Datasheet for the decision of 23 January 2007

Case Number: T 1285/05 - 3.4.02
Application Number: 98306958.4
Publication Number: 0982583
IPC: G01N 21/35
Language of the proceedings: EN
Title of invention: Measurement of spectrometer background profile
Applicant: PERKIN-ELMER LIMITED
Opponent:
Headword:
Relevant legal provisions: EPC Art. 52(1), 54
Keyword: "Novelty (yes)"
Decisions cited:
Catchword:
Case Number: T 1285/05 - 3.4.02

DECISION
of the Technical Board of Appeal 3.4.02
of 23 January 2007

Appellant: PERKIN-ELMER LIMITED
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Decision under appeal: Decision of the Examining Division of the European Patent Office posted 6 May 2005 refusing European application No. 98306958.4 pursuant to Article 97(1) EPC.

Composition of the Board:
Chairman: A. G. Klein
Members: F. J. Narganes-Quijano
C. Rennie-Smith
Summary of Facts and Submissions

I. The appellant (applicant) has lodged an appeal against the decision of the examining division to refuse European patent application No. 98 306 958.4 (publication No. 0982583).

In the decision under appeal the examining division referred to document D1: WO-A-9207275

and found that the subject-matter of claim 1 filed with the letter dated 11 April 2005 was anticipated by the disclosure of document D1 (Articles 52(1) and 54 EPC).

The examining division referred in particular to the principal components analysis performed in document D1 on correction spectra to separate real measurement process data from random measurement noise (page 10, lines 5 to 11) as well as to the eigenspectrum 5 represented in Figure 8 of the document, and concluded that the claimed creation of background profiles with lower noise levels was anticipated by document D1.

II. In the statement setting out the grounds of appeal the appellant requested setting aside of the decision under appeal and the grant of a patent on the basis of the set of claims filed with its letter dated 11 April 2005 and of the remaining application documents on file.

III. Claim 1 according to the request of the appellant reads as follows:
"An FT-IR spectrometer of the single beam type, which is arranged to measure the spectrum of a sample by comparing a background spectrum obtained without a sample present with a spectrum obtained with the sample present, said spectrometer including a source of analysing radiation (10), means (14) for receiving radiation transmitted through or reflected from a sample station, and processing means (16) for processing signals from the receiving means to provide spectral data, characterised in that the processing means is arranged so that it can record a plurality of background spectral profiles measured by the spectrometer over a period of time without a sample present and to analyse statistically said profiles in order to generate background profiles based on said collected background data, said statistical analysis including a data reduction technique arranged to extract principal components from the recorded profiles, and a step of reconstructing the original profiles from the data reduction step so as to create background profiles with lower noise levels."

The appellant's request includes dependent claim 2 referring back to claim 1.

IV. The arguments of the appellant in support of its requests can be summarised as follows:

The background spectrum with which the present invention is concerned is the instrument background spectrum measured when no sample is present in the spectrometer, and it is the processing of this background spectrum which lies at the heart of the present invention. The only reference in document D1 to
the background spectrum is on page 37, lines 26 to 28 and nowhere else in the document is such background spectrum referred to or discussed in any way. Document D1 is aimed primarily at baseline variations arising from perturbations of the background profile of the instrument and the document does not give any consideration to the actual instrument background itself.

In addition, document D1 proposes a different procedure involving, among other things, an orthogonalisation step that corrupts the true spectra. Eigenspectrum 5 in Figure 8 of the document shows strong evidence of water vapour in the sharp peaks in the left half of the spectrum and yet traces of these peaks can be found in eigenspectrum 4 and in eigenspectrum 2. This shows that the background cannot be identified alone in the space directions generated by the PCA (principal components analysis) procedure followed in the document. Furthermore, the eigenspectrum 5 in Figure 8 is not a background profile, but at the most one spectral component of background variance. The basis of the approach of document D1 to making spectrally derived measurements more robust is to orthogonalise the measured spectra against spectra of unwanted perturbations such as baseline variations of the instrument and contaminants.
**Reasons for the Decision**

1. The appeal is admissible.

2. **Amendments**

   After due consideration of the amendments made to the application documents, the Board is satisfied that the application documents as amended according to the appellant's request comply with the formal requirements of the EPC, and in particular with those set forth in Article 123(2) EPC. In particular, claim 1 is based on claims 1 to 3 and the passages on page 1, lines 3 to 6 and page 6, lines 9 to 13 of the description of the application as originally filed; and dependent claim 2 is based on claim 4 as originally filed.

   Furthermore, the description has been appropriately amended pursuant to Article 84 EPC, second sentence and Rules 27(1) (b) and (c) EPC.

3. **Novelty**

   3.1 Document D1 discloses a spectrometer arranged to measure the spectrum of a sample (paragraph bridging pages 4 and 5) by processing spectral signal data representative of the absorption, reflection or scattering radiation from the sample (page 14, line 12 et seq.), the spectrometer being exemplified by a FT-IR spectrometer of the single beam type (page 37, lines 22 to 28).

   The document discloses the correction of the measured spectral data of samples for the effects arising from
the measurement process itself (page 3, last paragraph, page 4, second paragraph, page 6, first paragraph, and page 17, second paragraph), and in particular for the effects caused by spectral baseline variations (changes in instrument performance due for instance to temperature variations and to changes in cell window transmittance, see page 3, first paragraph and page 5, lines 12 to 18) and by the presence of "ex-sample" chemical compounds (water vapour and carbon dioxide in the atmosphere and/or contaminants in the sample, see page 3, first paragraph, and page 5, lines 18 to 36). The correction spectral data may result from spectra collected on the instrument to simulate background variations and interferences due to ex-sample chemical compounds (page 6, lines 25 to 28, and page 9, lines 7 to 13) and the correction spectral data is subject to an orthogonalisation procedure (page 6, first and second paragraphs).

The document further discloses separating the sample spectral data from the spectral noise present in the measured sample spectral data (page 7, lines 6 to 11) by means of analytical methods based on principal components analysis (PCA) such as PCR (principal components regression) (page 2, second and third paragraphs) and CPSA (constrained principal spectral analysis) (page 16, line 7 et seq.).

According to the disclosure of document D1, the measured sample spectral data (matrix X) is first corrected for baseline variations and ex-sample chemical compounds (matrix Uₘ) to obtain corrected sample spectra data (matrix Xₙ) (page 4, lines 9 to 28, and page 15, lines 3 to 7), and then the resulting
corrected sample spectral data is subject to principal components analysis for correction of noise (page 7, second paragraph, and page 15, lines 3 to 9, see also claims 1 and 9 as well as claims 10 and 14 where the principal components analysis is applied to the corrected spectral matrix $X_c$ which is orthogonal to the correction matrix $U_m$ representative of spectral data of the measurement process itself).

3.2 In the decision under appeal the examining division held that in document D1 the principal components analytical procedures are applied to background spectral profiles obtained without a sample present in the sample station of the spectrometer as required by claim 1 of the appellant's request.

However, the Board is not able to agree with the examining division's view in this respect. Even assuming that - as held by the examining division but contested by the appellant - the spectral data representative of the baseline variations and the ex-sample chemical compounds referred to in document D1 (second paragraph of point 3.1 above) represent background spectra profiles within the meaning of the claimed subject-matter, the document would then disclose at the most subjecting the background spectra profiles to an orthogonalisation procedure (second paragraph of point 3.1 above) and not to a principal components analytical procedure and to a noise-reduction reconstructing procedure as required by the claimed subject-matter. Indeed, document D1 discloses the application of the latter procedures to the sample spectral data already corrected for baseline variations and ex-sample chemical compounds (third and fourth
paragraphs of point 3.1 above), but is silent as to the application of these procedures to the spectral data representative of both baseline variations and ex-sample chemical compounds.

This conclusion is not altered by the further disclosure of document D1 relating to the possibility of performing principal components analysis on measured correction spectra due to ex-sample chemical compounds to correct for random measurement noise (page 9, line 10 to page 10, line 11) because the corresponding disclosure only refers to correction spectra due to ex-sample chemical compounds and does not include the (remaining) "background variations" (page 9, lines 7 to 13, and page 10, lines 20 to 29). Similar considerations apply to the eigenspectrum 5 represented in Figure 8 of the document and referred to by the examining division in the decision under appeal as representing background spectral profile creation with lower noise levels; the eigenspectrum 5 represents only water vapour spectra (page 38, lines 24 and 25) and, in addition, this eigenspectrum has been obtained by PCA analysis (page 38, lines 16 to 19) of the measured spectrum of an actual sample (page 37, line 19 et seq.; see also page 46, lines 24 to 26), and not of background spectral profiles obtained without a sample present in the spectrometer as required by the subject-matter of claim 1. As a matter of fact, and as submitted by the appellant, document D1 mentions working with "empty beam background spectra" to be factored out of the measured sample spectra (page 37, lines 26 to 28), but the document is silent as to any principal components analytical treatment or processing of these "empty beam background spectra".
3.3 In view of the above, the Board concludes that document D1 fails to anticipate the extraction of principal components from measured background spectral profiles and the subsequent reconstruction of background spectral profiles with lower noise levels as required by claim 1. For this reason at least, the claimed subject-matter is novel over the disclosure of document D1 (Articles 52(1) and 54 EPC).

3.4 None of the remaining documents on file anticipates the subject-matter of claim 1 either (Articles 52(1) and 54 EPC). The same conclusion applies to dependent claim 2 by virtue of its dependence on claim 1.

4. Other requirements

During the first-instance examination proceedings the examining division only considered the issue of novelty of the claimed subject-matter. Notwithstanding, the Board is satisfied that the subject-matter of claim 1 as well as that of dependent claim 2 involve an inventive step over the available prior art (Articles 52(1) and 56 EPC). In particular, none of the documents on file discloses or suggests processing the background spectrum of a spectrometer as claimed nor the technical effects achieved therewith, namely a reduction in the time required to obtain noise-corrected sample spectral data (see description of the application, page 1, line 14 to page 2, line 13, and the paragraph bridging pages 7 and 8).

The Board is also satisfied that the patent application as amended according to the present request of the
appellant and the invention to which it relates meet
the remaining requirements of the EPC within the
meaning of Article 97(1) EPC.

5. In view of the above conclusions and considerations,
the decision under appeal is to be set aside. In
addition, the Board, in accordance with Article 111(1)
EPC, considers it appropriate to exercise favourably
the power within the competence of the examining
division to order grant of a patent.
Order

For these reasons it is decided that:

1. The decision under appeal is set aside.

2. The case is remitted to the department of first instance with the order to grant a patent in the following version:
   - claims 1 and 2 filed with the letter dated 11.04.2005,
   - description pages 1 and 5 to 9 as originally filed and pages 2 to 4 filed with the letter dated 11.04.2005, and
   - drawing sheets 1/2 and 2/2 filed with the letter dated 30.11.1998.

The Registrar

The Chairman:

M. Kiehl

A. G. Klein