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Published in:
Rapid Communications in Mass Spectrometry

DOI:
[10.1002/rcm.7232](https://doi.org/10.1002/rcm.7232)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2015

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Faghihi, V., Meijer, H. A. J., & Groening, M. (2015). A thoroughly validated spreadsheet for calculating isotopic abundances (H-2, O-17, O-18) for mixtures of waters with different isotopic compositions. *Rapid Communications in Mass Spectrometry*, 29(15), 1351-1356. <https://doi.org/10.1002/rcm.7232>

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Rapid Commun. Mass Spectrom. 2015, 29, 1351–1356
(wileyonlinelibrary.com) DOI: 10.1002/rcm.7232

A thoroughly validated spreadsheet for calculating isotopic abundances (^2H , ^{17}O , ^{18}O) for mixtures of waters with different isotopic compositions

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RATIONALE: Oxygen and hydrogen stable isotopes are widely used tracers for studies on naturally occurring and laboratory mixtures of isotopically different waters. Although the mixing calculations are straightforward to perform, there are ample possibilities to make mistakes, especially when dealing with a large number of mixed fluids. To facilitate isotope mixing calculations and to avoid computational mistakes, a flexible tool to carry out these calculations is in demand.

METHODS: We developed, in three independent efforts, spreadsheets to carry out the mixing calculations for a combination of waters with different isotopic compositions using the isotope mass balance equation. We validated our calculations by comparison of the results of the three spreadsheets for a large number of test calculations. For all the cases, we obtained identical results down to the 12th to 14th significant digit.

RESULTS: We present a user-friendly, thoroughly validated spreadsheet for calculating ^2H , ^{17}O and ^{18}O stable isotopic abundances and respective isotope delta values for mixtures of waters with arbitrary isotopic compositions. The spreadsheet allows the mixing of up to 10 different waters, of which up to five can be specified using their isotopic abundances and up to five others using their isotope delta values. The spreadsheet is implemented in Microsoft Excel and is freely available from our research groups' websites.

CONCLUSIONS: The present tool will be applicable in the production and characterization of singly and doubly labeled water (DLW) mother solutions, the analysis of isotope dilution measurements, the deduction of unknown isotope values of constituents for mixtures of natural waters, and many other applications. Copyright © 2015 John Wiley & Sons, Ltd.

Stable isotope mixing calculations are used for studies on naturally occurring interactions between different water bodies: ground water with surface waters (river, lake, stream, wetland, or sea water),^[1–6] ground water/surface water and precipitation interactions,^[7–10] river and lake/ocean interactions,^[11–15] and in addition, in laboratory applications such as the use of the isotope dilution technique, and the production of enriched and diluted mixtures for pharmaceutical and biological studies.^[16–20]

Isotopic compositions mix conservatively. The isotopic abundances of a mixture are simply related to the isotopic abundances of the isotopes in each component and the mole fraction of the individual components. While the calculations seem straightforward to perform using simple expressions, they are nevertheless complicated, with ample possibilities of making mistakes. This is especially the case when dealing with the mixing of waters of which some are specified with their isotopic abundances and others with delta values. Also, the calculations become more complex when the number of

mixed fluids increases. To facilitate isotope mixing calculations and to avoid computational mistakes, we developed a flexible spreadsheet. The spreadsheet allows users to compute the isotopic abundances and respective isotope delta values for a mixture of isotopically different waters based on the exact masses and the isotopic compositions of the constituents of the mixture. We are not the first to develop and disseminate such tools; earlier approaches were, however, limited to a rather specific area, such as C and N isotopes for ecology,^[21,22] and hydrogen isotopes in biogeochemistry.^[23,24] These authors, however, have not adapted their spreadsheets for isotope-enriched compounds, nor did they facilitate gravimetric mixing of multiple compounds. To our knowledge, this spreadsheet is also the first that facilitates specification of the compounds to be mixed in both isotope delta and isotope abundance statements. Our product is, however, limited to the mixing of water (although extension to other isotopes would be straightforward).

In the following sections, we first explain our calculation procedure and the way in which we checked our calculations. We then describe the structure of the spreadsheet. Some example applications of the spreadsheet are provided at the end of the paper.

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COMPUTATIONAL PROCEDURE

The isotopic abundances of a mixture are calculated using the isotope mass balance equation:^[25]

$$\chi^{(i)E}_T = x_1\chi^{(i)E}_1 + x_2\chi^{(i)E}_2 + \dots + x_n\chi^{(i)E}_n \quad (1)$$

where x is the mole fraction of the individual substances combined to generate the mixture T and $\chi^{(i)E}_n$ represents the isotopic abundance of isotope iE of element E in each substance, labeled here by the subscripts $n=1, 2$, and so on. This equation is in principle all that is required to determine the isotopic compositions of a mixture. However, the necessary input variables need to be computed first. Normally the masses (or weights) of the individual waters are known, and the mole amounts need to be computed using the molar mass of the specific water. Table 1 provides the isotopic masses required for these calculations.^[26] Next, the isotopic content of the individual waters will not always be expressed as isotopic abundances, but often as isotope delta values. In the latter case, their values refer to the international reference material, the water VSMOW (Vienna Standard Mean Ocean Water).^[27] Using the isotopic abundances of VSMOW, also given in Table 1, we can compute the isotopic abundances.

While the conversion of mass to moles is simple, it depends on the isotopic composition of the waters. The calculation of isotopic abundances from delta values is somewhat more complicated. Isotope delta values are defined as:

$$\delta^iE = \left(\frac{R_{\text{sample}}}{R_{\text{reference}}} - 1 \right) \quad (2)$$

where R_{sample} and $R_{\text{reference}}$ are the absolute ratios of the rare isotope i to the most abundant isotope of element E , in sample and reference (VSMOW), respectively. The isotope ratio of the sample, as the only unknown, can then be calculated by using the known delta value and the $R_{\text{reference}}$ of VSMOW (see Table 1). This ratio can then be converted into the isotopic abundances by using the following formulae for a two-isotope element (e.g., hydrogen, $i=1, 2$):

$${}^2F = \frac{{}^2R}{1 + {}^2R} \quad (3)$$

$${}^1F = 1 - {}^2F \quad (4)$$

Table 1. Data needed for the conversion of water masses to moles, and from isotope delta values to isotopic abundances

Isotope	Isotopic mass (g/mol)	Absolute isotopic ratio of VSMOW	Isotopic abundance of VSMOW
${}^1\text{H}$	1.0078250		0.99984426
${}^2\text{H}$	2.0141018	0.00015574	0.00015574
${}^{16}\text{O}$	15.9949146		0.99762058
${}^{17}\text{O}$	16.9991317	0.0003799	0.00037900
${}^{18}\text{O}$	17.9991610	0.0020052	0.00200043

and, for a three-isotope element (e.g., oxygen, $i=16, 17, 18$):

$${}^{18}F = \frac{{}^{18}R}{1 + {}^{17}R + {}^{18}R} \quad (5)$$

$${}^{17}F = \frac{{}^{17}R}{1 + {}^{17}R + {}^{18}R} \quad (6)$$

$${}^{16}F = 1 - ({}^{17}F + {}^{18}F) \quad (7)$$

As can be seen in the equation above, ${}^{18}F$ is a function of both ${}^{18}R$ and ${}^{17}R$ which makes it impossible to calculate ${}^{18}F$ without knowing ${}^{17}R$. However, the determination of $\delta^{17}\text{O}$ values is less common than for $\delta^{18}\text{O}$ values, because of experimental difficulties and because the $\delta^{17}\text{O}$ value in general does not yield extra information. Where the $\delta^{17}\text{O}$ value is not known, it is derived from its natural relationship with the $\delta^{18}\text{O}$ value using:

$$1 + \delta^{17}\text{O} = (1 + \delta^{18}\text{O})^\lambda \quad (8)$$

where λ is 0.5281.^[28] (we use all four digits for the sake of numerical exactness). Of course this relationship will only hold for natural waters, as all production processes for isotopically enriched oxygen (enriched in ${}^{18}\text{O}$) change the natural ${}^{17}\text{O}/{}^{18}\text{O}$ proportion significantly. For non-natural waters (such as highly ${}^{18}\text{O}$ -enriched waters) the $\delta^{17}\text{O}$ value (or ${}^{17}F$ directly) must be provided separately. Using the $\delta^{17}\text{O}$ value, ${}^{17}R$ and the oxygen isotopic abundances follow using Eqns. (2) and (5)–(7).

When the isotopic abundances are known (either directly, or through the calculations illustrated above), the masses U of oxygen and hydrogen in the individual fluids are calculated by:

$$U = \sum u_i\chi^{(i)E}, \quad i = 1 \text{ to } n \quad (9)$$

where $\chi^{(i)E}$ refers to the isotopic abundance of isotope i of element E and u is its respective atomic mass. For example, the average atomic mass of the element hydrogen in its natural composition = $((1 - 0.00015574) \times 1.0078250) + (0.00015574 \times 2.0141018) = 1.00798175$.

Then the molar mass of water is calculated as the sum of the average atomic masses of 2 hydrogen atoms and 1 oxygen atom. Subsequently, the number of moles for each component is obtained by dividing the mass^a of the component used in the mixture by the calculated molar mass of the component. Given the number of moles for each component in the mixture, and the total number of moles in the mixture by taking the sum of all the moles, we calculated the mole fraction x_n ($n=1, 2, \dots$) of each component in the final mixture.

Eventually, using the calculated mole fractions x_n and the isotopic abundances of hydrogen and oxygen $\chi^{(2,17,18)E}_n$ in each component, Eqn. (1) yields the isotopic abundances of the mixture. From these, the isotope ratios of the mixture can be calculated:

^aFor the preparation of laboratory mixtures of natural and highly enriched water one has to be cautious when weighing the amounts of water: as the density of the waters is different, one has to apply a slightly different buoyancy correction. See Faghihi *et al.*^[29] and Davis.^[30]

$${}^2R = \frac{{}^2F}{1 - {}^2F} \quad (10)$$

$${}^{17}R = \frac{{}^{17}F}{1 - {}^{17}F - {}^{18}F} \quad (11)$$

$${}^{18}R = \frac{{}^{18}F}{1 - {}^{17}F - {}^{18}F} \quad (12)$$

and, finally, from these ratios the delta values are determined using Eqn. (2) and the absolute ratios for VSMOW (see Table 1).

Using these equations assumes a pure stochastic distribution: all stable isotopes are randomly distributed over all possible isotopologues. This assumption is generally considered to be valid beyond any achievable measurement precision.

SPREADSHEET DEVELOPMENT

It is not difficult to implement the calculations explained above into an Excel spreadsheet. Nevertheless, as all researchers in the field of isotopes will admit, it is a complicated task to fulfil, with ample possibilities to make slight mistakes that remain unnoticed.

Therefore, the three authors deliberately performed this task fully independently in three approaches. We then compared the results of the three spreadsheets for a large number of test calculations. For all the cases, the three spreadsheets give identical results down to the 12th to 14th significant digit, which is the numerical precision one can expect. After this convincing evidence that all calculations were correct, we developed the present tool as a user-friendly version of the independent spreadsheets.

The spreadsheet is organized in five sections:

- Isotopic abundances inputs
- Isotope δ -values inputs
- Basic data and calculation cells
- Isotopic abundances outputs
- Isotope δ -values outputs

For the calculation of the isotopic abundances in a mixture of waters with different isotopic compositions, the user can enter delta values (with respect to VSMOW, Eqn. (2)) and/or elemental isotopic abundance fractions for the elements hydrogen and oxygen in waters (see Eqns. (3)–(7)). Note that the isotopic abundance fractions of all the isotopes of any given element add up to 1.

The spreadsheet allows the input of up to 10 fluids in which up to five fluids are entered with their isotopic abundance fractions and masses in the first section and up to five others with their delta values and masses in the second section.

The spreadsheet's inputs can only handle waters that are either fully specified in terms of isotopic abundances or in terms of isotope delta values. In case a water is specified by, for example, ${}^2\text{H}$ as abundance and ${}^{18}\text{O}$ (and ${}^{17}\text{O}$) as delta values, it is advised to convert the isotope delta values into their respective isotopic abundances using the isotope ratios of VSMOW, as given in Table 1 and Eqns. (2) and (5)–(7). This

calculation can easily be done using the spreadsheet, by entering the delta value(s) and any mass in the appropriate fields. The spreadsheet will then produce the correct isotopic abundances that are equivalent to the delta values. The abundance(s), together with the known abundance(s) of the other isotope(s), can subsequently be entered in the abundance input fields of the spreadsheet for mixture calculations.

All the data needed for calculations (Table 1) are present in the basic data section. They are visible to the user, but cannot be altered. They can, however, be copied into other fields. The calculations follow the line as presented above. All calculation cells have been made invisible. Further, the sheet has been protected in such a way that none of the cells except data entry cells can be changed by the user. For the final mixture, both the calculated isotopic abundance fractions and the delta values are shown in the spreadsheet outputs. The protection has been arranged only to prevent accidental changes and errors. However, the password is provided, such that the data and calculations can be inspected should a user desire to do so (in addition to unprotecting the worksheet, the calculations should be restyled to "general" to make them visible). The total spreadsheet occupies 26 rows of cells and is 27 columns wide. It can be copied and pasted in its entirety (when protection is turned off) such that a single worksheet can hold multiple mixing calculations. In Fig. 1 we present calculations using the spreadsheet for three quite different input cases, in which we mix some waters from the following list: distilled natural water ($\delta^2\text{H} = -42.7$ ‰, $\delta^{18}\text{O} = -6.32$ ‰), two other natural waters: slightly depleted ($\delta^2\text{H} = -120$ ‰, $\delta^{18}\text{O} = -13.5$ ‰) and strongly depleted water ($\delta^2\text{H} = -424.5$ ‰, $\delta^{18}\text{O} = -53.99$ ‰), pure ${}^2\text{H}$ water (${}^2\text{H}$ fraction = 99.993 ‰, ${}^{18}\text{O}$ fraction = 0.8998 ‰, ${}^{17}\text{O}$ fraction = 0.0874 ‰), and ${}^{18}\text{O}$ -enriched water (${}^{18}\text{O}$ fraction = 96.05 ‰, ${}^{17}\text{O}$ fraction = 1.176 ‰, ${}^2\text{H}$ fraction = 0.1791 ‰). The latter two are examples of commercially available products, of which we determined the isotopic abundances.

APPLICATIONS OF THE SPREADSHEET

The immediate cause for developing and thoroughly testing this spreadsheet was our recent production of a new series of stable isotope labeled reference waters from gravimetric mixing of natural water with pure ${}^2\text{H}$ and highly ${}^{18}\text{O}$ -enriched waters.^[29] For this work, many, and sometimes iterative, calculations of the isotope values of mixtures had to be performed, and we developed the present spreadsheet as a versatile tool for this work. As it is Excel-based, it can also easily be incorporated into larger Excel calculation structures, which was indispensable for the work presented in Faghghi *et al.*^[29] The isotopic values of both the pure ${}^2\text{H}$ water and the highly ${}^{18}\text{O}$ -enriched water were not accurately known from certifications, and were not specified at all for the non-enriched isotopes. Figures 1(b) and 1(c) are screenshots of the spreadsheet for this case study. As the water in the second set of rows is natural, the spreadsheet uses the natural relationship between the $\delta^{18}\text{O}$ and $\delta^{17}\text{O}$ values to calculate the $\delta^{17}\text{O}$ value for that natural water. This equally holds for the natural waters in the other examples.

Another application, somewhat related to the previous, is the production and characterization of doubly labeled water (DLW) mother solutions for administration to subjects of

ITEM	FLUID	Isotopic abundance 2H	Isotopic abundance 18O	Isotopic abundance 17O	Mass (g)
	FLUID 1				
	FLUID 2				
	FLUID 3				
	FLUID 4				
	FLUID 5				
ITEM	fluid	δ^{2H} (‰)	δ^{18O} (‰)	δ^{17O} (‰)	Mass (g)
natural water	fluid 1	-42.7	-6.32		15.36636
slightly depleted	fluid 2	-120	-13.5		9.745
strongly depleted	fluid 3	-424.5	-53.99		5.2326
	fluid 4				
	fluid 5				
Constants :					Mixture :
Isotopes	Isotopic masses (g/mol)	Absolute isotopic ratios of VSMOW	Isotopic abundances of VSMOW		isotopic abundance 2H
1H	1.0078250		0.99984426		0.0001349685
2H	2.0141018	1.5576E-04	0.00015574		isotopic abundance 17O
16O	15.9949146		0.99762058		0.0003756100
17O	16.9991317	3.799E-04	0.00037900		isotopic abundance 18O
18O	17.9991610	2.0052E-03	0.00200043		0.0019668006
					δ^{2H} (‰)
					-133.3675
					δ^{17O} (‰)
					-8.9711
					δ^{18O} (‰)
					-16.8470
					total mass of mixture
					30.34396

(a)

ITEM	FLUID	Isotopic abundance 2H	Isotopic abundance 18O	Isotopic abundance 17O	Mass (g)
2H enriched	FLUID 1	0.99993	0.008998	0.000874	20.9764
	FLUID 2				
	FLUID 3				
	FLUID 4				
	FLUID 5				
ITEM	fluid	δ^{2H} (‰)	δ^{18O} (‰)	δ^{17O} (‰)	Mass (g)
natural water	fluid 1	-42.7	-6.32		20041.4
	fluid 2				
	fluid 3				
	fluid 4				
	fluid 5				
Constants :					Mixture :
Isotopes	Isotopic masses (g/mol)	Absolute isotopic ratios of VSMOW	Isotopic abundances of VSMOW		isotopic abundance 2H
1H	1.0078250		0.99984426		0.0010888111
2H	2.0141018	1.5576E-04	0.00015574		isotopic abundance 17O
16O	15.9949146		0.99762058		0.0003782009
17O	16.9991317	3.799E-04	0.00037900		isotopic abundance 18O
18O	17.9991610	2.0052E-03	0.00200043		0.0019944028
					δ^{2H} (‰)
					5997.9321
					δ^{17O} (‰)
					-2.1048
					δ^{18O} (‰)
					-3.0192
					total mass of mixture
					20062.37640

(b)

ITEM	FLUID	Isotopic abundance 2H	Isotopic abundance 18O	Isotopic abundance 17O	Mass (g)
2H enriched	FLUID 1	0.99993	0.008998	0.000874	27.9682
18O enriched	FLUID 2	0.001791	0.9605	0.01176	45.4676
	FLUID 3				
	FLUID 4				
	FLUID 5				
ITEM	fluid	δ^{2H} (‰)	δ^{18O} (‰)	δ^{17O} (‰)	Mass (g)
natural water	fluid 1	-42.7	-6.32		10024.7
	fluid 2				
	fluid 3				
	fluid 4				
	fluid 5				
Constants :					Mixture :
Isotopes	Isotopic masses (g/mol)	Absolute isotopic ratios of VSMOW	Isotopic abundances of VSMOW		isotopic abundance 2H
1H	1.0078250		0.99984426		0.0026465779
2H	2.0141018	1.5576E-04	0.00015574		isotopic abundance 17O
16O	15.9949146		0.99762058		0.0004252809
17O	16.9991317	3.799E-04	0.00037900		isotopic abundance 18O
18O	17.9991610	2.0052E-03	0.00200043		0.0059050916
					δ^{2H} (‰)
					16036.4720
					δ^{17O} (‰)
					126.5865
					δ^{18O} (‰)
					1963.6501
					total mass of mixture
					10098.13580

(c)

Figure 1. Three screenshots of the spreadsheet with examples of the mixing of different natural and isotope-enriched waters (see also text). The examples (b) and (c) have been applied for the case study of production of singly and doubly labeled waters (see Applications section). As the waters in the second set of rows are natural, and the δ^{17O} value has not been explicitly specified, the spreadsheet uses the natural relationship between the δ^{18O} and δ^{17O} values to calculate the δ^{17O} value for those natural waters.

whom the energy expenditure is to be analyzed using the DLW method. For such mother mixtures, fixed amounts of pure ^2H water and (highly) enriched ^{18}O water need to be mixed, and the final isotope abundances need to be calculated. For such work the spreadsheet is instrumental.

Still other possible applications lie in the field of the analysis of isotope dilution measurements. Last but not least, the isotope values for naturally occurring mixtures of different water bodies can easily be determined (see Fig. 1(a)). In case the fractions of two (or more) mixing water bodies need to be determined based on isotope measurements of the original and the mixed water bodies, the spreadsheet can be used in an iterative way to match the relative amounts of the individual water bodies such that the isotope values for the final mixed water body agree with the measured values.

Many more applications are thinkable, one of the nicest being that it can replace rough "back-of-the-envelope" isotopic calculations that many researchers still tend to make.

CONCLUSIONS

We developed a user-friendly, thoroughly validated spreadsheet that serves to calculate the isotope delta values and corresponding isotopic abundances for a mixture of waters with different isotopic compositions. It can be put to use in direct computations of mixtures, but since it has been programmed in Excel and is fully accessible, it can also be incorporated in other Excel-based calculations and iterative processes. The spreadsheet has been successfully tested for various versions of Excel. The spreadsheet, along with a small manual, is available free of charge from websites of the authors' research groups.^[31,32]

Acknowledgments

This project was a spin-off of the IAEA-funded project (contract NET-17151) for the production of new isotope-enriched reference waters.^[29] V. Faghihi would like to acknowledge the support of the Iranian Ministry of Science, Research and Technology.

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