Response to comments from the Referee 1:

I agree with the other reviewer of the manuscript, Bettina Schaefli (further refereed as BS), that it is too condensed in its current form. This factor makes the development of the system of equations' solution difficult to follow, and this must be improved. In addition, I am a bit concerned that this method and the presented illustration example have been reported previously by (Correa et al., 2019). Therefore, I strongly encourage the authors to: 1) mention openly whether their uncertainty estimation method is different than/similar to (the same?) the one applied in the aforementioned paper and ii) to apply their method to 1-2 additional illustration examples from the published literature or, at the very least, include the evaluation of outliers suggested by BS to differentiate this work from the one of (Correa et al., 2019).

R: We are very thankful to the Referee's useful remarks, which greatly helped to improve our Technical Note. We appreciate the comment that the Technical Note is condensed, and it should be extended and clarified to provide the community with an easy-to-follow reading material, mainly in the description of the system of equations', their development and solution.

Regarding 1) We thank the Referee for highlighting that we based our application on the example published in Correa et al (2019). However, the authors calculated the uncertainties based only on the application of a final equation. The main objective of this Technical Note is therefore to explicitly describe the mathematical development in all detail that allows the calculation of partial derivatives, degrees of freedom and confidence interval limits for each source fraction contribution as well as to provide the code and example data for their calculation and reproducibility.

Regarding 2) An evaluation of outliers as well as four additional examples from the same data set were included in the new version of the Technical Note. Additionally, a new figure (Figure. 2) was included showing Boxplots of end-members projected in the three-dimensional mixing space as a basis for clarity and a better understanding of the example calculations.

Please find at the end of this document the description of the examples and tables with input information (Table 1 to Table 4) and results (Table 5 to Table 8) that have been included and discussed in the Technical Note.

Major Comments:

The authors claim the robustness of their method (P.2, L.34), but do not discuss this consideration in comparison for example, to the commonly applied Gaussian error propagation approach. I think it would be great to evaluate and discuss this in the manuscript to add value to the usefulness of the presented methodology. This could also help differentiate this work from the work of (Correa et al., 2019).

R: We agree with the Reviewer that an exhaustive comparison of different methods should be attempted at some point, but after careful consideration we did not follow this suggestion here due to the length of this technical note. We on purpose used this format and not a full research paper to present our novel methodology in more mathematical detail than usual, step-by-step with an example application and we also provide the codes. This uncertainty assessment method was not presented in Correa et al. (2019), only parts of the dataset.

System of equations and resolution: please make sure to define clearly all of the notation in the set of equations to facilitate the readability of their resolution throughout the paper. All the considerations within the resolution of the system must also be clearly stated.

R: We appreciate this suggestion and have extended and updated the manuscript to clarify the notation and also to include more details in the descriptions of equations and variables to improve the readability of the technical note.

Specific comments:

Page 1, Lines 12-13: this sentence is incomplete. Please correct.

R: We have edited the phrase. It now reads: "[…], Bayesian approaches to estimate such source uncertainty only exist only sound methods for two and three sources."

P.1, L15: "dataset".

R: In this context the word "set" refers to the set of equations used to calculate the uncertainty of the source's contributions to a mixture, not to the data set, therefore we have omitted this change.

P.2, L.7: Replace "novel" by "the availability of".

R: This has been corrected to "the availability of"

P.2, L.12: Delete "novel".

R: The word "novel" has been deleted.

P.2, footnote: I think "M" refers to the mixture, not to a source. Correct if necessary.

R: This has been corrected to "mixture"

P.7, L.4: n is approximately 30 for each source, or among all sources

R: We have edited the phrase to clarify this point. It now reads: "[…] and spring water (SW) (n ~ 30, for each end-member) were collected".

P.7, L.21 and L.23: I think you refer to streamflow (or mixture, M), and not to spring water (SW). Correct if necessary.

R: We have edited the phrase to correct this error. "SW" was replaced by "M".

Table 2: report λ values

R: By λ we assumed that the Referee refers to degrees of freedom (γ). These values are reported in the Table 5.

Application examples

We have generated 6 examples to analyze the sensitivity of the uncertainty calculation to the source sample size, the artificial inclusion of outliers (upper and lower extremes) and the increased standard deviations of the sources datasets. The first example considers 50% of the samples from the initial data sets of sources (Table 1). The median, standard deviation and sample size are input data (Table 2) to calculate the uncertainty ranges (Table 6). The second considers the remaining 50% of samples and was similarly executed (Table 2). In the third example, outliers were artificially included at the positive end of data sets from each source at each coordinate, respectively. The outliers consisted of twice the maximum positive value of the observed data (Table 3). Using the same criteria, the negative extremes were included in the fourth example (Table 3). In order to take into account the effect of sources with dispersed data clouds, the increase of the standard deviation was considered in two cases, the first, in the example five, increasing three times the value of the standard deviation of the initial data set (Table 4) and finally, increasing the standard deviation five times in the sixth example (Table 4).

Table 1. Median and standard deviation (std.dev.) of end-members and stream projected in three-dimensional space for the study period 2013–2014.

End-member		Coordinates			Naming
		U1	U2	U3	in equations
SW (n = 25)	median	26,25	7,29	7,00	A
	std.dev.	0,46	0,36	0,39	
HS (n = 33)	median	0,23	5,48	1,97	B
	std.dev.	0,85	1,29	0,69	
AN (n = 37)	median	-2,24	-3,93	3,71	C
	std.dev.	0,55	0,58	0,45	
RF (n = 36)	median	-5,38	-6,10	-4,84	D
	std.dev.	0,27	0,56	0,15	
Stream (n = 257)	median	-0,61	-1,04	0,94	M
	std.dev.	2,06	1,10	0,66	

Table 2. Median and standard deviation (std.dev.) of end-members and stream projected in three-dimensional considering 50% of the data sets (examples 1 and 2)

Naming		1)	End	Coordinates			2)	End	Coordinates		
in equations			member	U1	U2	U3		member	U1	U2	U3
A	median		SW	26.18	7.29	6.66		SW	26.28	7.29	7.1
	std.dev.		(n = 12)	0.34	0.39	0.48		(n = 13)	0.51	0.36	0.21
B	median		HS	0.23	5.41	1.87		HS	0.28	5.9	2.26
	std.dev.		(n = 17)	0.74	1.19	0.52		(n = 17)	0.96	1.33	0.74
C	median		AN	-2.37	-3.93	3.69		AN	-2.2	-3.94	3.89
	std.dev.		(n = 19)	0.59	0.4	0.49		(n = 19)	0.46	0.73	0.41
D	median		RF	-5.37	-6.26	-4.78		RF	-5.35	-5.99	-5.01
	std.dev.		(n = 18)	0.26	0.58	0.07		(n = 18)	0.28	0.53	0.15
M	median		Stream	-0,61	-1,04	0,94		Stream	-0,61	-1,04	0,94
	std.dev.		(n = 257)	2,06	1,10	0,66		(n = 257)	2,06	1,10	0,66

The example 1) considers the initial 50% and 2) the remaining 50% of the sample sets.

Table 3. Median and standard deviation (std.dev.) of end-members and stream projected in three-dimensional including artificial outliers (examples 3 and 4)

Naming in equations		3)	End member	Coordinates			4)	End member	Coordinates		
				U1	U2	U3			U1	U2	U3
A	median		SW	26.25	7.3	7.02		SW	26.21	7.29	6.95
	std.dev.		(n = 26)	5.51	1.73	1.68		(n = 26)	10.28	2.87	2.54
B	median		HS	0.27	5.47	1.98		HS	0.23	5.45	1.97
	std.dev.		(n = 34)	0.99	2.45	1.03		(n = 34)	1.12	1.99	0.8
C	median		AN	-2.24	-3.92	3.79		AN	-2.26	-3.95	3.74
	std.dev.		(n = 38)	0.78	1.17	0.92		(n = 38)	1.07	1.43	1.15
D	median		RF	-5.36	-6.08	-4.84		RF	-5.37	-6.11	-4.86
	std.dev.		(n = 37)	1.7	1.89	1.58		(n = 37)	1.09	1.42	0.94
M	median		Stream	-0,61	-1,04	0,94		Stream	-0,61	-1,04	0,94
	std.dev.		(n = 257)	2,06	1,10	0,66		(n = 257)	2,06	1,10	0,66

The example 3) considers outliers included at the positive extreme of the dataset of each source and 4) outliers included at the negative extreme.

Table 4. Median and enlarged standard deviation (std.dev.) of end-members and stream projected in three-dimensional (examples 5 and 6)

Naming in equations		5)	End member	Coordinates			6)	End member	Coordinates		
				U1	U2	U3			U1	U2	U3
A	median		SW	26,25	7,29	7,00		SW	26,25	7,29	7,00
	std.dev.		(n = 25)	1.39	1.07	1.19		(n = 25)	2.32	1.78	1.99
B	median		HS	0,23	5,48	1,97		HS	0,23	5,48	1,97
	std.dev.		(n = 33)	2.56	3.87	2.06		(n = 33)	4.27	6.45	3.43
C	median		AN	-2,24	-3,93	3,71		AN	-2,24	-3,93	3,71
	std.dev.		(n = 37)	1.65	1.73	1.34		(n = 37)	2.75	2.88	2.24
D	median		RF	-5,38	-6,10	-4,84		RF	-5,38	-6,10	-4,84
	std.dev.		(n = 36)	0.8	1.69	0.46		(n = 36)	1.34	2.81	0.77
M	median		Stream	-0,61	-1,04	0,94		Stream	-0,61	-1,04	0,94
	std.dev.		(n = 257)	2,06	1,10	0,66		(n = 257)	2,06	1,10	0,66

The example 5) considers 3-times the standard deviation of the original data set and 6) 5-times the standard deviation of the original data set.

Table 5. Uncertainty of individual end-member contributions to the stream and Satterthwaite (1946) approximation for the degrees of freedom calculated for the study period 2013–2014

	EM1	EM2	EM3	EM4
	SW	HS	AN	RF
Fraction of end-members contribution	0.06	0.3	0.35	0.29
Upper 95% confidence limit	0.21	0.57	0.58	0.46
Lower 95% confidence limit	0.00	0.03	0.12	0.12
Degrees of freedom	291	536	749	628

Table 6. Uncertainty of individual end-member contributions to the stream and Satterthwaite (1946) approximation for the degrees of freedom computed considering 50% of the data sets

	1)	EM1	EM2	EM3	EM4	2)	EM1	EM2	EM3	EM4
		SW	HS	AN	RF		SW	HS	AN	RF
Fraction of end-members contribution		0.06	0.3	0.35	0.28		0.06	0.28	0.35	0.3
Upper 95% confidence limit		0.21	0.57	0.58	0.45		0.21	0.55	0.58	0.46
Lower 95% confidence limit		0.00	0.03	0.12	0.11		0.00	0.02	0.12	0.14
Degrees of freedom		289	493	676	589		288	491	679	537

The example 1) was computed considering the initial 50% and 2) the remaining 50% of the sample sets.

Table 7. Uncertainty of individual end-member contributions to the stream and Satterthwaite (1946) approximation for the degrees of freedom computed after including artificial outliers

	3)	EM1	EM2	EM3	EM4	4)	EM1	EM2	EM3	EM4
		SW	HS	AN	RF		SW	HS	AN	RF
Fraction of end-members contribution		0.06	0.3	0.35	0.29		0.06	0.3	0.35	0.29
Upper 95% confidence limit		0.22	0.62	0.64	0.5		0.22	0.61	0.63	0.49
Lower 95% confidence limit		0.00	0.00	0.06	0.08		0.00	0.00	0.07	0.08
Degrees of freedom		350	448	640	529		353	554	757	621

The example 3) was computed after including outliers at the positive extreme of the dataset and 4) including outliers at the negative extreme.

Table 8. Uncertainty of individual end-member contributions to the stream and Satterthwaite (1946) approximation for the degrees of freedom computed with enlarged standard deviations

	5)	EM1	EM2	EM3	EM4	6)	EM1	EM2	EM3	EM4
		SW	HS	AN	RF		SW	HS	AN	RF
Fraction of end-members contribution		0.06	0.3	0.35	0.29		0.06	0.3	0.35	0.29
Upper 95% confidence limit		0.23	0.68	0.69	0.52		0.26	0.83	0.83	0.61
Lower 95% confidence limit		0.00	0.00	0.01	0.05		0.00	0.00	0.00	0.00
Degrees of freedom		372	225	362	312		335	122	211	172

The example 5) was computed considering 3-times the standard deviation of the original data set and 6) 5-times the standard deviation of the original data set.