

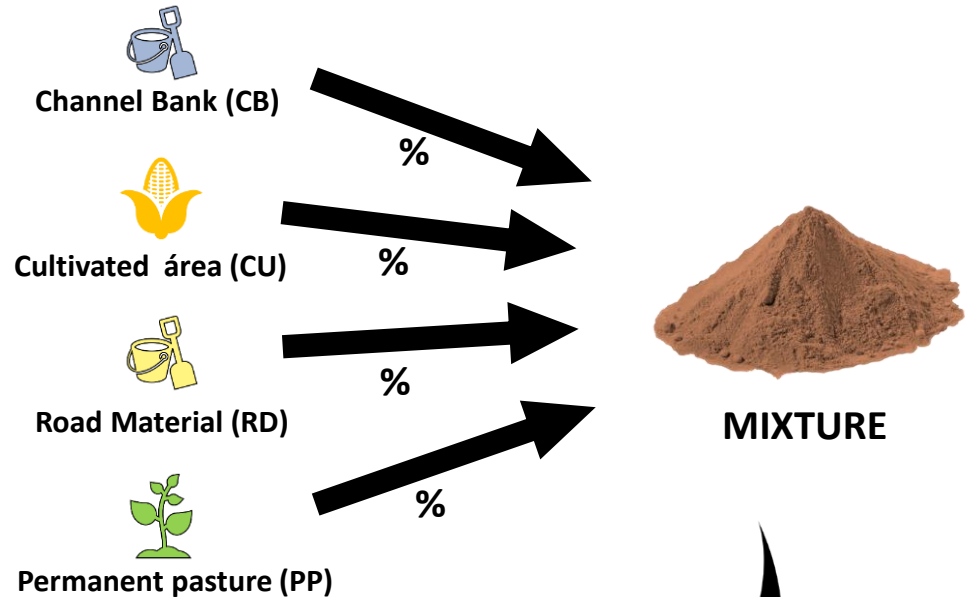
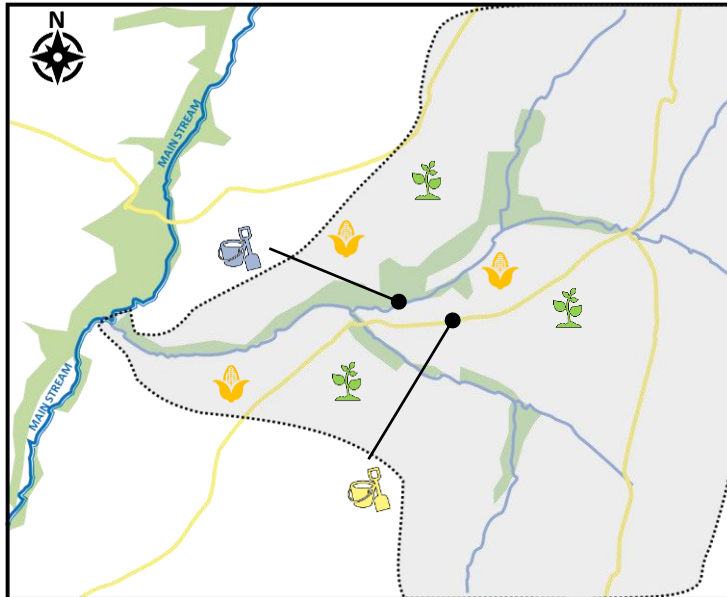
Comparing different error structures in MixSIAR analysis using artificial mixtures from real sediment sources

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Sampling and design



River Allen Sub-catchment (Cornwall)



ARTIFICIAL MIXTURES

	Code	CB	CU	RD	PP
Central Point	CP	25%	25%	25%	25%
Mixture 1 (4 scenarios)	M1S1	85%	5%	5%	5%
	M1S2	5%	85%	5%	5%
	M1S3	5%	5%	85%	5%
	M1S4	5%	5%	5%	85%
Mixture 2 (6 scenarios)	M2S1	40%	40%	10%	10%
	M2S2	40%	10%	40%	10%
	M2S3	40%	10%	10%	40%
	M2S4	10%	40%	40%	10%
	M2S5	10%	40%	10%	40%
	M2S6	10%	10%	40%	40%
Mixture 3 (4 scenarios)	M3S1	10%	30%	30%	30%
	M3S2	30%	10%	30%	30%
	M3S3	30%	30%	10%	30%
	M3S4	30%	30%	30%	10%

Chemical Analysis



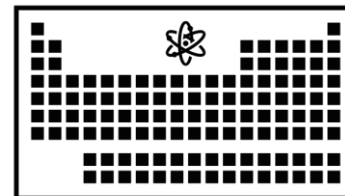
MIXTURE
($<63\mu\text{m}$ sieved)

Milling and
Pressing



PELLET
(Sample:Wax 4:1)

Elemental
Analysis



XRF

Unmixing model

**XRF
data**

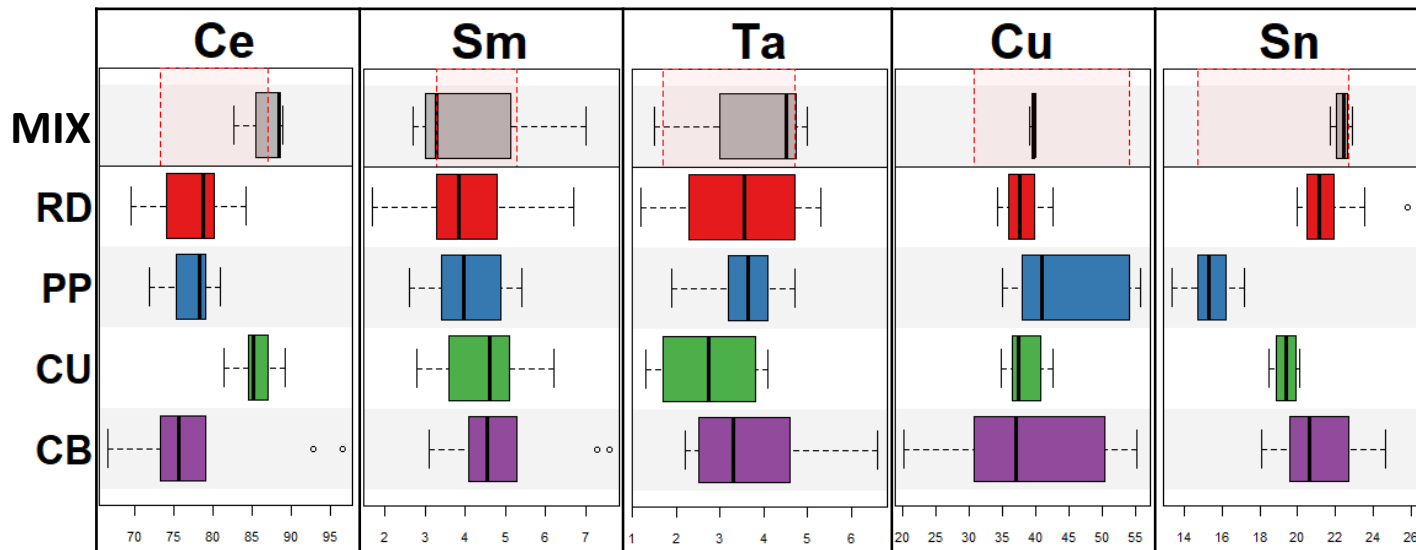
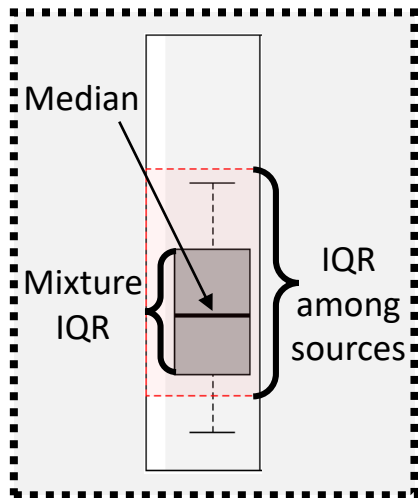
Tracer selection
(Boxplots)

**MixSIAR
analysis**

OUTPUT 1
+ Residual Error

OUTPUT 2
+ Residual Error
+ Process Error

TRACER SELECTION CRITERIA USING BOXPLOTS



Small Mixture IQR (mixture come from lab replicate)					
At least one non overlaped IQR among sources					
Median from Mixture, inside IQR among sources					

MixSIAR RESULTS



OUTPUT 1

Residual Error only

Code	% CB	% CU	% PP	% RD
CPC	21 ± 8	35 ± 8 ▲	18 ± 6 ▼	26 ± 8
M1S1	82 ± 14	8 ± 10	2 ± 4	8 ± 10
M1S2	5 ± 8	85 ± 6	4 ± 6	5 ± 8
M1S3	2 ± 6	12 ± 8	2 ± 4	84 ± 8
M1S4	5 ± 8	8 ± 8	81 ± 6	6 ± 8
M2S1	43 ± 10	42 ± 8	7 ± 6	8 ± 8
M2S2	38 ± 10	13 ± 8	11 ± 8	39 ± 10
M2S3	38 ± 10	12 ± 8	39 ± 8	11 ± 8
M2S4	10 ± 8	40 ± 6	17 ± 6 ▲	33 ± 8
M2S5	11 ± 8	42 ± 6	42 ± 6	5 ± 8
M2S6	14 ± 10	8 ± 8	45 ± 8	32 ± 8
M3S1	4 ± 8	38 ± 6 ▲	25 ± 6	33 ± 8
M3S2	27 ± 10	12 ± 8	29 ± 8	32 ± 8
M3S3	30 ± 8	30 ± 6	31 ± 6	9 ± 8
M3S4	34 ± 8	29 ± 6	11 ± 6	26 ± 8

OUTPUT 2

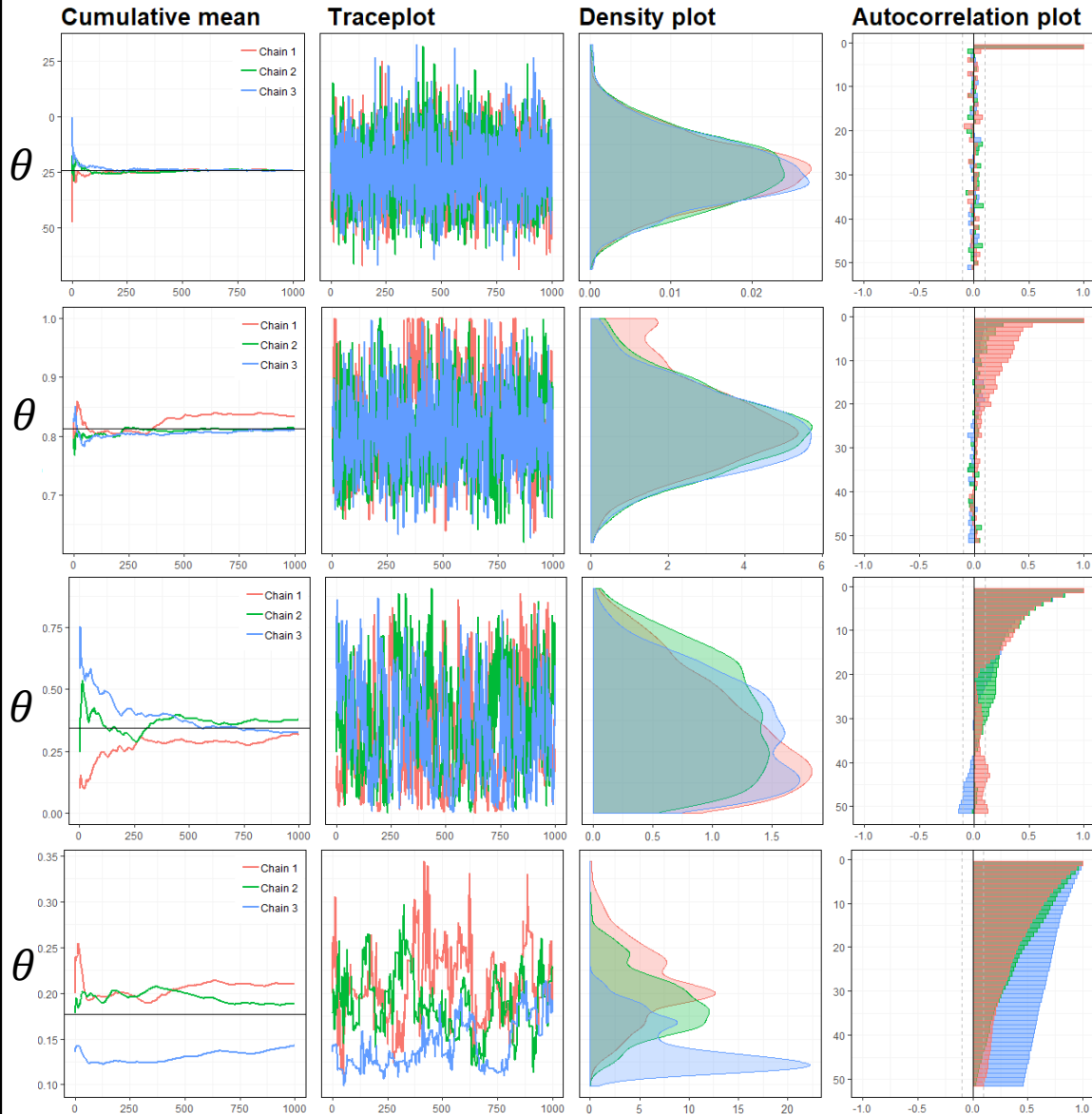
Residual Error x Process Error

Code	% CB	% CU	% PP	% RD
CPC	19 ± 4 ▼	33 ± 4 ▲	23 ± 4	25 ± 4
M1S1	60 ± 12 ▼	20 ± 10 ▲	3 ± 4	17 ± 8 ▲
M1S2	4 ± 2	86 ± 4	6 ± 2	3 ± 1.6 ▼
M1S3	8 ± 6	11 ± 6	9 ± 6	72 ± 8 ▼
M1S4	2 ± 4	12 ± 6 ▲	78 ± 6 ▼	7 ± 4
M2S1	27 ± 6 ▼	49 ± 4 ▲	10 ± 2	14 ± 4
M2S2	30 ± 8 ▼	20 ± 8 ▲	12 ± 6	37 ± 6
M2S3	28 ± 6 ▼	20 ± 8 ▲	35 ± 6	16 ± 4 ▲
M2S4	7 ± 10	44 ± 6	15 ± 4 ▲	34 ± 8
M2S5	8 ± 4	43 ± 4	40 ± 4	10 ± 4
M2S6	11 ± 6	13 ± 6	43 ± 6	32 ± 6 ▼
M3S1	8 ± 4	35 ± 4 ▲	30 ± 4	27 ± 4
M3S2	21 ± 6 ▼	19 ± 8 ▲	31 ± 6	29 ± 4
M3S3	22 ± 4 ▼	36 ± 6 ▲	30 ± 4	13 ± 4
M3S4	25 ± 6	35 ± 6	13 ± 4	27 ± 4

▲ Over-estimated value ($\mu - 2\sigma > \text{Real value}$)
 ▼ Under-estimated value ($\mu + 2\sigma < \text{Real value}$)

CONVERGENCE CRITERIA FOR θ

Visual Criteria



Gelman-Rubin Diagnostic [Reference: Value < 1.05]

1.000



1.029



1.019



1.759



CONVERGENCE RESULTS

OUTPUT 1

Residual Error only

	CB	CU	PP	RD
CP				
M1S1				
M1S2				
M1S3				
M1S4				
M2S1				
M2S2				
M2S3				
M2S4				
M2S5				
M2S6				
M3S1				
M3S2				
M3S3				
M3S4				

OUTPUT 2

Residual Error x Process Error

	CB	CU	PP	RD
CP				
M1S1				
M1S2				
M1S3				
M1S4				
M2S1				
M2S2				
M2S3				
M2S4				
M2S5				
M2S6				
M3S1				
M3S2				
M3S3				
M3S4				



Gelman-Rubin diagnostic value < 1.05



Gelman-Rubin diagnostic value > 1.05

POSTERIOR TRACER SELECTION

(Only apply for Output 2)

OUTPUT 2

Residual Error x Process Error

	CB	CU	PP	RD
CP				
M1S1				
M1S2				
M1S3				
M1S4				
M2S1				
M2S2				
M2S3				
M2S4				
M2S5				
M2S6				
M3S1				
M3S2				
M3S3				
M3S4				



Discard tracers where the residual error estimation (ϵ) did not converge and re-run

New Results

Code	% CB	% CU	% PP	% RD
CPC	17 ± 7 ▼	35 ± 6 ▲	25 ± 6	24 ± 6
M1S1	50 ± 22 ▼	23 ± 14 ▲	5 ± 8	23 ± 12 ▲
M1S2	4 ± 4	86 ± 4	7 ± 4	3 ± 4
M1S3	8 ± 8	11 ± 10	8 ± 8	73 ± 10 ▼
M1S4	3 ± 4	10 ± 6	79 ± 6	7 ± 6
M2S1	29 ± 10 ▼	48 ± 8	11 ± 6	12 ± 8
M2S2	23 ± 12 ▼	24 ± 12 ▲	12 ± 8	40 ± 10
M2S3	28 ± 10 ▼	18 ± 7 ▲	37 ± 6	17 ± 8
M2S4	10 ± 6	42 ± 8	15 ± 6	33 ± 8
M2S5	6 ± 4	45 ± 6	39 ± 6	11 ± 6
M2S6	11 ± 8	14 ± 8	43 ± 6	32 ± 8
M3S1	9 ± 6	35 ± 6	30 ± 6	25 ± 6
M3S2	16 ± 10 ▼	22 ± 10 ▲	25 ± 10	37 ± 10
M3S3	17 ± 8 ▼	40 ± 8 ▲	30 ± 6	13 ± 6
M3S4	25 ± 10	34 ± 8	12 ± 8	29 ± 8

New Convergence chart

	CB	CU	PP	RD
CP				
M1S1				
M1S2				
M1S3				
M1S4				
M2S1				
M2S2				
M2S3				
M2S4				
M2S5				
M2S6				
M3S1				
M3S2				
M3S3				
M3S4				

OUTPUT 1

Residual Error only

Short time of analysis

More precise

More convergence achieved

Increasing time of analysis
improve convergence



OUTPUT 2

Residual Error x Process Error

Longer time of analysis

Less precise (first run)

Some parameters do not converge
(first run)

Discarding tracers where the
estimation of ε did not converge
and re-run, improve convergence