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Reply to comment

Reply to comment on 'Characterization of surface and ground water δ^{18}O seasonal variation and its use for estimating groundwater residence times' by R. E. Criss and W. E. Winston

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It is the nature of the scientific method to use a variety of models, procedures, techniques and data to quantify and analyse natural phenomena. Recently, in Reddy *et al*. (2006), we published a study in which δ^{18}O values for precipitation, surface- and ground-water samples from the Shingobee River Headwaters Area (SRHA) were analysed using an amplitude-attenuation (convolution integral) approach for estimating mean residence times (MRTs). This approach has been used in many small watershed studies (e.g. Stewart and McDonnell, 1991; DeWalle *et al*., 1997; Burns and McDonnell, 1998; McGuire *et al*., 2002; Rodgers *et al*., 2005; McGuire and McDonnell, 2006). In a comment, Criss and Winston (2006) disagree with our method and present an alternative approach for interpreting δ^{18}O values in the SRHA. We feel that this comparison with our methodology is unfair. Criss and Winston (2006) focus their attention on the weaknesses in our method and the strengths of theirs, while overlooking our detailed evaluation of model predictions with other independent watershed hydrologic properties.

The comment by Criss and Winston (2006) makes several points, some of which we agree are valid criticisms of our paper. In this response, we will address their concerns regarding (1) our interpretation of the current state of the literature, (2) the data we used in the analysis, and (3) the relative merits of the two modelling approaches. In so doing, we will update the dataset with precipitation δ^{18}O data from 1990 to 2004, and compare the two approaches to provide a fair basis for understanding the strengths and weaknesses of both methods. Additionally, we will discuss some technical issues that arise for scientists in choosing between simple and complex models.

CURRENT STATE OF THE LITERATURE

The goal of the Reddy *et al*. (2006) paper was to test the applicability of the δ^{18}O amplitude-attenuation approach for estimating MRTs in a well-characterized catchment with significant surface-water–ground water interactions, and to evaluate the limitations of this approach by comparison of model predictions and other

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hydrologic data. Because our paper was not intended as a review of alternative methods, there was no reason to cite the Frederickson and Criss (1999) paper, which was less relevant to our study than the other watershed studies cited, or to compare the merits of the two approaches. Recent publications reviewing catchment travel-time modelling approaches include Rodgers *et al*. (2005) and McGuire and McDonnell (2006).

We agree that the studies co-authored by Criss since 1999 are examples of isotope hydrology studies in well-instrumented catchments with significant surface-water–ground water interaction. We have a 25-year record of surface-water–ground water research accomplishments at the SRHA (Siegel and Winter, 1980; Winter, 1997; LaBaugh *et al*., 1997; Schuster *et al*., 2003). Furthermore, the very different nature of surface-water–ground water interactions in the thick glacial till aquifer at the SRHA, with its abundant lakes, compared with the very different nature of surface-water–ground water interactions in the karst-related systems studied by Criss and colleagues, qualifies our watershed isotope hydrology study as the first study showing significant surface-water–ground water interactions occurring in a long-term, fully instrumented, multidisciplinary, research field site.

DATA USED IN THE ANALYSIS

Criss and Winston (2006) correctly point out the 1-year offset of the precipitation data used in our model calculations. We are grateful that this was caught so quickly by Criss and Winston (2006) and have used the opportunity of this response to update the precipitation data used in our model calculations.

We began our work characterizing the MRTs in the SRHA in 2001, when complete sets of isotopic and chemical data from SRHA were limited in sample number and collection sites. Hence, in our report (Reddy *et al*., 2006) the isotopic analysis data used were for a specific group of samples analysed at the same time, in the same laboratory. In hindsight, it would have been beneficial to have updated our analysis with a more complete precipitation δ^{18}O dataset when it became available.

Based on the comment by Criss and Winston (2006), we have reanalysed and reinterpreted a larger SRHA isotope hydrology dataset. We took the available precipitation isotope record and compared the MRTs based on the sine function fit of the larger dataset with the estimated MRT for Shingobee Lake presented in our publication (Reddy *et al*., 2006). We found no substantial difference in MRTs calculated using the two datasets.

We note that Criss and Winston (2006) incorrectly attributed SRHA data to a US Geological Survey (USGS) website that does not contain data. Criss and Winston (2006) used SRHA data in their comment that have not been published or peer reviewed. They should have cited a personal communication with USGS staff as the source of the preliminary, unpublished SRHA isotope data that served as a basis of their comment. We are currently verifying the SRHA isotopic database, and a USGS report of the isotopic data will be forthcoming.

RELATIVE MERITS OF THE TWO MODELLING APPROACHES

Criss and Winston (2006) agree with our research premises and conceptual model as presented in our publication (Reddy *et al*., 2006), namely that the annual δ^{18}O variation in watershed precipitation can be characterized and that annual δ^{18}O variation propagates in the watershed surface water and ground water. Further, they agree that this δ^{18}O annual variation in surface water and ground water can be used to obtain meaningful information about water MRT. Criss and Winston (2006) disagree with our use of the sine function to characterize the δ^{18}O watershed inputs and the use of the amplitude-attenuation approach to estimate MRT. In their comment, Criss and Winston (2006) presented only the strengths of their model and only the weaknesses of ours. Here, we present the strengths and weaknesses of both models to give an unbiased analysis of the pros and cons of each approach.

For the amplitude-attenuation approach, seasonal variation in surface and ground water δ^{18}O is characterized by the generalized sine-function equation:

$$\delta^{18}\mathrm{O} = (\delta^{18}\mathrm{O})_{\mathrm{mean}} + A \sin[(2\pi t/b) + c] \tag{1}$$

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where $(\delta^{18}O)_{mean}$ is the annual mean $\delta^{18}O$ in the precipitation, ground or surface water, A is the seasonal amplitude of $\delta^{18}O$, b is the period of the seasonal cycle (i.e. 365 days), and c (radians) is the phase lag. Using A for surface or ground water and the value of A for precipitation A_p calculated using Equation (1), the MRT of surface or ground water can be calculated as

$$\mathrm{MRT} = (1/\mathrm{b}')[(A/A_\mathrm{p})^{-2} - 1]^{0.5} \tag{2}$$

where b' (rad day^{-1}) is a conversion factor. The assumptions underlying Equation (2) are that the hydrologic system is at steady state, that the infiltration water mixes immediately, and that there is an exponential distribution of water residence times in the surface or ground water system. The amplitude-attenuation approach is valid in the case of sparse data and as a first-order estimate to MRT. McGuire and McDonnell (2006) have examined limitations of the sine-function equation for the estimation of catchment water transit times.

It is clear that the key isotopic parameter in this approach to estimation of MRT for surface water and ground water is the ratio of the annual $\delta^{18}O$ amplitude in precipitation A_p to that of a selected watershed hydrologic compartment A, such as a closed basin lake or a ground-water flow path. Moreover, in a much more general sense, this key isotopic parameter ratio is available at local and regional scales worldwide, and when used it may serve an important role in water resource evaluations and assessments of drinking water susceptibility to contamination, especially in developing countries.

There are several advantages to using a sine function to characterize the annual variation of watershed $\delta^{18}O$ inputs. First, the sine-function equation has been applied by other investigators to describe seasonal phenomena (Stewart and McDonnell, 1991; DeWalle *et al.*, 1997; Burns and McDonnell, 1998; McGuire *et al.*, 2002), and it is easy to understand and to apply. Also, this approach facilitates the examination of average behaviour occurring over a period of years, providing a visual reference for determining whether a year had greater than or less than typical $\delta^{18}O$ values. The main advantage of this approach was that we were able to apply the model to estimate MRTs in a situation where only sparse data (i.e. $\delta^{18}O$ measurements determined at most twice a month) were available. Although amounts of precipitation and $\delta^{18}O$ values tend to follow a seasonal cycle, a key drawback of Equation (1) is its inability to describe the random component characteristic of natural phenomena (e.g. precipitation occurs at random times with events of varying length and intensity). Trigonometric modelling of periodic time-series is done often with strong theoretical and data-based justification. Because of a limited period of record, we fit only a single sine function; therefore, we sacrificed some of the goodness of fit that a more complex trigonometric model might have provided.

The precipitation isotopic record used by Frederickson and Criss (1999) may be strongly influenced by the urban precipitation sampling site (metropolitan St Louis). Moreover, the karst aquifer studied by Frederickson and Criss (1999) is very different hydrologically from the SRHA aquifer—karst conduit flow is very different from the flow of water in a thick calcareous glacial drift deposit. The model presented by Criss and Winston (2006) is an equation for a 'damped running average' of precipitation $\delta^{18}O$ inputs into a watershed or hydrologic response area ($\delta^{18}O_{output}$) (Frederickson and Criss, 1999):

$$\delta^{18}\mathrm{O}_{\mathrm{output}} = \frac{\sum_i P_i \delta_i \mathrm{e}^{-t_i/\tau}}{\sum_i P_i \mathrm{e}^{-t_i/\tau}} \tag{3}$$

where P_i is the amount, δ_i is the δ-value, and t_i is the time of the sequential precipitation events. This model contains one parameter that is not based on measured data, the residence time τ, not to be confused with the MRT estimated with Equation (2). The parameter τ represents, '... the annual period of formation, overturn and mixing of the lake's surface layer (epilimnion)', according to Criss and Winston (2006).

The use of Equation (3) has several advantages. The simplicity of the model, which has only one fit parameter, is appealing. Because the model relies on experimental data for each precipitation event, the

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randomness of discrete precipitation events is incorporated in the model. The model has been used with apparent success to describe $\delta^{18}O_{output}$ in surface water and several spring discharges in a karst aquifer (Frederickson and Criss, 1999). However, for optimal application of Equation (3), extensive data (time, amount and δ-value for every precipitation event) are needed. Although Equation (3) can be applied when these data are available on an infrequent basis, the model resolution and accuracy will be reduced. Particularly at short time intervals, when there has not been enough precipitation to affect the $\delta^{18}O$ value in surface water substantially, the model cannot describe $\delta^{18}O_{output}$ values accurately. Furthermore, Equation (3) does not account for the possibility of mixing between water close to the surface and deeper water.

According to the famous quote of George Box, '... all models are wrong, but some are useful'. Despite the relatively sparse data available to us in our publication for the estimation of surface and ground water MRTs in the SRHA, we were able to estimate MRTs using Equations (1) and (2) and learn something about SRHA in the process. A goal in the study of the SRHA is identification of ground water interaction with lakes in the watershed (LaBaugh *et al*., 1997; Schuster *et al*., 2003). The estimated MRT for Shingobee Lake suggests the importance of (older) ground water inputs to the lake. In addition, the MRT estimates for ground water vary considerably over relatively short distances because of aquifer heterogeneity. The ground water MRTs agree with independent watershed hydrologic observations (such as ground-water tritium contents and estimated Darcy transit times). Therefore, our model is useful. In contrast, the model of Criss and Winston (2006) requires a well-resolved input function. Also, the model of Criss and Winston (2006) can be used to estimate τ, not the MRT, and in our opinion τ is less useful than the MRT for many watershed management issues, including assessment of ground water contamination susceptibility and remediation potential. Therefore, although Equation (3) may have fewer parameters, we believe it is less useful than our approach. It is noteworthy that the Criss and Winston (2006) process-based estimated time constant for Shingobee Lake is 1 year, a value very similar to the value given in Reddy *et al.* (2006) of $1{\cdot}9 \pm 0{\cdot}3$ years, calculated using the $\delta^{18}O$ annual amplitude-attenuation approach (without process-based adjustments) using the limited dataset in (Reddy *et al*., 2006: table III).

In response to the comment of Criss and Winston (2006) 'that "well WL 18 was not considered because the data could not be fitted to the sine function" illustrate[s] the inadequacy of this approach', we note that water samples from well WL 18 are anomalous (in comparison with nearby water-table wells) with respect to isotopic and chemical composition. Water chemistry from well WL 18 is similar to that of Williams Lake, and yet the water tritium content, as noted in the Discussion section of our paper (Reddy *et al*., 2006), indicates that the age of water sampled from well WL 18 is greater (84 years) than the lake residence times (~3 years) reported by Rosenberry (1985). The Discussion section points out this anomaly and lends support to the heterogeneity of the SRHA aquifer material. Our acknowledgement that we cannot fit *all* the data to the sine function by no means illustrates 'the inadequacy of this approach'. On the contrary, it demonstrates the difficulties of applying the $\delta^{18}O$ amplitude model to estimating the MRT of ground water with an age greater than several decades.

There are significant gaps in the SRHA precipitation isotope record. However, we have reanalysed all available precipitation isotope data from 1990 to 2004 using the sine-function equation (Figure 1) (119 samples, with an R^2 of 0·71). The period of this extended data set is $366 \pm 1{\cdot}2$ days, the mean $\delta^{18}O$ value is $-13{\cdot}22 \pm 0{\cdot}26$‰, and the amplitude of the annual ^{18}O variation is $6{\cdot}41 \pm 0{\cdot}39$‰. This precipitation annual amplitude, based on all available Shingobee precipitation $\delta^{18}O$ values, yields an MRT for Shingobee Lake surface water of $1{\cdot}6 \pm 0{\cdot}3$ years, in comparison with a value of $1{\cdot}9 \pm 0{\cdot}3$ years (Reddy *et al*., 2006: table III). The difference in the MRT for Shingobee Lake surface water obtained using the short and full data set is within the estimated error of the MRT. The similarity of the MRT using a short and an extended precipitation isotope dataset suggests that the sine-function approach employed at the SRHA area is a robust method.

Criss and Winston (2006) suggest another apparent weakness in our approach that we would like to address. For three of the six sites where the sine-function equation was used with success (at one site, well WL 18, the method could not be applied), the period for the fit varied from the expected value of 365 days. They comment that, with a period different than 365 days, the fit would be out of phase with the lake after 15 years.

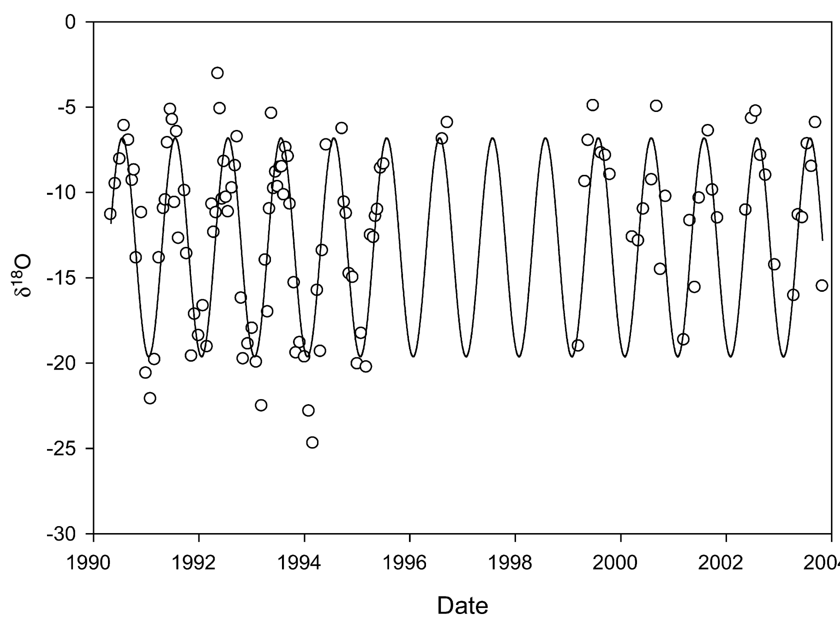

Figure 1. Plot of seasonal ^{18}O variations in precipitation from the SRHA as a function of time, with a sine function fitted to the dataset

However, it is incorrect for Criss and Winston to extrapolate the sine-function equation outside the period of record. For Shingobee Lake precipitation, for Shingobee Lake, and for Shingobee River, the periods were 387, 353, and 450 days respectively. The values of the time constants indicate that we are pushing the limits of the method in terms of the amount of data available. Data from the longer time-series show the anticipated time period of $366 \pm 1{\cdot}2$ days for SRHA precipitation. Second, the values of A_p and A, which are input for Equation (2) in the estimation of MRTs, are not highly sensitive to the value of the time period. Therefore, regardless of the period, the MRT estimate should be reasonable.

CHOOSING BETWEEN SIMPLE AND COMPLEX MODELS

Criss and Winston (2006) indicate that their model is superior to our four-parameter model because it has only one parameter. However, it is important to note, at least in this application, that the model of Criss and Winston (2006) has an additional parameter. Criss and Winston (2006) state that their δ^{18}O model of Shingobee Lake water is adjusted for both lake turnover and ^{18}O evaporative enrichment. Equation (3) did not describe the Shingobee Lake data (see Criss and Winston (2006: figure 2c); note the different scales on the Y axes) until the fit was offset by 1·5‰ to adjust for evaporative ^{18}O enrichment; this counts as a second model parameter. More importantly, a model with fewer parameters is not necessarily a better model.

Scientists often have to choose between a simple and a more complex model. It is at the modeller's discretion to determine whether a simple or more complex model is appropriate. The choice of models depends upon the amount of data available, the question being addressed, the theoretical basis of the models, and other factors. Criss and Winston (2006) state, 'Given enough free parameters, any type of curve, such as a complex polynomial or a cubic spline, can provide an accurate fit to a limited number of data points'. This statement is misleading, because data exhibiting an exponential increase cannot be described using an exponential decay function, nor can a straight line be described using a sine function (i.e. the functional form of the equation chosen affects the shape of the resulting curve). Modelling done properly can include multiple parameters without a loss of theoretical or physical significance. By choosing a model with theoretical meaning (e.g. a sine function to reflect seasonal variation), and then by verifying that enough data are available to estimate all parameters accurately (e.g. by using uncertainty measures, such as standard errors of the parameter estimates to verify that the dataset has sufficient information for proper model parameterization), a meaningful model with multiple parameters can be generated. The four fitting parameters were not chosen arbitrarily, but describe well-defined properties of periodically varying functions: mean, amplitude, phase and period. Our goal in this analysis was to obtain good estimates of the values of the amplitudes A_p and A. For comparing two models with different numbers of parameters, we prefer using a statistical approach to discriminate between models instead of a visual inspection. For example, the Akaike information criterion (AIC) compares model goodness of fit while also including a penalty function for the number of parameters. The AIC value provides a convenient index for choosing the model that properly balances simplicity and goodness of fit (Akaike, 1974; Burnham and Anderson, 2004).

CONCLUSION

In conclusion, although our model is not the only approach to understanding residence times in surface and ground water, it has been commonly applied in many other small catchment studies and we believe it is a useful approach. Time will tell whether the scientific community agrees with us.

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