kim et al., 2008; Richardson, 1981). Each peptide bond formation eliminates two theoretically exchangeable hydrogen atoms from the original amino acid molecules. The three-dimensional gluten structure is stabilized by hydrogen bonds between peptide chains, predominantly forming α-helices and β-sheets, which saturate the hydrogen bond donors and acceptors in the peptide backbone (Nivesse et al., 2021; Wieser, 2007). Additionally, buried hydrogen atoms within the gluten structure further reduce the pool of exchangeable hydrogen atoms. This aligns with Wolf et al. (2011) who reported that intramolecular hydrogen bonding in proteins significantly decreases the pool of exchangeable hydrogen atoms.

Interestingly, the noodles, which comprised 45% of gluten, exhibited a notable increase in hydrogen exchangeability. This result aligns with our previous studies (Yang et al., 2024), which showed that noodles with this specific gluten content had the highest depleted fractionation values ($\Delta\delta^2H$). This may be related to the presence of buried deuterium, as explained by the inertia of the exchangeability phenomenon derived from the local 3D structure, proposed and proved in studies of Nivesse et al. (2021).

3.5. Further discussion

3.5.1. Variability δ^2H and $\delta^{18}O$ in noodles with changes in formulation and cooking water abundance

Previous research has primarily focused on the isotopic characterization of unprocessed agricultural products, noting significant variability linked to geographical and climatic conditions (Bontempo et al., 2016; Camin et al., 2017). Wadood et al. (2019) noted that wheat's isotopic composition varies with water availability during growth, yet the current study illustrates that post-harvest cooking processes can further modify these isotopes significantly. However, the results suggest that processing conditions, specifically water composition and noodle formulation, play equally critical roles.

During cooking, isotopic fractionation may occur through different pathways. A study by van der Zanden et al. (2018) demonstrated that heating processes could lead to significant hydrogen isotope fractionation. The researchers observed up to 28‰ shifts in δ^2H values in organic materials when subjected to heating attributed to the degradation of substances like protein. Other studies demonstrated that isotopes in organic matter will exchange with the water resulting in changes in δ^2H (Filot et al., 2006; Krishnamurthy, 1993; Schimmelmann et al., 1993; Sessions et al., 2004). In our previous study, considering the heat effects solely, the impact of thermal processes like oven heating on

isotopic signatures in noodles were elucidated. Differently, it was found that thermal treatment such as 100 °C in an oven (the temperature when noodles are boiled) did not significantly alter the δ^2H and $\delta^{18}O$ in the noodles. Moreover, the results from this study demonstrate that the δ^2H values in cooked noodles are significantly influenced by the isotopic composition of the cooking water, validating the occurrence of hydrogen isotope exchange.

3.5.2. Hydrogen/oxygen isotope exchangeability between cooking water and noodles

3.5.2.1. Hydrogen isotope exchangeability. The analysis of hydrogen isotope exchangeability between cooking water and noodles provides critical insights into the isotopic dynamics during food processing. The observed exchangeability fractions (f $(H)_{ex}$) ranged from 11.1% to 19.3%, indicating that a notable portion of the hydrogen in the noodles is available for exchange during boiling. This variability suggests that different components within the noodles, such as starch and gluten, have distinct capacities for hydrogen isotope exchange. Specifically, noodles with a higher starch content showed higher exchangeability fractions, while pure gluten noodles exhibited the lowest exchangeability. This can be attributed to the molecular structures of starch and gluten. The variation in the exchangeability fraction across different noodle formulations highlights the complex nature of hydrogen isotope interactions within organic matrices.

Starch, primarily composed of amylose and amylopectin, has a structure that allows more accessible hydroxyl groups, which are prone to isotope exchange. On the other hand, gluten proteins form complex 3D networks with extensive intramolecular and intermolecular hydrogen bonding, limiting the availability of exchangeable hydrogen atoms. This can also explain why the precision of the prediction value varied. The significant hydrogen exchangeability observed in noodles with a 45% gluten composition indicates that the initial structure of the starch-gluten matrix may expose more hydrogen bonds, facilitating greater isotope exchange during cooking. This aligns with previous findings where noodles with this specific gluten content showed the highest depleted fractionation values ($\Delta\delta^2H$). The interplay between starch and gluten likely creates a matrix that balances the accessibility of hydrogen atoms for exchange while maintaining structural integrity.

3.5.2.2. Oxygen isotope stability. In the current study, the $\delta^{18}O$ in the samples remained stable despite water boiling processing. In food matrices, the quantity of exchangeable oxygen is typically limited, particularly when compared to exchangeable hydrogen. This is attributed to the fact that oxygen atoms in biomolecules are often involved in relatively stable chemical bonds, such as C-O, O-H, and P-O bonds. The exchangeability of oxygen atoms depends on their chemical environment within the molecule. In most biomolecules, oxygen is present in stable covalent bonds that are resistant to exchange (Wright, 2017). Even under conditions of heating or under acidic or alkaline environments, most oxygen atoms do not readily exchange, unless subjected to extreme conditions where certain chemical bonds might be broken (Hendry, 2010). Although water is a common medium in food processing, the direct exchange of oxygen between water and food is relatively rare.

The current results have important implications for food authenticity, traceability, and processing optimization. Understanding the isotopic behaviour of different food components can aid in developing robust methods to trace and authenticate the geographical and botanical origins of food products. Additionally, the knowledge of hydrogen isotope exchangeability can be used to refine food processing techniques to enhance product quality and consistency. Further research should focus on expanding the scope of isotope exchange studies to include other food matrices and processing conditions. Investigating the effects of different cooking times, temperatures, and water compositions on isotope exchange can provide a more comprehensive understanding of the factors influencing isotopic dynamics in food.

In summary, this study explored how variations in δ^2H and $\delta^{18}O$ values of cooking water affect the isotopic profiles of noodles with different gluten-to-starch formulations. Noodle formulation and the isotopic composition of cooking water significantly affected the δ^2H in cooked noodles ($p < 0.05$). Additionally, the δ^2H values of noodles varies with the cooking waters abundance changes, indicating that the hydrogen isotope exchanges occurred between noodles and cooking water during boiling. The formulation also had a significant impact on $\delta^{18}O$, however, $\delta^{18}O$ in the samples remained stable despite boiling processing and water abundance of cooking water.

An equation for determining the exchange factor ($f(H)_{ex}$) was developed in the study. The fraction of hydrogen atoms in different noodles for exchange was highest at 19.3% in noodles with the formulation of 45:55 (gluten-to-starch) and lowest at 11.1% in noodles with 100% gluten. The findings highlight the significant role of molecular structure in determining the exchangeability of hydrogen isotopes, with starch-rich noodles exhibiting higher exchangeability compared to gluten-rich noodles. This study also provides a new insight to understand the isotopic behaviour of different food components aiding in developing methods to trace and authenticate the geographical and botanical origins of food products. Additionally, the knowledge of hydrogen isotope exchangeability can be used to refine food processing techniques to enhance product quality and consistency.

CRediT authorship contribution statement

Jingjie Yang: Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft. **Sara W. Erasmus:** Formal analysis, Visualization, Writing – original draft, Writing – review & editing. **Qianqian Sun:** Formal analysis, Validation. **Yingquan Zhang:** Resources. **Ming Li:** Resources. **Bo Zhang:** Resources. **Boli Guo:** Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Supervision, Writing – original draft, Writing – review & editing. **Saskia M. van Ruth:** Conceptualization, Methodology, Supervision, Writing – original draft, Writing – review & editing.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.crfs.2025.101024.

Data availability

Data will be made available on request.

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