

Temperature-Dependent Particle Formation During Biomass Combustion: A Combined spICP-TOFMS and Magnetic Study

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Supplementary Information

Table 1SI: spICP-TOFMS parameters used for the analysis of leachate

PARAMETER (UNIT)

Sample Flow Rate (mL min ⁻¹)	≈ 0.18
Transport efficiency (%)	≈ 5-20%
RF power (W)	1300
Spray Chamber type	Quartz Cyclonic
Nebuliser type	PFA Microflow
Ar cool gas (L min ⁻¹)	13.0
Ar auxiliary gas (L min ⁻¹)	2.0
Ar nebulization gas (L min ⁻¹)	1.1
Collision cell gas (mL min ⁻¹)	Helium : 14 Hydrogen : 7
Dwell time (ms)	0.083
Acquired mass range	23 to 238 amu (blanked region: 32-40 amu)
Examined isotopes	²⁷ Al ²⁸ Si ⁴⁸ Ti ⁵⁵ Mn ⁵⁶ Fe

Table 2SI: Combustion condition

Code	Treatment	Average % mass loss
PN12	Fresh sample	-
PN13	5 min	39%
PN14	400°C 15 min	65%
PN15	30 min	73%
PN20	5 min	64%
PN21	550°C 15 min	79%
PN22	30 min	76%
PM4	800°C 5 min	84%
PM3	15 min	88%

Table 3SI: spICP-TOFMS detection limit and sensitivity

Code	Treatment		leachate wood (mg/mL)	dilution factor	LOD (fg)				
					Al	Si	Ti	Mn	Fe
PN12	Fresh sample		12,49	50,3	1,72	3,33	0,21	0,11	0,47
PN13		5 min	12,47	50,7	1,12	1,86	0,21	0,17	0,30
PN14	400°C	15 min	12,45	51,8	1,15	1,96	0,22	0,29	0,32
PN15		30 min	12,50	50,9	1,35	2,27	0,21	0,27	0,38
PN20		5 min	12,53	50,2	1,17	1,98	0,17	0,28	0,33
PN21	550°C	15 min	12,44	100,1	1,26	2,09	0,17	0,34	0,37
PN22		30 min	12,46	200,3	1,14	2,41	0,20	0,45	0,40
PM4	800°C	5 min	12,54	638,8	0,66	1,75	0,10	0,14	0,18
PM3		15 min	12,13	214,0	0,65	2,26	0,13	0,13	0,17

Analysis date	Sample ID	ionic response (cts/(µg/L))				
		Al	Si	Ti	Mn	Fe
26/02/2025	PN	0,464	0,304	2,526	4,876	4,051
19/05/2025	PM	0,241	0,142	1,418	2,428	2,188

Table 4SI: Bulk elemental concentration (mean \pm sd) in samples digested in nitric acid at different combustion temperatures: a) Reported per sample mass; b) Normalized to pre-combustion mass.

a)

Combustion temperature	Mn (ppm)	Si (ppm)	Al (ppm)	Fe (ppm)	Zn (ppm)	Ti (ppm)	Cu (ppm)	Pb (ppm)	Mn/Fe ratio
Fresh	175 \pm 1	138 \pm 2	205 \pm 1	43 \pm 1	12 \pm 1	9 \pm 1	5 \pm 1	0	4,0
400°C	248 \pm 1	521 \pm 10	386 \pm 8	166 \pm 1	14 \pm 1	8 \pm 1	7 \pm 1	3 \pm 1	1,5
550°C	859 \pm 8	484 \pm 10	277 \pm 6	195 \pm 1	23 \pm 1	11 \pm 1	14 \pm 1	8 \pm 1	4,4
800°C	711 \pm 8	712 \pm 19	326 \pm 11	219 \pm 1	15 \pm 1	12 \pm 1	23 \pm 1	30 \pm 1	3,2

b)

Combustion temperature	Combustion enrichment factor	Mn (ppm)	Si (ppm)	Al (ppm)	Fe (ppm)	Zn (ppm)	Ti (ppm)	Cu (ppm)	Pb (ppm)
400°C	1,738	143 \pm 15	300 \pm 32	222 \pm 24	96 \pm 10	8 \pm 1	5 \pm 1	4 \pm 1	2 \pm 1
550°C	4,714	182 \pm 19	105 \pm 11	59 \pm 6	41 \pm 4	5 \pm 1	2 \pm 1	3 \pm 1	2 \pm 1
800°C	9,166	77 \pm 6	78 \pm 8	35 \pm 4	24 \pm 3	2 \pm 1	2 \pm 1	2 \pm 1	3 \pm 1

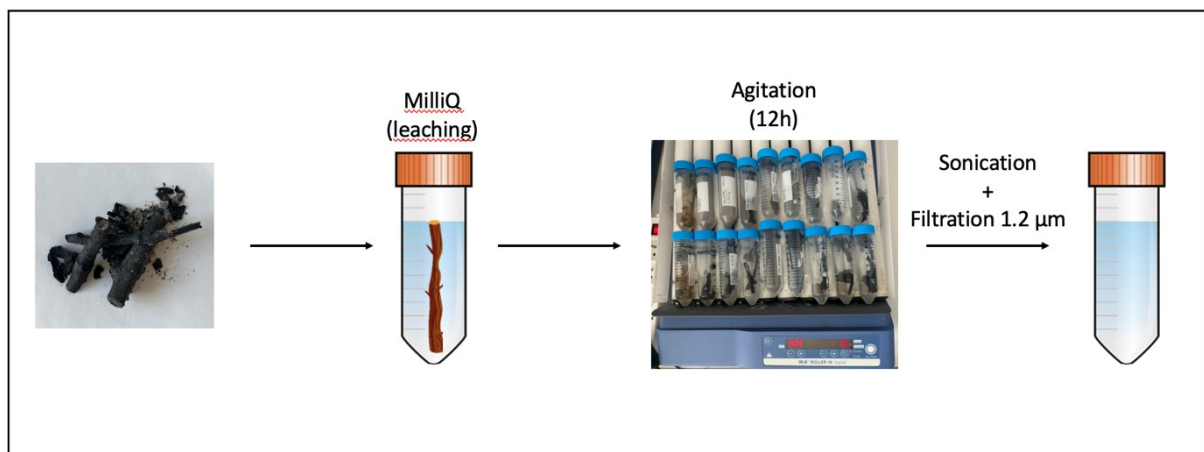
Of the elements measured, samples contained higher levels of manganese, silica, aluminium and iron, while copper, zinc, titanium and lead are only present in trace amounts. While these measurements should be treated with caution as the digested samples are not necessarily identical (more thorns or more wood), results indicate that an increase in combustion temperature leads to a concentration of the studied elements, suggesting that the loss of mass is not primarily due to these elements. However, if the bulk elemental concentration is normalized to the mass prior to combustion, the loss of Si as well as metals was evident during combustion. The temperature mostly impacted the aerosolization of aluminium and silica, which decreased by more than 65% between 400°C and 550°C. Conversely, manganese, copper and lead were affected the least, with a maximum loss of 50% between 450°C and 800°C.

Figure 1SI: High-temperature combustion facility and post-combustion residues a) Samples in the sample holder before combustion, on the left for combustions up to 550°C, on the right for combustions at 800°C; b) Sample after combustion; c) Horizontal furnace used for controlled soil heating.



Figure 2SI: a) Sample leaching procedure for analysis by spICP-TOFMS; b) Procedure for preparing samples for measuring magnetic properties (VSM).

a)



b)

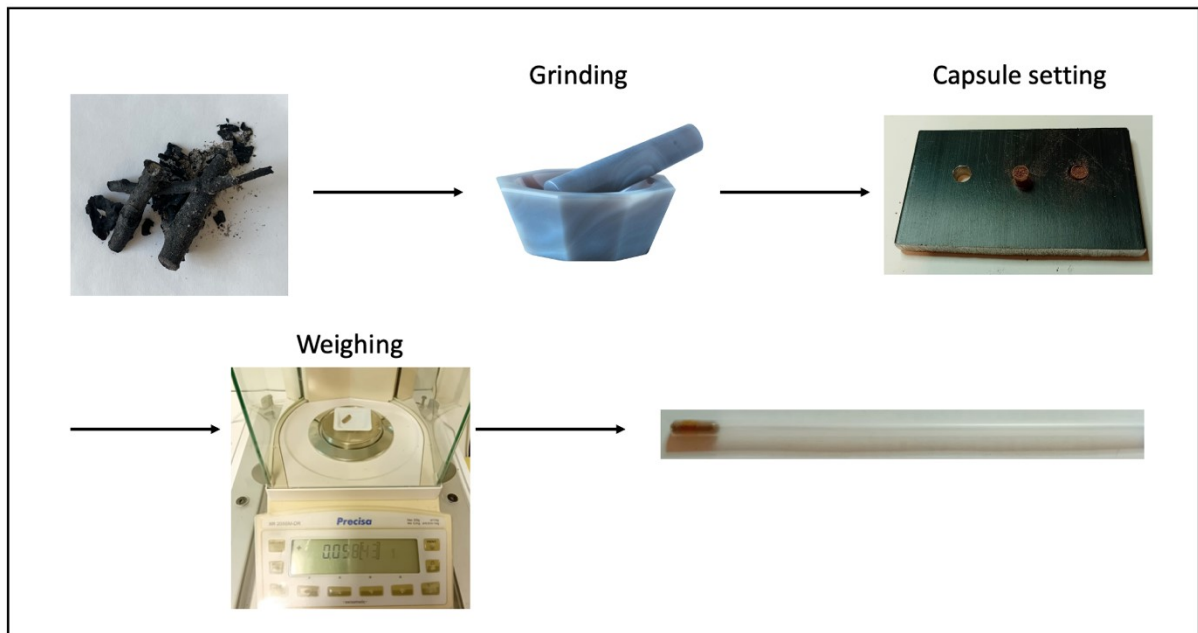


Figure 3SI: Photographs of fresh wood and combustion residues at different combustion intensities.

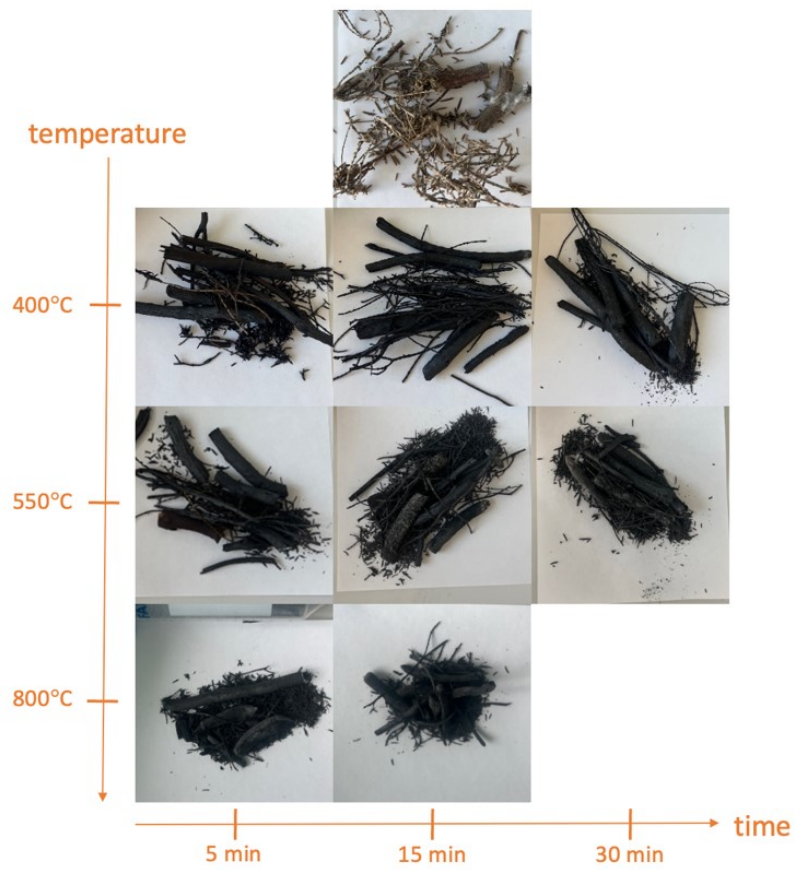


Figure 4SI: Total concentration (dissolved + nanoparticulate fractions) measured in the leachate. The values were converted to leachate concentrations by applying the dilution factor. The mass of wood leached per mL of water is 12.5 ± 0.07 mg/mL for all samples, except for those treated at 800 °C for 15 minutes, for which it is 12.13.

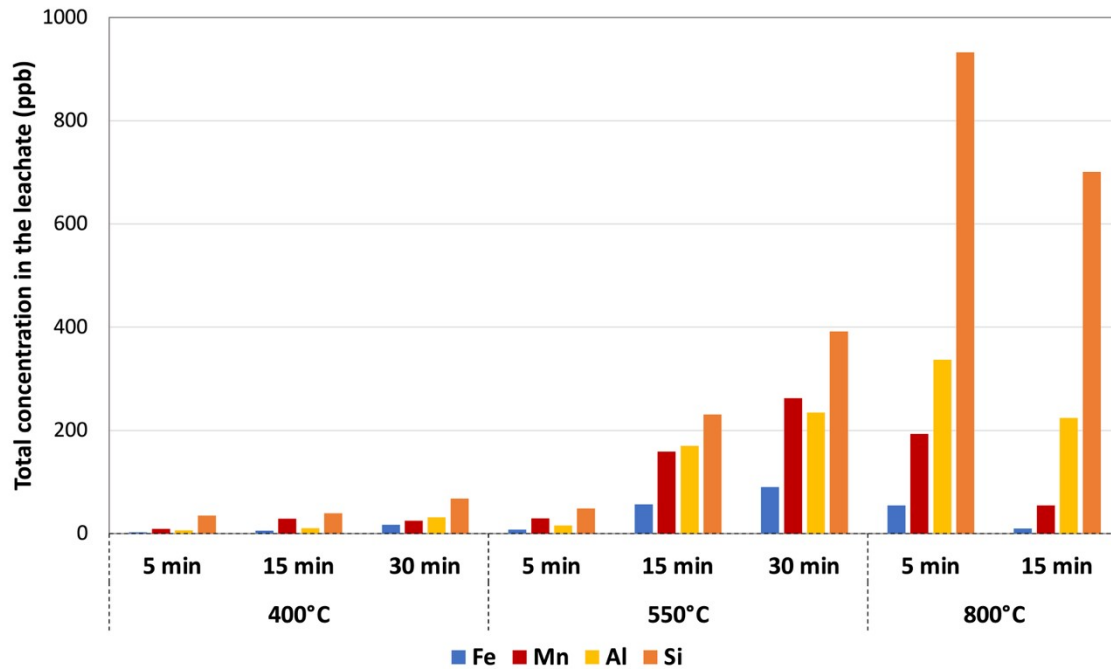


Figure 5SI: Data from magnetic measurements: change in normalized magnetic susceptibility relative to the mass of the calcined sample as a function of combustion condition.

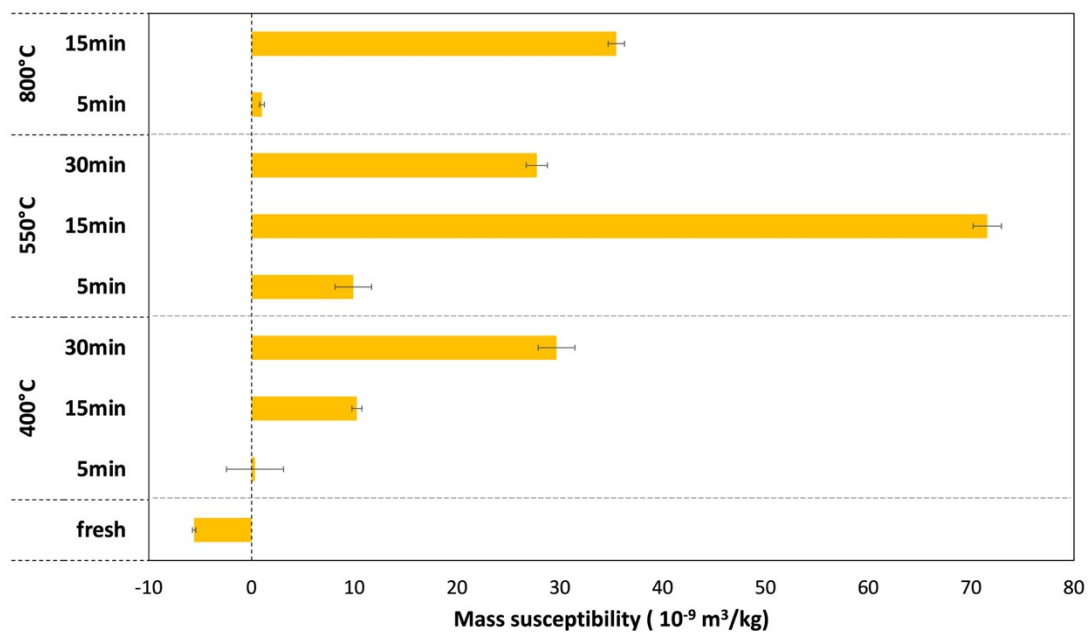


Figure 6SI: The particle families present in the leachate were identified using self-organizing maps (SOM) combined with k-means meta-clustering. For this purpose, the spICP-TOFMS raw data were converted into elemental mass fractions.

All samples were combined into a single matrix, and particles were projected onto the SOM according to their compositional similarity, evaluated using Euclidean distance. Panel a) shows the SOM hit histogram, where each particle is assigned to a neuron in the artificial neural network, while panel b) illustrates the spatial distribution of elemental composition across the network.

Clusters were then defined using the k-means algorithm applied to the SOM map. As the k-means approach functions as a measure of dissimilarity, the number of clusters was set manually to nine in order to optimally separate the particles of interest, visually maximize group consistency, and minimize internal variability while maintaining a sufficient number of particles per cluster. Each hexagon on the SOM is thus assigned to a cluster, as shown in panel c). The composition and particle count for each cluster are shown in panel d). Cluster 2, which represent less than 0.2% of the data, seems to correspond to trace components in carbonate particles.⁸⁹ It was excluded from further analyses and discussion. Clusters 5 and 8, have been merged to form a single cluster SiAl.

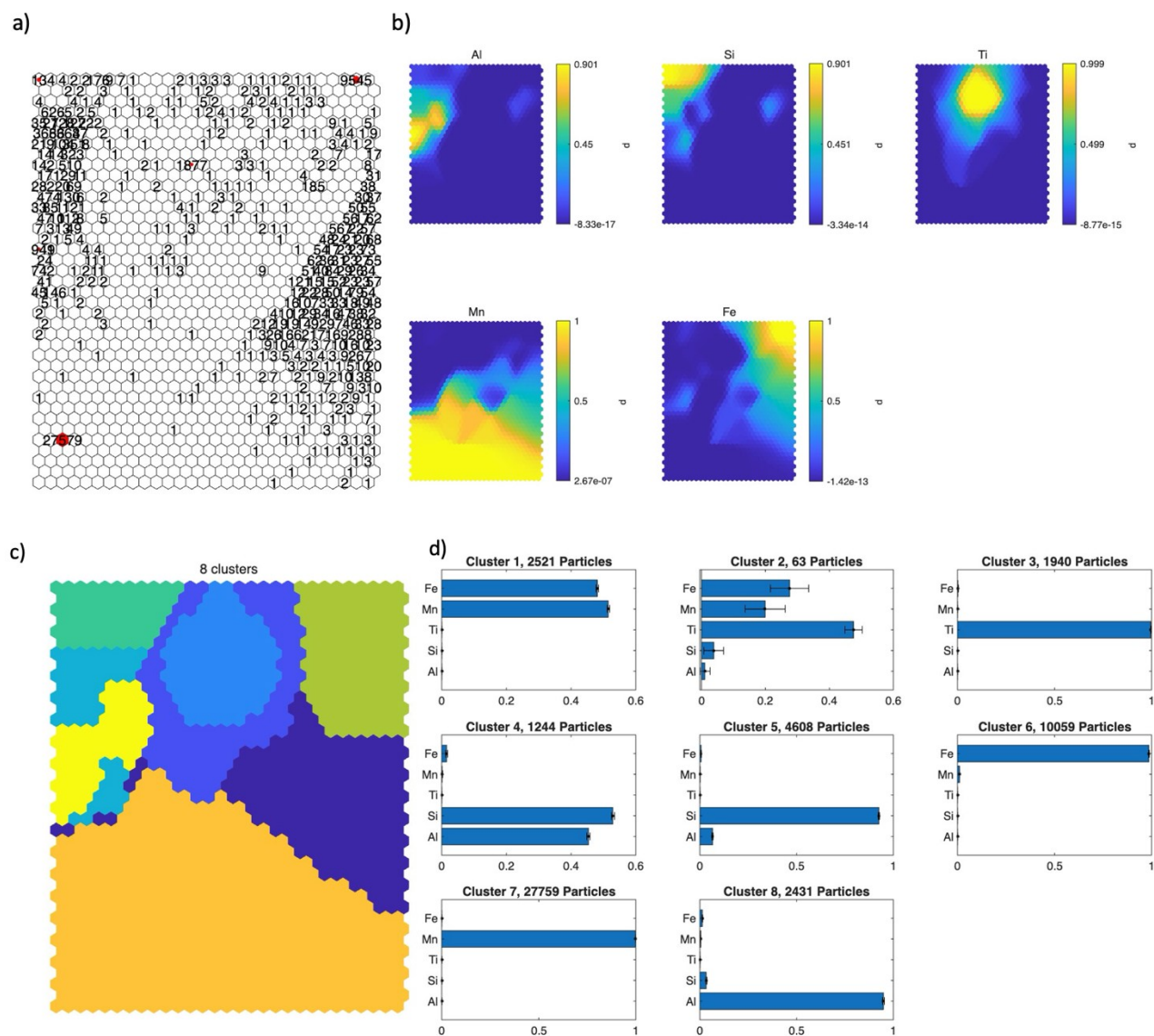
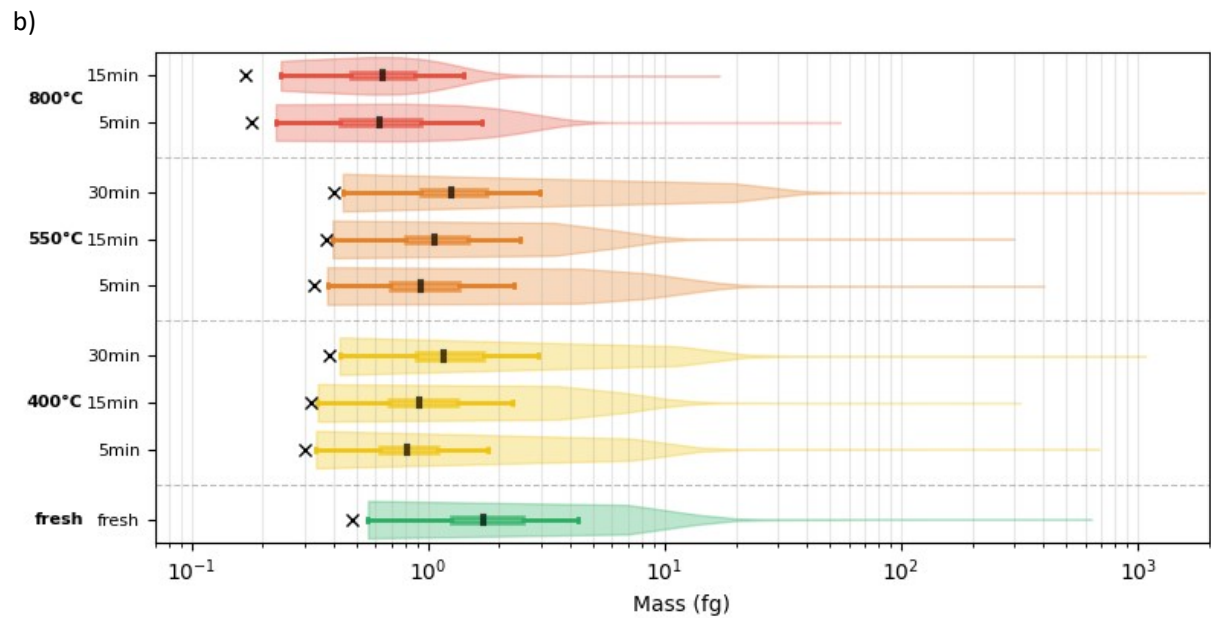
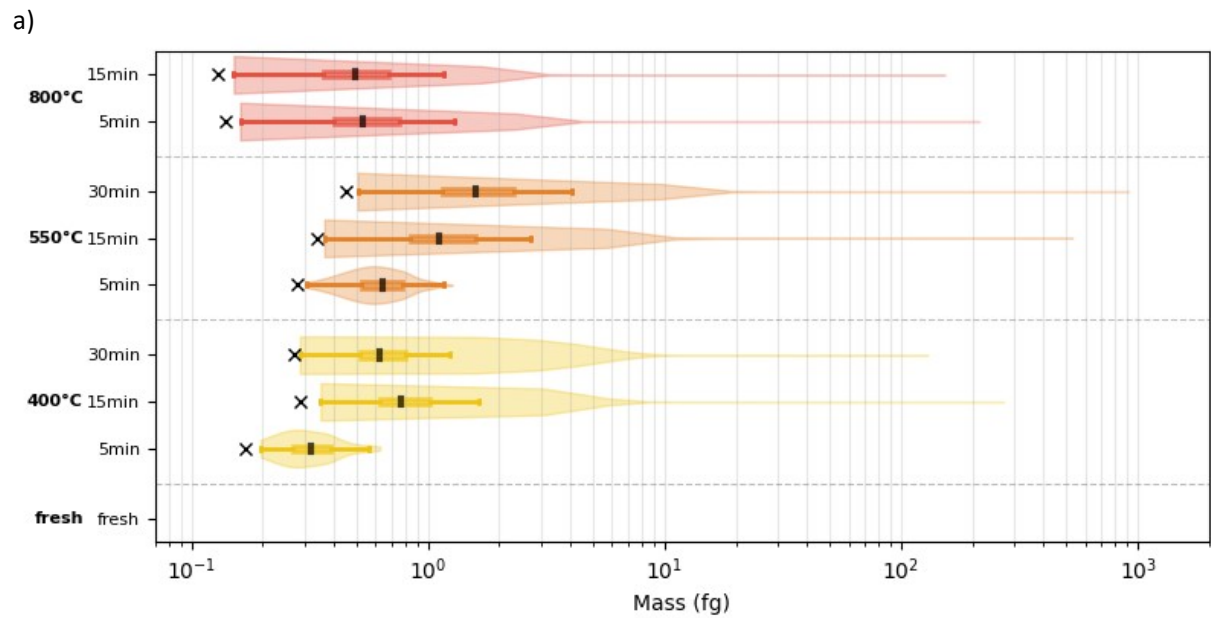
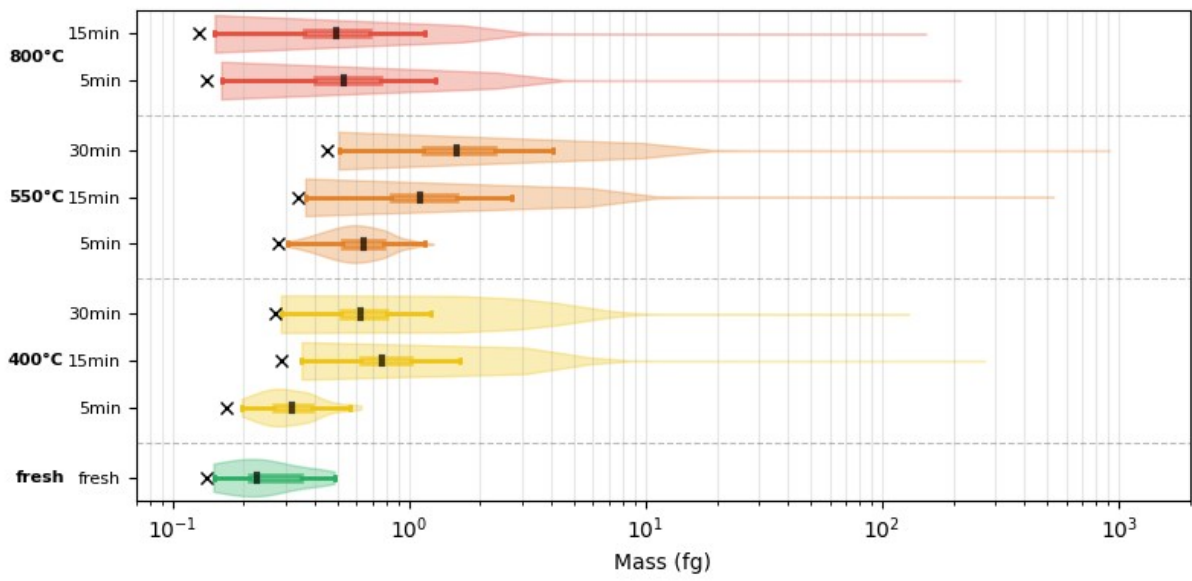


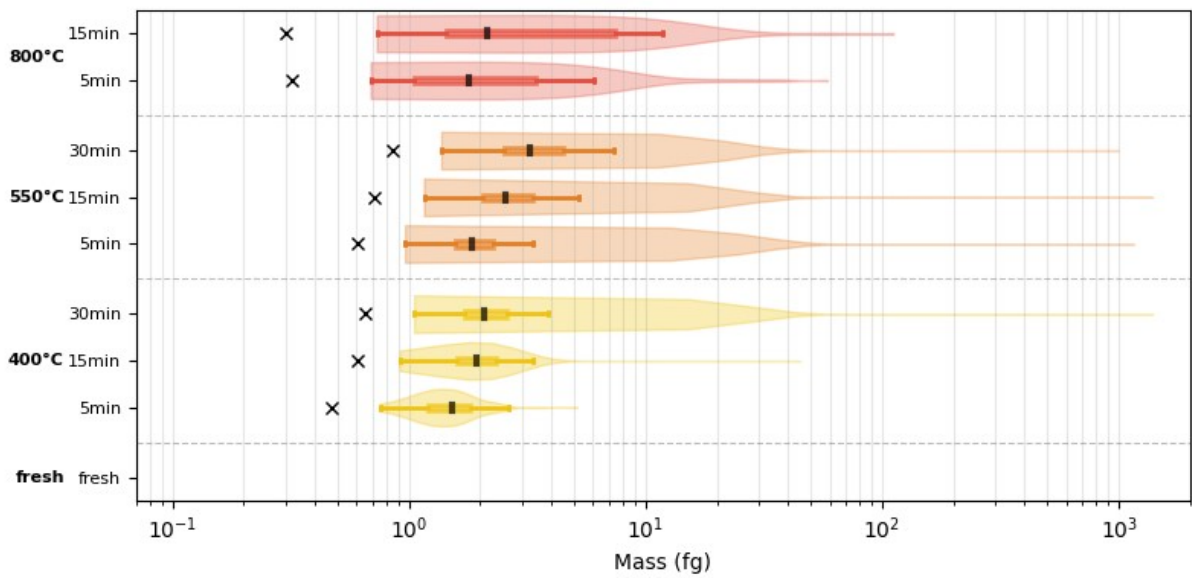
Figure 7SI: Violin plot representation of particle masses measured by spICP-TOFMS as a function of combustion conditions: a) Mn monoelemental; b) Fe monoelemental; c) Ti monoelemental; d) MnFe bielemental; e) SiAl bielemental; f) SiAlFe trielemental. The black crosses represent the detection limit of the particles during measurement.



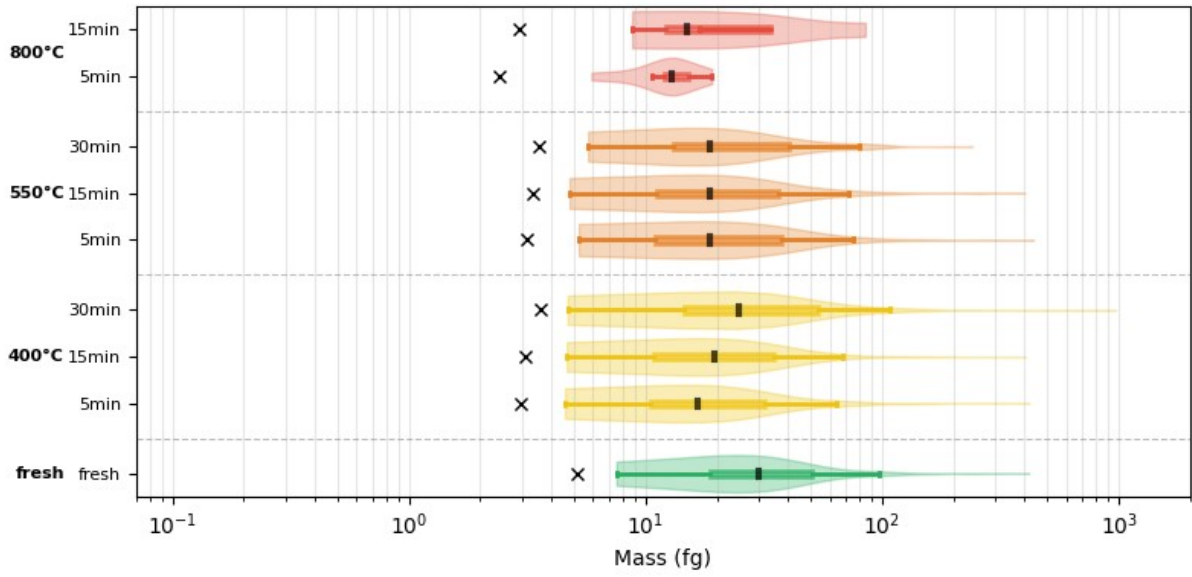
c)



d)



e)



f)

