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Modern stalagmite $\delta^{18}O$: Instrumental calibration and forward modelling

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ABSTRACT

The $\delta^{18}O$ isotopic composition of stalagmite calcite frequently contains a climate signal, but one that is difficult to interpret in terms of either rainfall or temperature. Over glacial–interglacial time periods and decadal sampling resolution, stalagmite $\delta^{18}O$ clearly contains a 'first order' climate signal where the magnitude of changes in temperature and ocean/atmospheric circulation dominate the $\delta^{18}O$ signature. However, at annual–biennial resolution sampling, and within interglacial periods, the magnitude of climate changes is smaller, and variability in $\delta^{18}O$ introduced by soil, karst groundwater and cave processes can introduce considerable uncertainty into the climatic interpretation of stalagmite $\delta^{18}O$ records. Here, two approaches that can quantify the climate signal contained with stalagmite $\delta^{18}O$ are discussed. Firstly, linear regression based approaches are reviewed, which correlate stalagmite $\delta^{18}O$ with instrumental climate parameters such as temperature and rainfall. The advantages and disadvantages of complex linear regression approaches that attempt to account for groundwater mixing within the karst aquifer are discussed. Secondly, a forward modelling approach is introduced, where stalagmite $\delta^{18}O$ is modelled from rainfall $\delta^{18}O$, surface climate parameters and a simple karst hydrology model. Using a case study from Gibraltar, this latter approach demonstrates that between stalagmite variability in $\delta^{18}O$ of the order of 1‰ can be explained solely by differences in karst hydrology. Forward modelling suggests that a similar variability in $\delta^{18}O$ might be observed between stalagmites within a cave, or between caves within a homogenous climate region, and highlights the difficulty in attempting to use $\delta^{18}O$ as a paleo-thermometer.

1. Introduction

Since the original work of Duplessy et al. (1970), there has been a long history of the analysis and interpretation of the record contained in $\delta^{18}O$ in speleothem calcite. Over the 40 years of research, it has become increasingly apparent that one single simple interpretation of speleothem $\delta^{18}O$ in terms of either temperature or rainfall, as originally interpreted (e.g. Duplessy et al., 1970; Gascoyne et al., 1980) is not possible. Instead, the complexity of processes that transform $\delta^{18}O$ signature of rainfall, in the soil, ground water and within cave, are increasingly recognised (Fairchild et al., 2006). The $\delta^{18}O$ of rainfall may be transformed in the soil zone, especially in drier climates through evaporation. Depending on the seasonality of the climate, this rain, that may be immediately considered soil water, will recharge the karst aquifer during periods when precipitation exceeds evapotranspiration. This 'hydrologically effective precipitation' is likely to vary seasonally, as well as over longer or shorter time periods. Once within the karst aquifer, percolating waters may follow complex flow routes, or pathways, due to the nature of the porosity of karst aquifers, with conduit, fracture and matrix flow all possible. This will mix waters, potentially of different ages, sometimes in a non-linear fashion. Moreover, storage of water in fissures and cave voids of varying sizes is likely, sometimes with prior calcite precipitation occurring. Finally, upon reaching a cave void where a speleothem may be sampled for scientific analysis, the dripwater $\delta^{18}O$ may be further transformed. This will most commonly be through non-equilibrium fractionation during calcite precipitation due to either rapid degassing or the effects of evaporation. For a full review of the effects of these processes in transforming $\delta^{18}O$, as well as other speleothem proxies, see Fairchild et al. (2006). Despite the number and complexity of processes that might transform speleothem $\delta^{18}O$, for regions with a strong climate forcing such as within the SE Asian Monsoon, it is clear that speleothem $\delta^{18}O$ can preserve a 'first order' climate signal over longer (glacial–interglacial) time periods (Spötl and Mangini, 2002; Wang et al., 2008).

Over shorter time periods (e.g. 100–10,000 years) and sampled at high resolution (e.g. annual), it is apparent that the climate derived $\delta^{18}O$ signal may be obscured by transformations in $\delta^{18}O$ in the soil, groundwater and cave, as described above. In cases where stalagmite $\delta^{18}O$ times series have been replicated for relatively climatically similar regions, such as for the last ~23 ka in New Zealand (Williams et al., 2005), a between-sample variability in $\delta^{18}O$ of the order of ~0.5‰ is observed around the 'first order' glacial–interglacial transition climate signal. Williams et al. (2005) caution that because of the many karst processes that might transform $\delta^{18}O$ between its source and an individual stalagmite, a more reliable record might be obtained by the compositing of several stalagmite records. The aim of this paper is to discuss two approaches that may enable us to understand better the extent to which there is a direct climate correlation with an individual stalagmite $\delta^{18}O$

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record. Maybe more important would be an improved understanding and quantification of the uncertainty in stalagmite $\delta^{18}O$ derived from transformations within the soil and karst system. For modern stalagmite samples, for which high resolution sampling can generate annual or better resolution records of $\delta^{18}O$, two approaches can be utilised. This paper firstly reviews empirical approaches that can be used to regress stalagmite $\delta^{18}O$ time series against instrumental climate data. Then, a more deductive approach is used to forward model stalagmite $\delta^{18}O$ from empirical climate and isotope data and using a simple karst hydrological model.

2. Calibrating stalagmite $\delta^{18}O$ against instrumental data using regression approaches

One approach to understanding the $\delta^{18}O$ record in speleothems would be to calibrate speleothem $\delta^{18}O$ against instrumental data, typically using classical linear regression. This has been made possible by the increasing recognition of annual growth banding in speleothems (Broecker et al., 1960; Genty, 1993; Baker et al., 1993) which provides the necessary chronological control. This is coupled with improvements in microdrilling technology, which permits the sampling of 50–100 µm thick wafers of speleothem calcite, which in most regions equates approximately to annual resolution. Therefore, time series of $\delta^{18}O$ of stalagmite calcite can be obtained at annual resolution, which for samples that are actively forming leads to the possibility of calibrating $\delta^{18}O$ against instrumental climate. Ideally, the $\delta^{18}O$ of speleothem calcite would be regressed against time series of $\delta^{18}O$ in precipitation. However, despite a significant global effort to collect monthly $\delta^{18}O$ precipitation samples, for example, the IAEA Water isotope database WISER (Water Isotope System for Data Analysis, Visualisation and Electronic Retrieval; www.iaea.org/water), such data are typically of insufficient temporal duration or continuity to be of practical use. An exception is the work of Mattey et al. (2008), who correlate winter dripwater $\delta^{18}O$, reconstructed from stalagmite calcite $\delta^{18}O$, against the weighted winter $\delta^{18}O$ of precipitation for the period 1962–2004 AD (in Gibraltar). Instead, researchers have focussed on calibration of stalagmite proxy data against the more widely available instrumental temperature and/or rainfall series. Only a few such studies utilise $\delta^{18}O$ (Baker et al., 2007; Jex et al., 2010-this issue), following earlier linear regression based calibrations of annual lamina width (growth rate) against climate (Proctor et al., 2000, 2002; Frisia et al., 2003; Tan et al., 2002). In all cases, regression between mean annual climate and stalagmite $\delta^{18}O$ using unsmoothed data yields a lower correlation than regressing smoothed climate data and unsmoothed stalagmite $\delta^{18}O$. The mixing and storage of water in the karst aquifer mean that it would be highly unlikely for a stalagmite to respond immediately to the climate of that year; it is more likely to represent an integrated signal of the proceeding *n* years. Historically, a fixed value for *n*, such as 10 years, has been used to enable comparison with other decadal averaged proxies: however, given our knowledge of karst hydrology such a fixed approach may increase the uncertainty associated with the regression.

Recently, the basic linear regression approach has been developed in an attempt to account for the mixing of ground water within the karst aquifer. Baker et al. (2007) and Jex et al. (2010-this issue) took the instrumental monthly rainfall and/or temperature series for the stalagmite location, and applied a simple function:

$$W_{t=n} = MI_n + (1-M)\sum I_{n-1 \text{ to } n-x} \tag{1}$$

where:

$W_{t=n}$	water at time *n*
M	proportion of fracture flow
I	monthly instrumental climate parameter (e.g. total precipitation (P), mean temperature (T), total evapotranspiration (ET))
x	variable length of storage flow component

The simple mixing model presumes just two flow components, a fracture flow component *M* that transfers the surface water to the cave drip in the same year, and a matrix flow component $(1-M)$ that has a slower transfer rate and mixes water of the preceding *x* years. Mixing models are run for monthly, seasonal and annual climate parameters, to reflect the fact that water recharge to the aquifer can be highly seasonal, and result in a large number of transformed time series *W*, with variable *x*, *M* and *I*. Baker et al. (2007) run this simple mixing model for Ethiopian instrumental rainfall series for the months March–October. In this region, where monthly temperature variability is low, temperature was not used as an input variable, nor was Nov–Feb rainfall as a significant soil moisture deficit develops during these seasonally dry months. Rather, transformed monthly rainfall series were regressed against stalagmite growth rate and ^{18}O time series. In contrast, Jex (2008) and Jex et al. (2010-this issue) explored the full range of monthly, seasonal and annual instrumental climate parameters for NE Turkey, and regressed these against ^{13}C, ^{18}O and growth rate time series. Both Baker et al. (2007) and Jex et al. (2010-this issue), found that the best correlations were observed when parameter *M* was set to <0.3 and $x<10$ years. Several factors can guide the expected range of these parameters. The proportion of preferential (i.e. fracture) to matrix flow may determine the stalagmite shape, with candlestick stalagmites expected to have *M* close to or equal to 0, and those with increasing widths a greater proportion of fracture flow. The presence of hydrologically generated annual growth laminae, fluorescent organic matter or soil derived trace elements, would infer $M>0.0$.

One of the disadvantages with the transformed parameter regression models detailed above is the decrease in degrees of freedom (*df*) within the regression model when the storage flow component *x* is introduced. For most regions of the world, the length of instrumental climate series is between 50 and 150 years. With $x=1$ and an instrumental series of 100 years, then $df=99$, and a regression yielding a correlation, $r=0.50$, would be statistically significant at 99% confidence. With $x=5$ and the same instrumental series, then *df* could be as low as 19, for which a statistically 99% confidence level significant correlation coefficient *r* would be 0.58. For many regions of the world, where the length of instrumental climate series is less than 100 years and with $5<x<20$, the *df* become unacceptably low: even when correlation coefficients are very high they would not achieve statistical significance. However, the approach still has several advantages. Through the analysis of a larger number of regressions between transformed instrumental series and a stalagmite proxy, one should expect to see similar correlations between regressions for adjacent calendar months, and between similar transformation functions *x* and *M*. If these are not observed, then it should lead to an investigation of the instrumental series for in-homogeneities. Secondly, even if the transformed regressions do not yield statistically significant correlations, the relationships that are observed between *x*, *M* and instrumental climate parameters should provide some insight into the processes affecting the stalagmite proxy under investigation.

The mixing of water within the karst aquifer therefore means that stalagmites will necessarily preferentially preserve a smoothed, or low frequency, climate signal, which may be less amenable to linear regression based calibration. Additionally, calibration approaches are needed that tackle the problems of equifinality and non-linearity. For stalagmites, the extent to which a proxy time series may be reached by more than one climate input is not known, but the known complexities of karst hydrology mean that the equifinality issue is one that cannot be ignored. Karst drip-water hydrology is known to be non-linear, with under and overflow type behaviour that has been both conceptualised (Tooth and Fairchild, 2003) and observed (Genty and Deflandre, 1998; Baker and Brunsdon, 2003). In these circumstances, linear regression approaches will not provide an appropriate solution, and alternative approaches are needed. One such approach would be to forward model the stalagmite proxy of interest from a series of

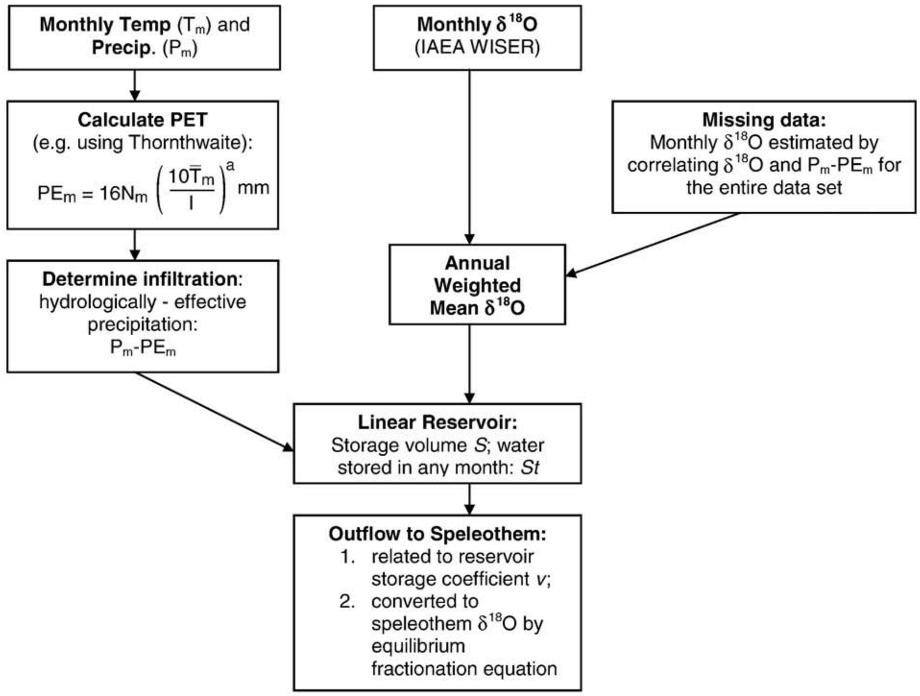

Fig. 1. Flowchart of the forward model.

input parameters and transformation functions. For example, for the stalagmite $\delta^{18}O$ proxy, where $\delta^{18}O$ of precipitation is available, one could attempted to forward model the $\delta^{18}O$ from rainfall to stalagmite using conceptual models of karst hydrology. This is the approach that is developed next.

3. Forward modelling of stalagmite $\delta^{18}O$

To explore the potential of forward modelling based approaches, a simple spreadsheet based approach has been followed. A flow chart for our forward model is presented in Fig. 1. Input data are monthly total precipitation, mean monthly temperature and rainfall $\delta^{18}O$ as obtained from the IAEA WISER. The rainfall and temperature data are used to calculate water excess using the Thornthwaite method. More complex models could use alternative methods to determine water excess, but Thornthwaite enables the significance of the ratio between precipitation and evapotranspiration to be explored. Working forward in time, recharge to the karst was presumed to occur in months when the water balance was positive (soil moisture deficit is presumed negligible). The $\delta^{18}O$ value of rainfall of that month was presumed to recharge the aquifer, and an annual weighted mean of the recharge water $\delta^{18}O$ was calculated for all hydrological years. This was defined as the total input to the aquifer and is presumed to enter the groundwater system in the same hydrological year.

The input water was then entered into a simple hydrological representation of a karst system which is modelled as a single linear reservoir (following Gilman and Newson, 1980), as illustrated schematically in Fig. 2, and again implemented in a simple spreadsheet (example spreadsheets are available from the authors on request). Recharge, or infiltration, is considered equivalent to 'hydrologically effective precipitation', determined as the difference between precipitation (P) and evapotranspiration (Evp) as calculated previously using the Thornthwaite approach. These infiltrating waters, of a known $\delta^{18}O$ composition, are considered to pass through a linear reservoir of total storage volume S. At any time, the amount of water stored within the reservoir is described by the parameter St, while the initial water stored within the reservoir at the start of the model run is St_i. The capacity of the reservoir (S) can be varied, as can the initial volume of water in the reservoir (St_i). Input to the reservoir is the annual water excess, whose $\delta^{18}O$ mixes linearly with any existing $\delta^{18}O$ held within the reservoir. Reservoir outflow rate, which is a function of

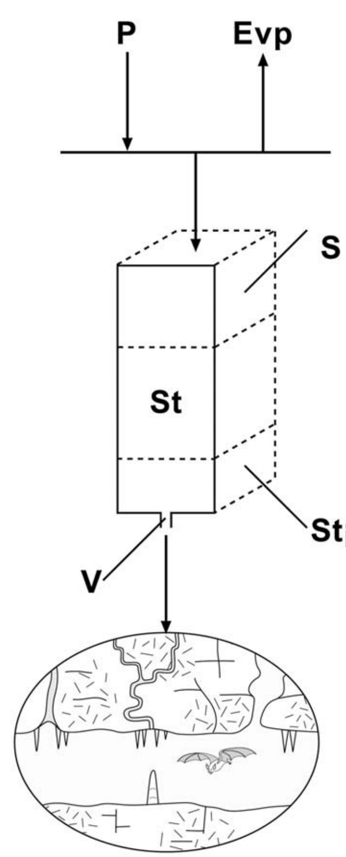

Fig. 2. Schematic representation of the linear reservoir model for dripwater $\delta^{18}O$ as a function of parameters total storage volume, S, water stored in the reservoir, St, initial volume of water stored in the reservoir, St_i, and outflow rate, v as described in the text.

the reservoir storage coefficient, is represented by the parameter v which describes how a volume of water is removed from the mixed reservoir and transported directly to the stalagmite where it is converted to stalagmite $\delta^{18}O$ using the equilibrium fractionation equations that Leng and Marshall (2004) derived from Kim and O'Neil (1997). Input, output and linear mixing are all implemented in the spreadsheet using basic equations, with the addition of logical operators to control boundary conditions (e.g. when $St = S$ or $St = 0$).

As a case study relevant to the Mediterranean region, we used the IAEA $\delta^{18}O$ precipitation dataset to forward model the stalagmite $\delta^{18}O$ that might be expected at Gibraltar. The advantage of this site is that not only does it have a relatively long and continuous IAEA $\delta^{18}O$ rainfall record, but also that different model outputs can be readily compared to a stalagmite $\delta^{18}O$ time series (Mattey et al., 2008). IAEA $\delta^{18}O$ precipitation data at Gibraltar are available from 1962 AD, but are very discontinuous until 1974 AD, from which time a near continuous dataset is available. The IAEA d18O precipitation data was used as the model input data, except for months where $\delta^{18}O$ data are missing post 1974 AD (37 months in total, with worst data quality in the period 1993–1995 AD). In these cases of missing data, a monthly mean $\delta^{18}O$ value was used which was calculated from the $\delta^{18}O$ vs. water excess correlation for the whole monthly data series ($\delta^{18}O = -3.92 - 0.00526 \times$ water excess). For the period 1962–1973 AD, IAEA data were used where available (1962–1965 AD), and for the remainder of the period rainfall $\delta^{18}O$ values were predicted from stalagmite $\delta^{18}O$ as given in Mattey et al. (2008). Given the poor quality data prior to 1974 AD, this period was used solely to allow the groundwater reservoir to achieve an equilibrium state.

Dripwater $\delta^{18}O$ was initially forward modelled for a small reservoir; given our lack of knowledge of the actual reservoir size this was defined as one with a capacity six times greater than mean annual water excess. Likewise, the reservoir was arbitrarily defined to be initially 66% full. Only one variable was changed: the outlet size (v) which varied between 20% and 100% of the mean annual input. Fig. 3 shows that for v within the range of 20% to 50%, there is muted variability in dripwater $\delta^{18}O$ of <0.3‰. Under these scenarios the reservoir fills quickly and remains close to capacity for the duration of the model run. However, as v is allowed to increase to 100% of the mean annual input, inter-annual variability of $\delta^{18}O$ increases and this variability increases in magnitude through time as reservoir water volume (s) decreases. For these values of v, the impact of individual years can be observed, for example, years of low water excess such as 1995 (annual P-ET = 29 mm) which decrease the volume of water in the reservoir to ~30% of its capacity. The $\delta^{18}O$ signature of recharge waters in subsequent years is reflected in the modelled dripwater $\delta^{18}O$ until the point when the reservoir approaches full capacity.

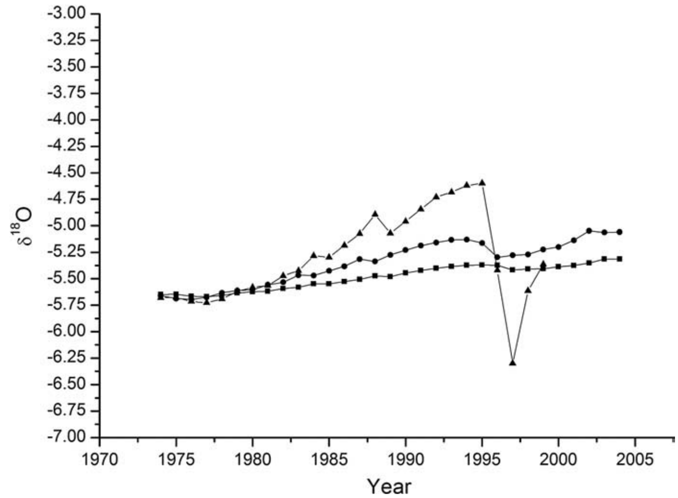

Fig. 4. Reservoir of capacity ×2000 that of the mean annual input and initially 10% full. Outlet size varies as 10% (squares), 100% (circles) and 150% (triangles) of mean annual water excess.

Secondly, stalagmite $\delta^{18}O$ was forward modelled, again by varying the outlet size (v), but for the situation where the reservoir storage capacity (S) is significantly greater than the mean annual water excess and initial volume of water stored remains constant. Fig. 4 shows that for v arbitrarily defined as being between 10% and 100% of mean annual water excess, dripwater $\delta^{18}O$ exhibits very low variability due to the relative dominance of stored water within the reservoir. Where v equals 150% of the annual water excess, and for the same initial reservoir water volume, the reservoir empties during the model run. From this point, dripwater $\delta^{18}O$ variability increases, so that during the latter part of the model run it reflects the mean annual recharge water.

The third set of forward model simulations investigated the importance of changes in the initial volume of water stored within the reservoir (St_i) for the situation where the reservoir volume capacity (S) was arbitrarily set to equal ×6 the mean annual water excess and the outlet size (v) defined to equal the mean annual water excess (Fig. 5). Here, a decrease in St_i increases the variability in dripwater $\delta^{18}O$ as the relative proportions of reservoir and recharge waters change. As in Fig. 2, the combination of a year of very low water

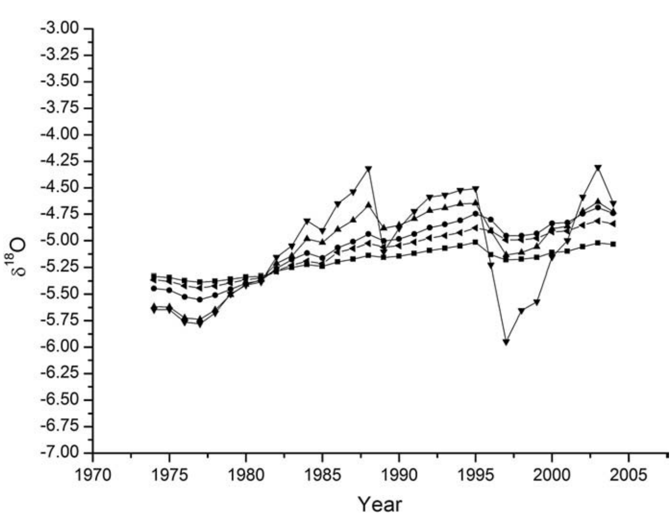

Fig. 3. Reservoir of volume ×6 that of mean annual water excess. Initial reservoir 66% full. Outlet size varied as a proportion of mean annual water excess. Squares: 20%, left triangle: (30%), circle: (50%), up triangle: (80%), down triangle: 100%.

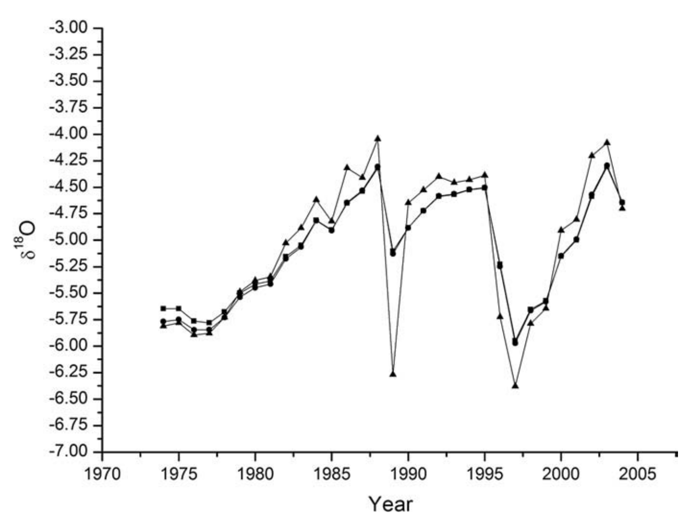

Fig. 5. Reservoir of volume of ×6 that of mean annual water excess. Initial reservoir 66% full (squares), 50% full (circles) and 33% full (triangles). Outlet size fixed and set to the mean annual water excess.

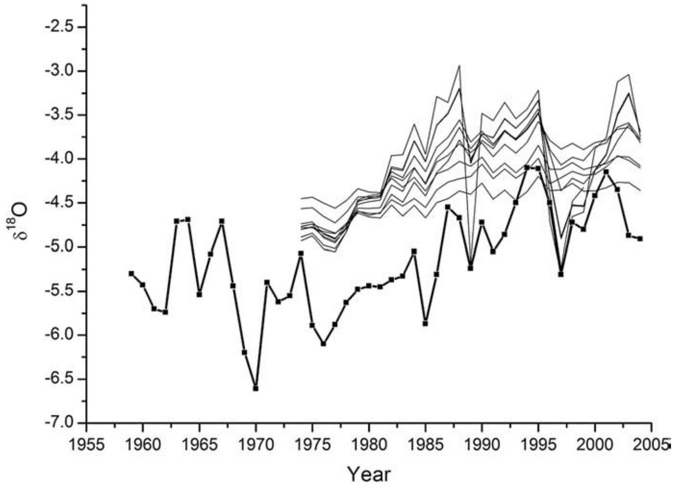

Fig. 6. Summary of output produced by all model runs, illustrated in Figs. 2–4, together with actual stalagmite δ^{18}O (from Mattey et al., 2008).

excess in 1995, followed by a year of high water excess (1061 mm) in 1996 is reflected in a dripwater δ^{18}O response that is highly sensitive to reservoir conditions at the time of the event.

Fig. 6 plots the results of all model runs presented in Figs. 3–5 to show the potential variability in stalagmite δ^{18}O predicted by fixed climate input parameters and which therefore depend solely upon variations in the karst reservoir input, output, volume and storage. δ^{18}O are those for stalagmite calcite, corrected for fractionation using Leng and Marshall (2004). Modelled δ^{18}O show a range of ~0.5–1.2‰ in any one year. The model results also suggest that a similar variability in δ^{18}O might be observed between stalagmites within a cave, or between caves within a homogenous climate region, and is the same magnitude as that observed by Williams et al. (2005). Remembering that our model is simplistic, without the separation of conduit fracture and matrix inputs of different isotopic composition, nor overflow or underflow behaviour, an even greater range in δ^{18}O might be expected in real karst systems. Such variability highlights why the use of δ^{18}O in the past as a simple palaeo-thermometer has been found to be futile. Also presented in Fig. 6 is the actual δ^{18}O of winter deposited calcite for stalagmite Gib04a (Mattey et al., 2008) for comparison with the model output. Modelled δ^{18}O is that of the mean annual calcite, and winter calcite would be expected to be isotopically lighter than this due to the seasonality of δ^{18}O of recharge. This is observed in Fig. 6. However, the difference between modelled and actual δ^{18}O of calcite actually appears less than the potential uncertainties introduced by different water–calcite fractionation correction factors (McDermott et al., 2006). Modelled δ^{18}O captures the lower δ^{18}O variability between 1975 and 1985 AD and models the impact of the dry/wet year combination of 1995/1996 AD. However, the trend of isotopically heavier δ^{18}O with time is less well captured in the model. There are a number of possible explanations for this. For example, the initial conditions may not have been represented correctly by the model, and if there had been a negative water balance in the preceding period, the reservoir would have been recharged with waters that were isotopically lighter. Alternatively, there may have been changes in the nature of 'hydrologically effective' events over the time period, which can only be represented at a relatively crude level given the use of monthly climate data. Further work is needed to investigate the relative significance of these factors.

4. Conclusion

Stalagmites have to potential to provide essential low frequency climate information, especially for the last hundreds to thousands of years, where an improved understanding of natural climate variability over the timescale of decades is essential to understand and model current greenhouse gas induced global warming. Although there have been many attempts to reconstruct temperature variability for the last ~1000 years, (e.g. Mann et al., 1998; Esper et al., 2002; Moberg et al., 2005; Mann et al., 2008), it remains the case that a key issue is the need to reliably extract the low frequency climate component. Christansen et al. (2009) recently demonstrated that all reconstruction methods contain a large element of stochasticity and an underestimation of low frequency component. Therefore there is a need to further refine the approaches used to calibrate stalagmite proxies against instrumental climate series, as discussed here. We propose that a combination of both linear regression of stalagmite δ^{18}O against instrumental climate series and forward modelling would help understand both the climate signal contained within stalagmite δ^{18}O, and the sources of uncertainty in any climate reconstruction.

In our single linear reservoir model, we have demonstrated that stalagmite δ^{18}O is sensitive to the storage volume S, the initial amount of water stored (St) and the outlet size (v), the sensitivity of dripwater δ^{18}O to each factor depending on its relative volume. With respect to forward modelling approaches, further complexity can be added to the model presented here to reflect a wider range of potential processes affecting stalagmite δ^{18}O. These include: (1) a parameter to reflect the input of a fraction of isotopically heavy water that might have undergone evaporation in the soil or near surface groundwater, and a vegetation component that could model δ^{18}O evapotranspired by this route; (2) the input of both conduit and diffuse water into the reservoir store; the former of more variable isotopic composition depending on the time of recharge; (3) a more complex groundwater flow behaviour including threshold responses such as overflow or underflow behaviour from the reservoir; (4) a parameter to reflect non-equilibrium conditions during speleothem formation. Both (1) and (4) can potentially relate to surface climate, particularly temperature, and therefore be parameterised in relation to this input parameter. Ultimately, it can be envisaged that a forward modelling approach can be used: (1) to generate more realistic stalagmite δ^{18}O pseudoproxies than those generated by purely stochastic methods (Moberg et al., 2008); (2) to better understand hypothetical stalagmite δ^{18}O responses to rapid climate changes such as the '8.2 ka event'; (3) as well as to model stalagmite parameters other than δ^{18}O.

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