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# RAPID ANALYSIS OF IMPORTANT FUEL PROPERTIES OF PEAT BY FT-IR SPECTROSCOPY

## Turpeen tärkeiden polttoaineominaisuuksien nopea analysointi FT-IR-spektroskopian avulla

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Several important fuel properties of peat were rapidly determined by FT-IR spectroscopy, using the multicomponent analysis program CIRCOM. The following correlations ($r^2$) were found between FT-IR data and data obtained by traditional analytical methods, for 16 standard peat samples: calorific value 0.93, carbon content 0.95, volatiles 0.92 and nitrogen content 0.98. Determinations of hydrogen and ash contents in peat did not give satisfactory results ($r^2 = < 0.7$).

Keywords: FT-IR spectroscopy, fuel analysis, peat

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## INTRODUCTION

Infrared spectroscopy makes possible a rapid determination of important fuel properties of dried and milled peat, with only slightly lower precision than by traditional methods. The accuracy is high enough to allow comparison of the samples although it is insufficient for tasks such as the calculation of the efficiency of a specific power plant.

A multicomponent analysis program CIRCOM (computerized infrared characterization of materials) for obtaining quantitative data from infrared spectra of coals was developed at Broken Hill Proprientary Co. Ltd in Australia. Quantitative results are obtained by a statistical approach which identifies those characteristics of the spectra that are correlated with specific properties of the samples, and separates them from those that are not. The procedure starts with a representative set of preanalysed samples, whose spectra form a learning set from which the program finds correlations of interest. The program extracts a maximum amount of information from the infrared spectra with the aid of factor analysis followed by multiple linear regression.

CIRCOM has been applied successfully for the analysis of many important properties of coal (Fredericks et al. 1985a, b, Fredericks et al. 1985, Verheyen et al. 1987). The following properties of brown coal were analysed with a higher correlation than 0.9 ($r^2$): ash content (0.93), carbon content (0.94), specific energy (0.93) and oxygen content (0.95). In addition, a study of samples from individual brown coal fields gave good correlations for volatiles (0.97), moisture content (0.94) and the contents of $Al_2O_3$ and several functional groups (Verheyen et al. 1987).

Fourier-transform infrared spectroscopy has also been used for the rapid characterization of peat. Intensity values from selected wavenumber regions of the infrared spectra of Swedish peats were correlated with calorific value, degree of decomposition, carbon content, nitrogen content and content of amino acids and amino sugars, with the use of partial least-squares modelling with latent variables (PLS). The correlations ($r^2$) obtained with 40 peat samples were as follows: calorific value 0.86, degree of decomposition 0.73, nitrogen content 0.94, carbon content 0.84, galactose amine content 0.95 and glutamic acid content 0.98 (Holmgren and Norden 1988).

The fuel properties of peat have also been analysed rapidly by near infrared spectroscopy, with PLS used to calculate the water content and calorific value from the n.i.r. spectra. (Johansson et al. 1987).

In this work the multicomponent analysis program CIRCOM was used for the rapid determination of important fuel properties of peat.

## MATERIAL AND METHODS

Selected fuel properties of 16 peat samples collected in central Finland (*Sphagnum*- and *Carex*-based peats) and northern Finland (peats containing *Bryales*-peat) were analysed by traditional methods and, after drying (105°C, 24 h) and milling, by FT-IR technique. Determinations by traditional methods were as follows: calorific value by DIN 51900, volatiles by DIN 51720, ash content by DIN 51719 and the contents of carbon, hydrogen and nitrogen by Carlo Erba elemental analyser.

The infrared spectra were obtained using KBr pellet technique with the sample amount of 2.0 mg in 200 mg KBr. The spectra obtained by this technique were slightly better than those obtained by diffuse reflectance. Spectra were recorded with a Perkin-Elmer 1760 instrument equipped with a CIRCOM multicomponent analysis program. The combined spectral regions used were 4 000–2 500 and 2 000–450 $cm^{-1}$. The range 2 500–2 000 $cm^{-1}$ was excluded because of possible disturbances due to $CO_2$ in the air. The number of data points was 1 525 per one standard.

Three analytically determined values which correlated poorly with the calculated values of nitrogen content, calorific value and carbon content were excluded (two of these values were the properties of SC H 3-peat with a very high ash content and the third value was the very low nitrogen content in LS H 8–9 peat, Table 1).

## RESULTS AND DISCUSSION

Table 1 shows the results of fuel analysis of the peats obtained by traditional methods. There are some exceptions to the general rule that, for a single type of peat, carbon content and calorific value increase with degree of humification. Probably the discrepancies are due to variation in the content of inorganic material. Nitrogen contents are higher in *Carex*- and *Bryales*-peats than in *Sphagnum*-peats.

Figs. 1–4 show the correlation between the analytically determined and the calculated values of the studied fuel properties. The correlations ($r^2$) were as follows: calorific value 0.93, volatiles 0.92, carbon content 0.95 and nitrogen content 0.98. The correlation between analysed and calculated data was poor (< 0.7) for hydrogen and ash.

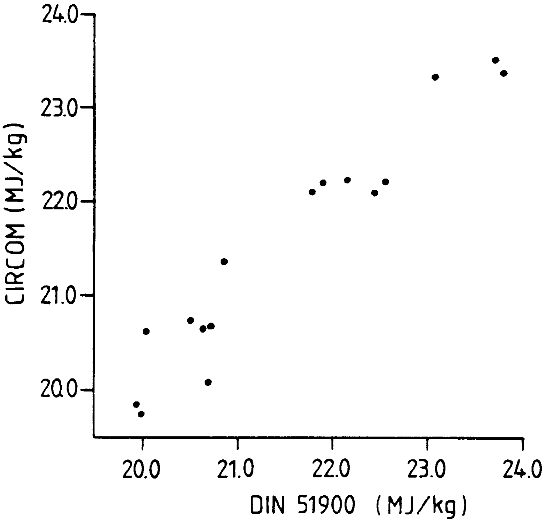


Fig. 1. The correlation between the calorific values of the samples analysed by DIN 51900 and the values calculated from FT-IR spectra by the multicomponent analysis program CIRCOM.

*Kuva 1. DIN-normin 51900 mukaisesti määritettyjen kalorimetristen lämpöarvojen korrelointi FT-IR spektreistä moniyhdiste-analyysiohjelma CIRCOM'lla saatuihin arvoihin*

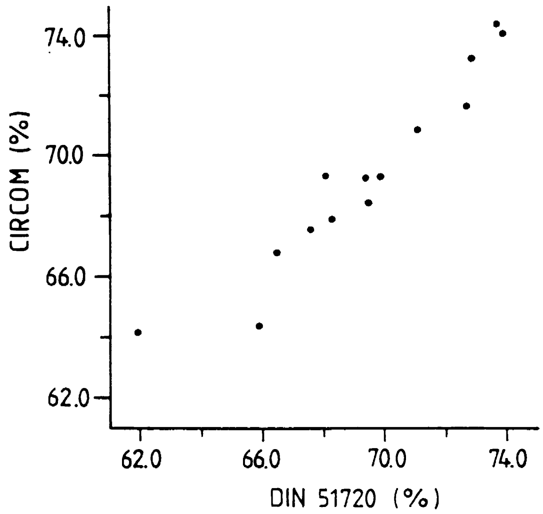


Fig. 2. The correlation between the contents of volatiles determined by DIN 51720 and those calculated by CIRCOM.

*Kuva 2. DIN-normin 51720 mukaisesti määritettyjen haihtuvien aineiden määrien korrelointi FT-IR spektreistä CIRCOM-ohjelmalla saatuihin arvoihin.*

Table 1. The important fuel properties of the peat samples analysed by traditional methods. S = *Sphagnum*, C = *Carex*, B = *Bryales*, Er = *Eriophorum*, L = Woody peat, H= degree of humification, by von Post's method, * = value not used in calculations due to poor correlation.

*Taulukko 1. Turvenäytteiden tärkeät polttoaineominaisuudet perinteisillä menetelmillä analysoituna. S = rahkaturve, C = saraturve, B = ruskosammalturve, Er = tupasvillaturve, L = puuturve H = maatumisaste von Postin menetelmällä analysoituna, * = arvoa ei ole käytetty laskuihin huonon korrelaation takia.*

| Peat – *Turve* | | Cal. value – *Lämpöarvo* MJ/kg | Volatiles – *Haihtuvat* | C | H % | N | Ash – *Tuhka* |
|---|---|---|---|---|---|---|---|
| S | H2–3 | 20.0 | 73.9 | 51.6 | 5.19 | 1.06 | 2.9 |
| ErS | H3–4 | 20.5 | 72.9 | 52.6 | 5.29 | 1.10 | 1.9 |
| ErS | H8–9 | 23.7 | 68.3 | 57.8 | 5.77 | 1.46 | 2.9 |
| ErS | H6–7 | 23.1 | 68.1 | 56.6 | 5.41 | 0.91 | 2.0 |
| ErS | H2 | 20.6 | 72.7 | 52.4 | 5.43 | 1.02 | 2.1 |
| ErS | H4 | 23.8 | 69.4 | 56.9 | 6.20 | 1.48 | 3.5 |
| ErS | H6 | 21.9 | 65.9 | 54.9 | 5.48 | 1.46 | 3.0 |
| LS | H8 | 22.4 | 61.9 | 53.9 | 5.67 | 1.78 | 8.8 |
| S | H3 | 22.5 | 69.5 | 55.0 | 6.19 | 1.31 | 4.6 |
| SC | H6 | 20.7 | 67.6 | 51.9 | 5.39 | 2.88 | 8.3 |
| C | H5 | 21.8 | 63.4 | 52.9 | 5.66 | 1.99 | 7.9 |
| LS | H8–9 | 22.2 | 66.5 | 55.0 | 5.37 | 0.67* | 4.9 |
| B | H4 | 20.9 | 69.9 | 50.4 | 5.95 | 3.16 | 6.3 |
| S | H1–2 | 19.9 | 73.7 | 50.5 | 5.40 | 0.86 | 1.5 |
| BC | H4 | 20.7 | 71.1 | 50.9 | 5.60 | 2.92 | 5.1 |
| SC | H3 | 20.1 | 65.3* | 50.2* | 5.72 | 1.62 | 11.2 |

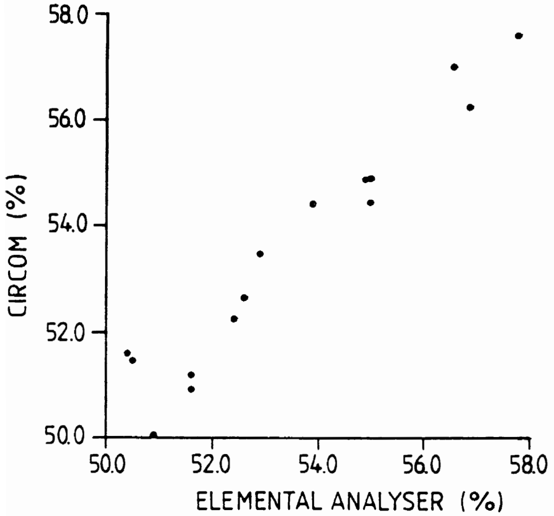


Fig. 3. The correlation between the carbon contents determined by elemental analyser and those calculated by CIRCOM.

*Kuva 3. Alkuaineanalysaattorilla analysoitujen hiilipitoisuuksien korrelointi CIRCOM-ohjelmalla saatuihin arvoihin.*

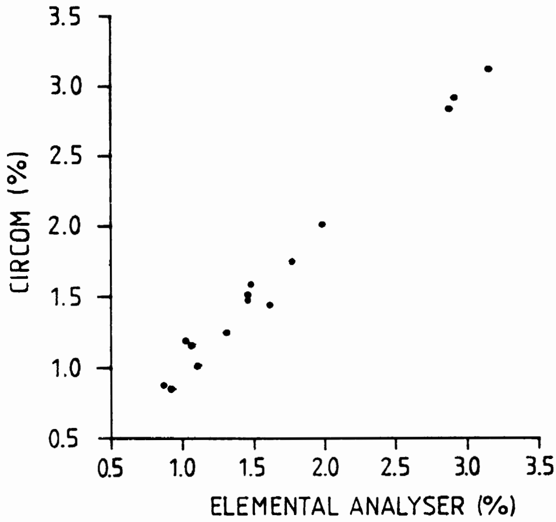


Fig. 4. The correlation between the nitrogen contents determined by elemental analyser and those calculated by CIRCOM.

*Kuva 4. Alkuaineanalysaattorilla analysoitujen typpipitoisuuksien korrelointi CIRCOM-ohjelmalla saatuihin arvoihin.*

## CONCLUSIONS

The correlations between FT-IR data and measured values obtained by traditional analytical methods are shown to be good ($r^2 > 0.9$) in the analysis of carbon content, calorific value and volatile content, and excellent in the analysis of nitrogen ($r^2 = 0.98$). The rapid analysis is uncertain for peats of exceptionally high ash content (> 9%) or low nitrogen content (< 0.8%). Holmgren and Norden (1988) earlier found a good correlation between analytically determined and calculated nitrogen concentrations ($r^2 = 0.94$) when using the diffuse reflectance technique in conjunction with the PLS regression method.

## REFERENCES

Fredericks, P.M., Lee, J.B., Osborn, P.R. & Swinkels, D.A. 1985a, b: Materials characterization using factor analysis of FT-IR spectra. Part 1: Results. — Applied Spectroscopy 39: 303–310 (1985a); Part 2: Mathematical and statistical considerations. — Applied Spectroscopy 39:311–316 (1985b).

Fredricks, P.M., Osborn, P.R. & Swinkels, D.A. 1985: Rapid chracterization of iron ore by Fourier Transform Infrared Spectrometry. — Anal. Chem. 57:1947–1951.

Holmgren, A. & Norden, B. 1988: Characterization of peat samples by diffuse reflectance FT-IR spectroscopy. — Applied Spectroscopy 42:255–261.

Johansson, E., Persson, J.-Å. & Albano, C. 1987: Determination of water content and calorific value of peat by near i.r. spectroscopy. — Fuel 66:22–27.

Verheyen T.V., Heng, S., Perry, G.J. & Fredericks, P.M. 1987: Rapid analysis of brown coal properties by statistical correlation of their infrared spectra. — In: Moulijn, J.A., Nater, K.A. & Chermin, H.A.G. (eds.), Proceedings of the 1987 International Conference on Coal Science. Maastrict, The Netherlands, October 26–30, 1987: 127–129. Elsevier, Amsterdam.

## TIIVISTELMÄ

## TURPEEN TÄRKEIDEN POLTTOAINEOMINAISUUKSIEN NOPEA ANALYSOINTI FT-IR SPEKTROSKOPIAN AVULLA

Työssä tutkittiin kuinka tarkasti FT-IR spektrometrilla, joka on varustettu moniyhdiste-analyysiohjelmalla (CIRCOM) voidaan analysoida nopeasti turpeen tärkeitä polttoaineominaisuuksia. Tarkastellut ominaisuudet (kalorimetrinen lämpöarvo, haihtuvien aineiden pitoisuus, hiili-, typpi-, vety- ja tuhkapitoisuus) määritettiin ensin perinteisillä menetelmillä kuudestatoista turvenäytteestä. Tämän jälkeen näytteistä ajettiin infrapunaspektrit ja analysoidut tulokset syötettiin spektrien ohella CIRCOM-ohjelman käsiteltäväksi. Hyvä korrelaatio spektrien ja analyysitulosten välillä ($r^2 > 0.9$) saatiin lämpöarvolle (0.93), haihtuvien aineiden sisällölle (0.92) ja hiilipitoisuudelle (0.95). Typpipitoisuudet korreloivat erittäin hyvin IR-spektrien kanssa ($r^2 = 0.98$). Tuhka- ja vetypitoisuuksien korrelaatiot IR-spektreihin olivat huonot ($r^2 < 0.7$).

Tulokset osoittivat, että turpeen kalorimetrinen lämpöarvo, haihtuvien aineiden pitoisuus, hiilipitoisuus ja typpipitoisuus voidaan määrittää suhteellisen hyvällä tarkkuudella ja nopeasti CIRCOM-ohjelmalla varustetulla FT-IR spektrometrillä. Turpeen suuri tuhkapitoisuus (> 9% kuivapainosta) aiheuttaa epätarkkuutta. Jos typpipitoisuus on hyvin pieni (< 0.8%), saatu tulos saattaa myös olla epätarkka.

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