We thank the associate editor and reviewer for their continued efforts to improve our manuscript. We have considered the minor suggestions from the recent round of reviews and followed all of them. Please see a detailed response to all remaining concerns below.

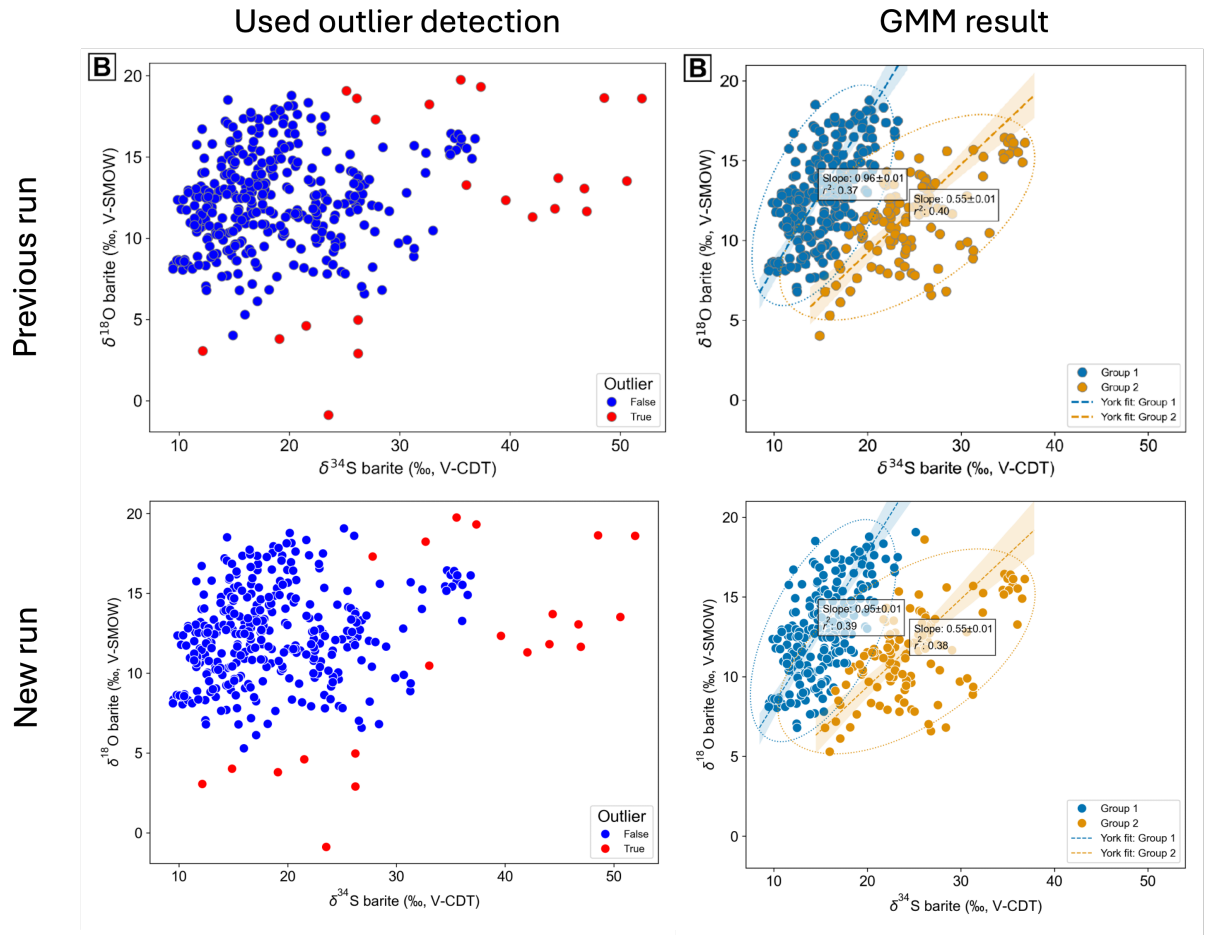
Associate Editor comments

1. Improved justification for why this clustering outlier method (DBSCAN) was chosen that includes reference to relevant literature. In the revised manuscript, I would like to see the authors justify this selection by citing other literature that has used this method, preferable at least one citation for a similar application.

We now cite the original reference that developed the DBSCAN method (Ester et al. 1996) (line 145), and a justification of why this method was chosen. We also added a reference to a previous application of this method to bivariate isotope data (Valentine et al. 2015) (lines 146-147).

2. Sensitivity analysis of DBSCAN parameterization. The minimum points to form a cluster was selected at four, and the neighbourhood radius was selected at 0.5. However, the authors provide no justification (descriptive or via citations) as to why these parameter values were selected. I appreciate the sensitivity analysis that was undertaken for the GMM-localities; as such, I would like to see something similar with the DBSCAN parameterization. These values (4 and 0.5, respectively) may be the most appropriate values. However, to improve the objectivity of the analyses and to understand the sensitivity of the DBSCAN method to changes in these parameters, other parameter values (higher and lower for both parameters) should be assessed.

We conducted a sensitivity test for the outlier detection by varying the minimum points to form a dense cluster (minPts) (see new Fig. S1). We chose the appropriate neighborhood radius (ε) by the heuristic suggested by Ester et al. (1996), based on the distance to the k-nearest neighbor. To increase objectivity, we added a function to select ε numerically for each minPts, rather than selecting it visually (as previously). We also added the Ester et al. 1996 reference in that context (line 144). Our test suggested changing the input parameters for DBSCAN from minPts = 4, epsilon 0.5 (previous run) to minPts= 13, epsilon = 0.586 (see explanation in lines 161-166). The effect of these changes on outlier detection and the subsequent GMM clustering was minimal (outliers: n =21 in the new run, vs. 22 in the previous run; cluster slopes 0.96 & 0.55 vs. 0.95 & 0.55) (see Figure below). Nevertheless, we think our new, formalized approach was valuable in increasing the reproducibility for future studies.



Reviewer comments

1. My only remaining comment relates to the outlier analysis presented in Fig. S1. For clarity, I suggest using a more consistent colour scheme between Fig. S1a and Fig. S1b so that the identified outliers can be more easily tracked between panels. In addition, it would be helpful to briefly discuss the 22 excluded outlier datapoints in the manuscript, even if only to explain their significance (or lack thereof) and the rationale for their exclusion. This would further improve the statistical transparency of the study.

We now use more consistent coloring across figures, particularly for detected outliers between Fig. 4A and Fig. S2 (old Fig. S1). We also noticed that the outliers were not included in Fig. 4B, C despite some having associated $\delta^{18}O$ and $\delta^{13}C$ data, which we corrected.

GMM is sensitive to outliers, which could affect the number, shape, and slope of the resulting clusters. We excluded the outliers from the GMM to avoid an influence on the interpretation of the clustered data, since GMM is sensitive to outliers. We clarified this in the method section (lines 143-144). Nevertheless, the outliers carry meaning, and we agree that despite their exclusion from GMM, they should not be ignored: We added a brief discussion at the end of section 3.2 (lines 310-314) on why the outliers are not discussed within the same framework as Groups 1 and 2: *"The outliers identified via DBSCAN (n = 21) are strongly heterogeneous and do not follow a common $\delta^{18}O/\delta^{34}S$*

trend (Fig. 4A, Table 2). Thus, the outliers do not form a coherent group and likely reflect highly variable fluid compositions and fractionation processes. Moreover, a relationship of the outliers with fluid sources and MSR pathways is unclear because only four outliers have associated $\delta^{18}O_{calcite}$ and $\delta^{13}C_{calcite}$ values (Fig. 4B, C).

Additionally, our discussion of the highest $\delta^{34}S_{barite}$ values in Section 3.4 addresses the data points in the outlier group. Now, we explicitly state this earlier in that paragraph (Line 439): "*The $\delta^{34}S_{barite}$ values of up to +52.0 ‰ observed among the outliers suggest that the SRR at times exceeded the sulfate resupply, decreasing the steady-state sulfate concentration (i.e., closed-system conditions) (Fig. 4A).*"

2. My remaining comments are limited to language and copy-editing issues. There are still some inconsistencies in spelling throughout the manuscript, particularly with respect to the use of British and American English (e.g., analysed vs. analyzed, modelling vs. modeling, behaviour vs. behavior). I recommend choosing one convention and applying it consistently throughout.

We double-checked the manuscript for grammar and language errors, including inconsistent use of British and American English. Several issues were resolved throughout the manuscript.

Page 3: "thermodynamically table" should read "thermodynamically stable".

Corrected.

Section 3.2: "effects SRR" should read "effects of SRR".

Corrected.

Section 3.4: "due its association" should read "due to its association".

Corrected.

Section 3.4: "increase … imply" should read "increase … implies".

Corrected.