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Data Article

Data on physical and chemical characterization of wood combustion products derived at cogeneration power plants

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ABSTRACT

The data presented in this article are related to the research paper "Granulation of fly ash and biochar with organic lake sediments – A way to sustainable utilization of waste from bioenergy production" [1] in the context of waste material investigation and possible valorization instead of disposal. This article provides a comprehensive chemical and physical characterization of wood combustion products – fly ashes, bottom ashes, mixed ashes and biochar. Multiple analytical techniques and methodology were exploited to investigate the composition of wood combustion products, among them a loss on ignition, potentiometry, colorimetry, X-ray diffractometry, X-ray fluorescence spectrometry, inductively coupled plasma optical emission spectrometry, gas chromatography. General parameters detected were the content of dry matter, gravimetric water, volatile matter, amount of ash and fixed carbon. The elemental analysis involved determining C, H, N and O. Physical properties were described by bulk density, solid density, total porosity, electric conductivity, specific weight and mass ratio assessment of particle size distribution. The mineralogical composition was described by major crystalline phases of samples and content of oxides. Chemical properties and composition were characterized by pH,

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the content of ammonium, nitrates, nitrites, exchangeable elements and cation exchange capacity as well as after the 3-step speciation and analytical quantification of trace and major elements (Al, As, Ba, Ca, Cd, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Sb, Se, Sr, Ti, Tl, V and Zn) and detection of polycyclic aromatic hydrocarbons.

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Specifications Table

Subject	Materials science; Environmental science
Specific subject area	Waste material characterization
Type of data	Table and figure
How data were acquired	Loss on ignition (LOI), sieving, pycnometer method, potentiometry, colorimetry, powder X-ray diffractometry (XRD), X-ray fluorescence spectrometry (XRF), inductively coupled plasma optical emission spectrometry (ICP-OES), gas chromatography (GC)
Data format	Raw and analyzed
Parameters for data collection	Ten consolidated samples of wood combustion products obtained at cogeneration power plants and prior investigation were dried at 105 °C for two hours; selected samples (2F, 2B, 3B, 4 M, 5 M and 6 M) were subjected for the full-scale analyses, while for the others, selection of the analyzed parameters was applied
Description of data collection	General characteristics of samples were described by dry matter, gravimetric water, volatile matter, content of ash; Elemental analysis involved determination of C, H, N and O; Physical properties were described by bulk density, solid density, total porosity, electric conductivity, specific weight and mass ratio assessment of particle size distribution; Mineralogical composition was described by major crystalline phases of samples and content of oxides; Chemical properties and composition was described by pH, content of ammonium, nitrates, nitrites and exchangeable elements as well as speciation and quantification of chemical elements and polycyclic aromatic hydrocarbons (PAHs)
Data source location	Samples were collected at cogeneration plants in Latvia and Lithuania; analyses were performed at the University of Latvia, Riga, Republic of Latvia
Data accessibility	Data are deposited in a public repository: Mendeley Data Z. Vincevica-Gaile, K. Stankevica, M. Klavins, A. Trubaca-Boginska, Analysis of wood combustion products, https://doi.org/10.17632/3ngwcbj5r7.1
Related research article	Z. Vincevica-Gaile, K. Stankevica, K. Irtiseva, A. Shishkin, V. Obuka, S. Celma, J. Ozolins, M. Klavins, Granulation of fly ash and biochar with organic lake sediments – A way to sustainable utilization of waste from bioenergy production, Biomass Bioenerg. 125 (2019) 23–33. https://doi.org/10.1016/j.biombioe.2019.04.004

Value of the Data

- The data involve comprehensive chemical and physical characterization of wood combustion waste samples derived from energy and heat producing power plants.
- The data are valuable for engineers and researchers working on ash and biochar investigation and utilization, waste valorization, and innovative products from secondary raw materials. The data are valid for comparison with other results of similar materials.

- The data are useful for various purposes including life cycle analysis (LCA), secondary raw material assessment, waste description and potential use.
- The data, as well as applied methodology, can act as a basis for further investigation or processing of biomass combustion products relevant for construction, geoengineering, agricultural purposes.

1. Data Description

The data involved in this article provide a versatile characterization of 10 consolidated samples of wood combustion products – fly ashes (1F, 2F), bottom ashes (1B, 2B, 3B), mixed ashes (4 M, 5 M, 6 M) and biochar (7BJ, 8BT). Selected samples (2F, 2B, 3B, 4 M, 5 M and 6 M) were subjected for the full-scale analyses, while for the others, selection of the analyzed parameters was applied. Table 1 compiles the general parameters such as the content of moisture, dry matter, volatile matter, ashes and fixed carbon characterizing the samples. Elemental composition regarding the content of C, H, N and O is provided in Table 2. Physical properties are described by density, porosity, specific weight and electrical conductivity (see Table 3).

Mass ratio assessment of particle size distribution is shown in Fig. 1. Mineralogical description of the samples is demonstrated in Figs. 2 and 3.

Table 1
General parameters characterizing samples ($n = 3$) of wood combustion products.

	Fly ashes	Bottom ashes		Mixed ashes			Biochar	
Parameter, unit	2F	2B	3B	4M	5M	6M	7BJ	8BT
Dry matter, %	98.49	99.73	80.14	93.80	91.43	99.70	96.49	98.57
Gravimetric water content, %	1.51	0.27	19.86	6.20	8.57	0.30	3.51	1.43
Volatile matter, %	8.82	2.84	5.14	8.89	5.08	12.66	31.21	30.65
Ash content, %	62.14	94.41	73.00	84.64	86.30	78.46	13.97	19.35
Fixed carbon, %	27.53	2.48	2.00	0.27	0.04	8.58	51.31	48.57

Table 2
Elemental composition characterizing samples ($n = 12$ and $n = 6$, depending on a sample) of wood ashes (ND – not detected).

	Fly ashes	Bottom ashes		Mixed ashes		
Parameter, unit	2F	2B	3B	4M	5M	6M
Organic carbon (C_{org}), %	49.38	1.62	0.73	6.19	2.02	21.43
Hydrogen, %	0.66	0.12	0.12	0.79	0.63	0.31
Nitrogen, %	0.22	ND	ND	ND	ND	0.05
Oxygen, %	49.74	98.26	99.15	93.02	97.35	78.21
H/C_{org}, molar ratio	0.16	0.89	1.93	1.52	3.72	0.17
O/C_{org}, molar ratio	0.76	45.82	100.59	11.28	36.18	2.74

Table 3
Physical properties of wood combustion product samples ($n = 3$; N/A – not analyzed).

	Fly ashes	Bottom ashes		Mixed ashes			Biochar	
Parameter, unit	2F	2B	3B	4M	5M	6M	7BJ	8BT
Bulk density, kg/m^3	367.97	1306.85	833.11	964.46	1021.98	764.76	210.01	190.00
Solid density, kg/m^3	2434.25	2558.63	2615.63	2689.15	3037.77	2817.27	1970.34	1850.11
Total porosity, m^3/m^3	0.843	0.487	0.681	0.635	0.644	0.728	0.891	0.897
Electric conductivity, S/m	1.36	0.32	0.22	0.62	0.47	0.53	N/A	N/A
Specific weight, kN/m^3	23.88	25.10	25.66	26.38	29.80	27.64	19.33	18.15

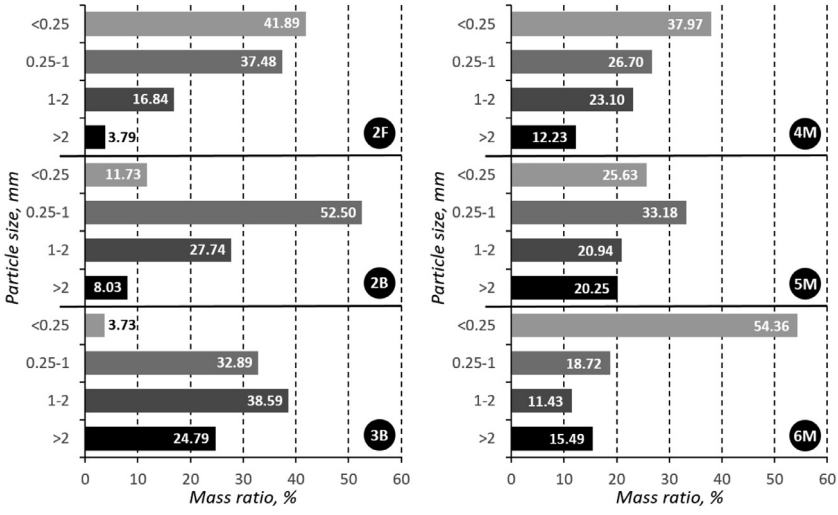

Fig. 1. Mean weighted particle size and the mass ratio of wood ash samples ($n = 2$).

Table 4
Content of oxides in wood ash samples ($n = 1$ in each fraction) by fractions detected using XRF (ND – not detected).

Element in the form of oxide	Fly ashes		Bottom ashes		Mixed ashes					
	2F		2B	3B	4M		5M		6M	
Fraction, mm	<0.25	>2	<0.25	<0.25	<0.25	0.25–1	<0.25	0.25–1	<0.25	0.25–1
CaO, %	44.8	11.9	45.6	43.8	40.8	26.1	28.2	21.2	18.4	8.4
SiO_2, %	11.6	0.8	13.9	13.3	17.0	35.7	34.1	44.4	39.9	52.6
K_2O, %	4.9	5.1	5.0	4.9	5.0	6.4	4.1	5.1	5.5	3.8
MgO, %	5.9	0.5	6.8	4.8	3.1	2.4	4.1	3.0	2.1	1.3
Fe_2O_3, %	1.3	0.5	2.1	1.5	2.8	2.7	2.7	2.0	1.6	0.9
SO_3, %	2.9	0.6	1.2	0.3	2.0	0.9	0.8	0.6	1.1	0.2
P_2O_5, %	3.6	0.6	3.1	4.0	2.0	1.3	1.6	1.3	2.5	1.2
Al_2O_3, %	2.0	ND	2.0	2.1	1.8	2.1	2.7	3.0	3.3	2.1
MnO, %	3.4	1.1	1.8	1.4	1.2	0.9	0.7	0.6	1.1	0.5
Na_2O, %	ND	ND	ND	ND	1.1	2.0	ND	ND	ND	0.8
Cl, %	ND	ND	ND	ND	1.1	0.5	ND	ND	ND	ND
Other, %	1.7	0.3	1.0	0.8	1.0	0.5	0.4	1.6	0.6	0.1
Total, %	82.1	21.4	82.5	76.9	78.9	81.5	79.4	82.8	76.1	71.9

Table 5
Detected acidity of wood combustion products ($n = 3$; N/A – not analyzed).

	Fly ashes	Bottom ashes		Mixed ashes			Biochar	
Parameter	2F	2B	3B	4M	5M	6M	7BJ	8BT
pH in water	12.57	11.84	11.71	12.08	12.03	11.98	12.41	12.63
pH in KCl	12.51	12.03	11.91	12.41	12.39	12.22	N/A	N/A

XRF analysis (Table 4) revealed that the main mineral components in the form of oxides in wood ashes were Ca and Si with a significant amount of K and Mg. Chemical characterization of samples involved detection of pH (Table 5), the content of ammonium, nitrites and nitrates (Table 6), exchangeable elements (Table 7) and quantification of trace and major elements (Al, As, Ba, Ca, Cd, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Sb, Se, Sr, Ti, Tl, V and Zn) by fractions (Supplement 1).

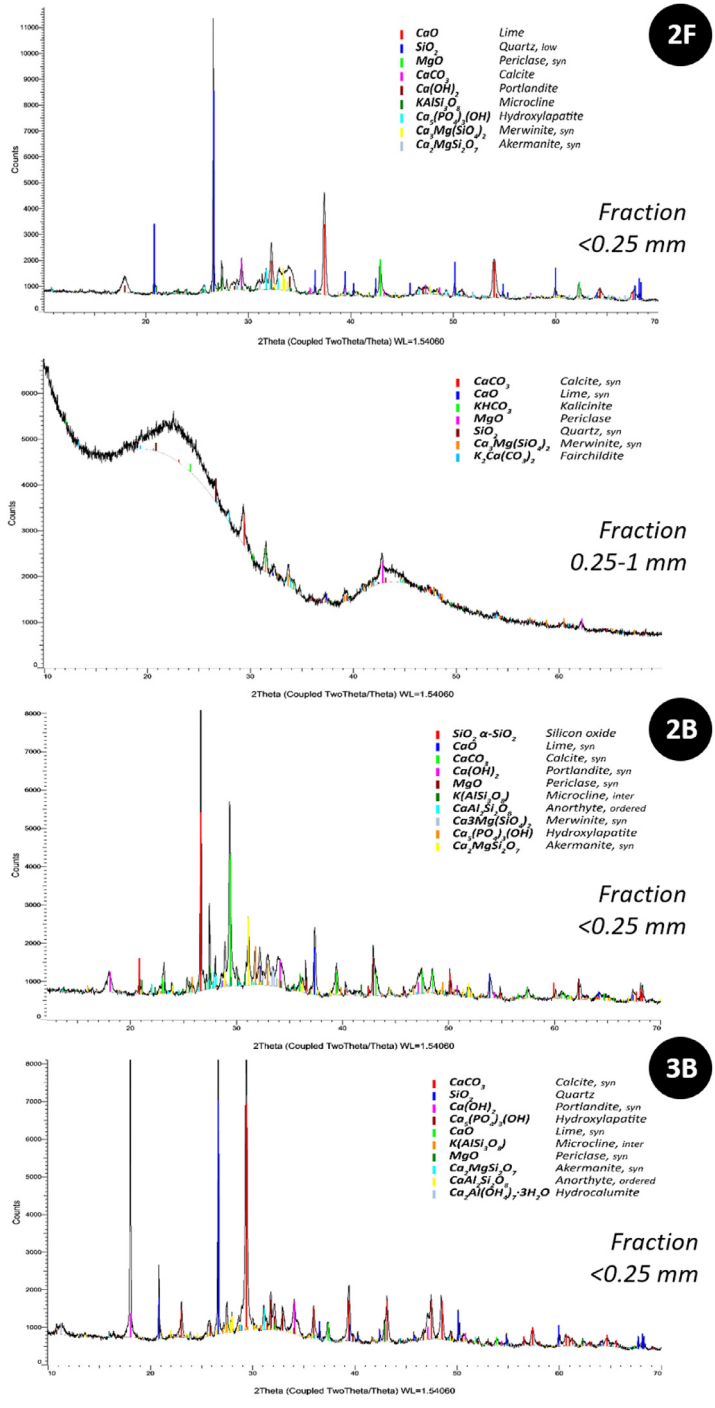

Fig. 2. Mineralogical composition of fly ash and bottom ash samples ($n = 1$ in each fraction) according to XRD analysis.

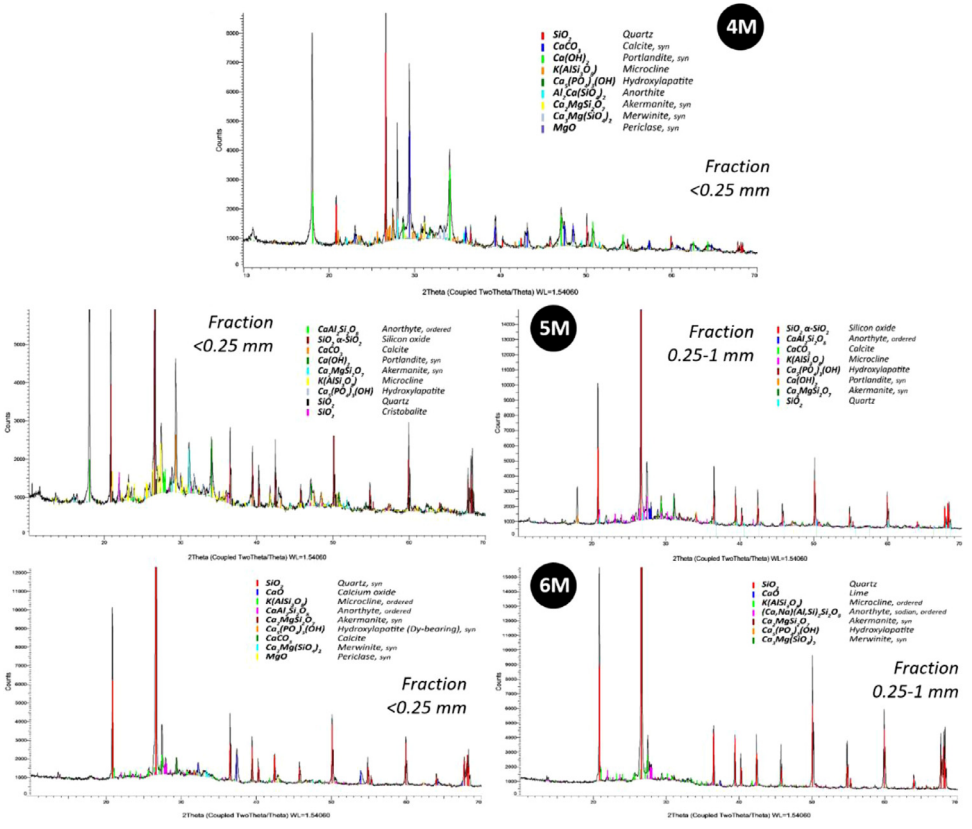

Fig. 3. Mineralogical composition of mixed ash samples ($n = 1$ in each fraction) according to XRD analysis.

Table 6
Content of ammonium, nitrates and nitrites in wood ash samples ($n = 3$).

	Fly ashes	Bottom ashes		Mixed ashes		
Parameter, unit	2F	2B	3B	4M	5M	6M
N-NH_4, mg/kg	1.83	3.24	3.79	5.33	2.67	3.28
NH_4, mg/kg	2.36	4.17	4.88	6.86	3.44	4.22
N-NO_3, mg/kg	59.97	93.10	13.23	99.87	89.84	93.24
NO_3, mg/kg	265.45	412.13	58.57	442.12	397.72	412.77
N-NO_2, mg/kg	0.47	3.16	1.09	2.39	1.10	1.37
NO_2, mg/kg	1.53	10.39	3.59	7.86	3.61	4.49

Table 7
Content of exchangeable elements in wood ash samples ($n = 3$) and cation exchange capacity (CEC).

Parameter, unit	Fly ashes	Bottom ashes		Mixed ashes		
	2F	2B	3B	4M	5M	6M
K_{ex}, cmol/kg	39.09	13.08	13.94	30.92	8.95	17.00
Ca_{ex}, cmol/kg	371.49	115.51	28.53	258.64	235.87	125.49
Mg_{ex}, cmol/kg	42.71	9.38	2.53	8.50	4.72	10.17
Na_{ex}, cmol/kg	1.64	0.55	0.72	10.02	1.25	0.94
CEC, cmol/kg	3.33	1.09	1.02	1.28	0.77	1.47

Table 8
Specification of sampled wood combustion products and their origin.

Type of sample	Sample description	Producer	Fuel used	Thermochemical process applied
1F: Fly ash	Grey powder with some inclusions of stones	'Fortum Jelgava', Ltd. (Jelgava, Latvia)	Variable wood waste chips	Combustion at 850–1000 °C
2F: Fly ash	Dark grey to black powder with lustre	'Oil Investment Projects', Ltd. (Vilnius, Lithuania)	Coniferous softwood chips	Combustion at 950 °C
1B: Bottom ash	Dark grey grainy powder	'Fortum Jelgava', Ltd. (Jelgava, Latvia)	Variable wood waste chips	Combustion at 850–1000 °C
2B: Bottom ash	Light grey powder with a small amount of coal remains	'Oil Investment Projects', Ltd. (Vilnius, Lithuania)	Coniferous softwood chips	Combustion at 950 °C
3B: Bottom ash	Brownish grey, wet sandy substance	'Technology Projects', Ltd. (Vilnius, Lithuania)	Variable wood waste chips	Combustion at 950 °C
4M: Mixed ash	Light grey powder with quartz grains	'SSPC Taika', Ltd. (Kaunas, Lithuania)	Coniferous softwood chips	Combustion at 950 °C
5M: Mixed ash	Light grey powder with quartz grains	'GECO Kaunas', Ltd. (Kaunas, Lithuania)	Coniferous softwood chips	Combustion at 950 °C
6M: Mixed ash	Dark grey to black powder	'GECO Vilnius', Ltd. (Vilnius, Lithuania)	Coniferous softwood chips	Combustion at 950 °C
7BJ: Biochar	Dark grey to black powder with lustre	Cogeneration Station 1 (Jekabpils, Latvia)	Non-coniferous hardwood chips	Pyrolysis at 800 °C
8BT: Biochar	Dark grey to black powder with lustre, with pieces of coal	Cogeneration Station 2 (Taurene, Latvia)	Non-coniferous hardwood chips	Pyrolysis at 600 °C

None of analyzed PAHs (naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benzo[a]anthracene, chrysenes, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene, benzo[a]pyrene, indeno[1,2,3-c,d]pyrene, dibenz[a,h]anthracene, benzo[g,h,i]perylene) was detected above the detection level in any of wood combustion products.

2. Experimental Design, Materials and Methods

2.1. Sampling and pretreatment

Samples of wood combustion products were obtained from commercial cogeneration power plants located in Lithuania and Latvia. Sample collection was performed based on the strict sampling procedure, which was developed according to the literature [2] and is described in the related research article [1]. The samples differed due to various fuel used at the energy production plant and various thermochemical process and temperature applied (Table 8).

Pretreatment involved, firstly, preparation of consolidated samples, secondly, screening using a sieve of mesh size 1500 µm, thirdly, each sample was dried at 105 °C in drying oven Plus II Oven (Labassco) for two hours until constant weight. For further investigation of wood combustion products, only dried samples were used.

2.2. Characterization of general parameters and physical properties

Estimating general characteristic parameters such as dry matter, volatile matter, the content of ashes and fixed carbon in the samples of wood combustion products was done by LOI [3-5]. Gravimetric water (moisture) and dry matter content was detected as a loss in weight after drying of samples at 105 °C for 2 h in a drying oven (Plus II Oven, Labassco). Content of volatile

matter was determined as a loss in weight at 950 °C under specified conditions in a muffle furnace (t_{max}=1100 °C, Omron). Ash content was determined as a residue after burning to constant weight at 750 °C for 6 h in a muffle furnace. Fixed carbon was calculated, taking into account detected values of gravimetric water content, volatile matter and ash content. Evaluation of physical properties involved detection of density and porosity [6,7]. To estimate bulk density, the measurements in a graduated cylinder were done [6]. The method involved detection of tapped density by mechanically tapping a graduated cylinder containing a dry sample in a powder consistency subsequently detecting the sample weight (after 3 drops of 0.15 m). Solid density was estimated using pycnometer method [8] that involved placement of a dry sample in a previously weighed borosilicate glass calibrated pycnometer (100±0.001 cm^3) and filling the rest of the volume with a liquid of known density, i.e., water. The density of a sample was determined from the known density of water, the weight of the pycnometer filled only with the liquid, the weight of the pycnometer filled with the sample and liquid, and the weight of the sample. Material porosity was calculated, taking into account the detected values of bulk and solid density [7,8]. Electrical conductivity was detected by potentiometry in water [7]. Mass ratio assessment was performed to detect particle size distribution applying sieve analysis, but the specific weight was calculated considering solid density value [9].

The elemental analysis involved detecting hydrogen, nitrogen, oxygen and total carbon content [7,8] by combustion-gas chromatography using the Elemental Analyser Model EA-1108 (Carlo Erba Instruments) calibrated with L-cystine (≥98%, TLC, Sigma Aldrich).

The phase composition of the samples was detected by XRD analysis [10] by using a Bruker D8 Advance X-ray diffractometer with Cu Kα radiation (λ=1.5418 Å) and a LynxEye detector, operating at 40 kV and 40 mA with 0.6 mm divergence slit and 8.0 mm anti-scatter slit. The scan was run from 3° to 70° (2Θ), with increments of 0.02 and a counting time of 1.0 s per step. Peak identification was carried out by comparing the experimental data with the International Centre for Diffraction Data (ICDD).

2.3. Characterization of chemical composition and properties

Methods for analysis of chemical composition and properties of wood combustion products involved detection of acidity, the concentration of ammonium, nitrates, nitrites, exchangeable elements, quantification and speciation of trace and major elements, as well as detection of PAHs. The main mineral components were detected by XRF. pH in water (<0.1 µS/cm, 18 MΩ/cm, Millipore Elix-3) and 1 M KCl solution (99.0–100.5%, ACS reagent, Sigma Aldrich) was detected applying potentiometry [7,11] using pH-meter pH 213 (Hanna Instruments).

XRF analysis was applied to detect elements in the form of oxides [12] using a Bruker S8 Tiger wavelength-dispersive spectrometer (equipped with Rh anode X-ray tube and using 4 kW excitation power). Measurements were performed under helium atmosphere at 50 kV and 50 mA tube settings and using 8 mm mask, LiF (200) crystal, 0.46° collimator, and scintillation counter.

Ammonium nitrogen was detected by Nessler method [13] measuring sorption by colorimeter DR 2800 (Hach Lange) at 420 nm. Nitrate nitrogen was detected by cadmium reduction method [13] measuring sorption by colorimeter at 500 nm. Nitrite nitrogen was detected using diazotization method [13] measuring sorption by colorimeter at 507 nm. Reagents used for these analyses were $KNaC_4H_4O_6 \cdot 4H_2O$ (≥99%, Reagent Plus, Sigma Aldrich) and K_2HgI_4 (Analytical Reagent, Sigma Aldrich), NitraVer 5 Nitrate Reagent Powder Pillow, 10-mL (Hach) and NitriVer 3 Nitrate Reagent Powder Pillow, 10-mL (Hach), respectively. Content of ammonium, nitrates and nitrites was calculated subsequently.

Exchangeable elements (K_{ex}, Ca_{ex}, Mg_{ex}, Na_{ex}) were detected after extraction with ammonium acetate (98%, AG, Penta) [7,11] measuring their concentration by ICP-OES (iCAP 7000, Thermo Scientific).Cation exchange capacity was calculated subsequently.

Speciation and total element content involved analytical detection of Al, As, Ba, Ca, Cd, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Sb, Se, Sr, Ti, Tl, V and Zn [14]. 3-step element

speciation analysis of samples was done based on adapted method resulting in three types of fractions: 1) Fraction of water-soluble (easily available) compounds (obtained by sample dissolution in heated-up deionised water (<0.1 μS/cm, 18 MΩ/cm, Millipore Elix-3)); 2) Fraction of weak acid-soluble compounds (obtained by dissolving the remains from the first step in 0.11 M acetic acid (99.8%, AG, Penta); 3) Residual fraction (obtained by dissolving the remains from the second step in *Aqua regia*, i.e., mixture of nitric acid (69%, ACS, ISO, Scharlau) and hydrochloric acid (37%, ACS, ISO, Scharlau) in a molar ratio of 1:3). Each analytical solution was made in triplicate and, at each step, blank samples were prepared in the same manner. The concentration of trace and major elements in solutions was measured using ICP-OES (iCAP 7000, Thermo Scientific) and expressed as mg/kg of sample dry matter. Quality of the analytical measurements was ensured by the analysis of certified reference material IAEA-336 Lichen (IAEA) containing reference values on broad spectra of major and minor elements. Total element content was counted as a sum of concentrations detected at the steps of speciation analysis.

Analysis of PAHs was performed by detecting in hexane using Soxhlet extractor (Behr ET2, labor-Technik) for 6 h at 850 °C [15]. After the extraction procedure, samples were evaporated at a room temperature, and the remains were dissolved in 1 mL of hexane (≥99%, ACS, Sigma Aldrich). Concentration of PAHs – naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benzo[a]anthracene, chrysenes, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene, benzo[a]pyrene, indeno[1,2,3-c,d]pyrene, dibenz[a,h]anthracene, benzo[g,h,i]perylene – was detected using gas chromatography (Clarus 580, Perkin Elmer) equipped with mass-selective detector with analyser of quadrupole type (Clarus SQ 8C, Perkin Elmer).

Ethics Statement

The authors declare that they have followed the general ethics rules of scientific research performance and publishing.

CRediT Author Statement

Zane Vincevica-Gaile: Conceptualization, Investigation, Data curation, Visualization, Writing – Original draft, Project administration, Funding acquisition. **Karina Stankevica:** Methodology, Validation, Formal analysis, Writing – Review and editing. **Maris Klavins:** Supervision, Resources. **Anna Trubaca-Boginska:** Formal analysis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.106994.

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