ABB Measurement & Analytics

MB3600-CH80 PET Packaging Analyzer Pre-Calibrated for %Crystallinity Determination in PET

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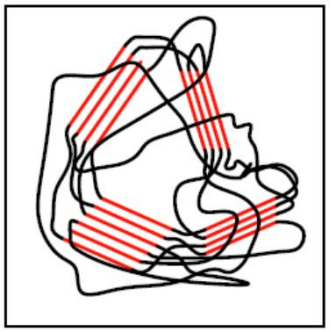
MB3600-CH80 PET Packaging Analyzer - Background

- FT-NIR is an attractive alternative as it allows to perform rapid determination of plastic bottles crystallinity in a fast and non-destructive manner. Each intact bottle can be analysed within a few seconds, and the test can be performed by an operator without analytical background.
- The MB3600-CH80 PET Packaging Analyzer is a rugged industrial FT-NIR solution for fast analysis of PET containers like jars, bottles and preforms. It is intended for R&D centers, QA/QC laboratories or production lines of companies performing a large number of daily measurements of key characteristics of PET packaging containers.

Crystallinity of PET Bottles and Preforms

- Crystallinity refers to the degree of structural order in a solid. Amorphous polymers (with no significant degree of crystallization) behave very differently than crystalline polymers.
- Many polymeric materials like plastic bottles can be prepared in such a way as to produce a mixture of crystalline and amorphous regions. In such cases, the degree of crystallinity can be controlled by modifying process techniques. It has a big influence on hardness, density, transparency and diffusion of a polymer. It is usually specified as a percentage of the volume of the material that is crystalline. For companies producing plastic bottles, it is important to verify the crystallinity of blown bottle walls in order to ensure product consistency, strength and overall quality.
- Crystallinity can be measured in a laboratory using X-ray diffraction, density measurements or calorimetric techniques, but those methods are sometimes inaccurate. In addition, they are slow and require chemical consumables, which means results are not always available in time to be included in a Certificate of Analysis for end-users.

Amorphous polymer – Random molecular orientation in solid phase



Crystalline polymer – Densely packed crystallites in solid phase

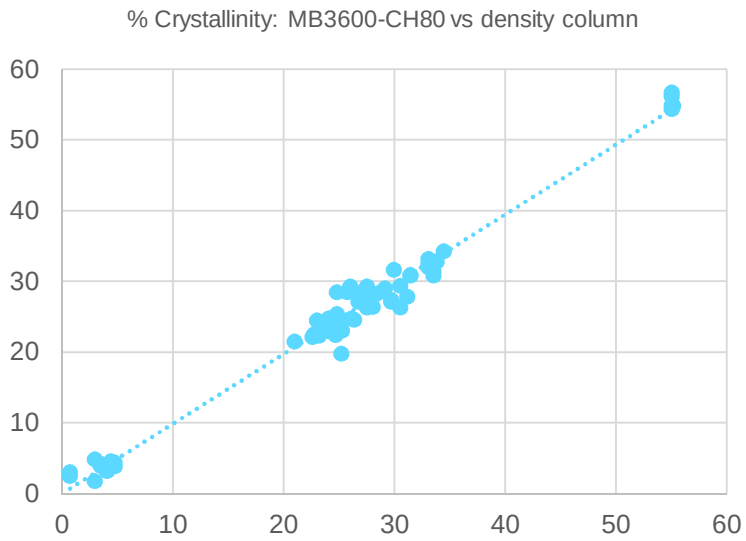
MB3600-CH80 PET Packaging Analyzer – Ease of Use

- Analysis with the MB3600-CH80 is performed within a few seconds, as an alternative to slower laboratory methods.
- No specific sample or instrument preparation is required, measurements are totally non-destructive. The operator just places the intact bottle or preform in the MB3600-CH80 sampling compartment and follows on-screen instructions.
- Analysis with MB3600-CH80 does not require any chemical reagent, waste disposal or consumable.

MB3600-CH80 PET Packaging Analyzer – Precision

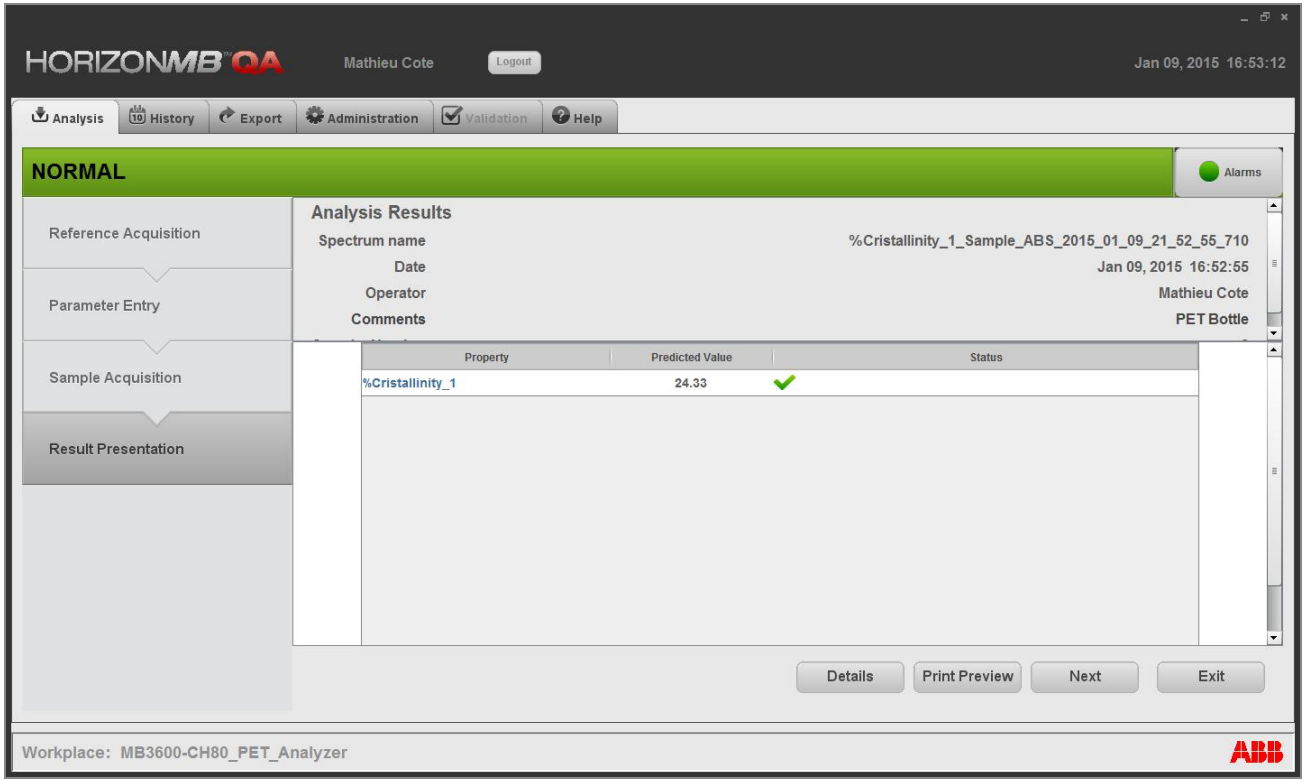
- ABB has developed an unrivalled FT-NIR calibration expertise and is able to offer a turnkey model for %crystallinity determination in PET bottles. This calibration is pre-loaded on the instrument and configured as starter method in the Horizon MB QA user-friendly operator interface.
- The FT-NIR technique will typically exhibit a reproducibility similar to traditional laboratory methods, but with a superior precision (repeatability) and robustness.
- From the day of installation, the user can analyse PET bottles with the MB3600-CH80.

Property	Samples	Units	SECV	Repeatability (*r*)	Range Min	Range Max
Crystallinity	PET Bottle & Preforms	%	1.41	<0.1	0.65	55.1



MB3600-CH80 PET Packaging Analyzer - Reliability

- For each assay, a statistical indicator is automatically calculated and allows to assess the quality of the sample recognition by the system. Automatic warnings are displayed for PET formulations that are unique or significantly different from the calibration database. This serves as an indication for the user that the FT-NIR calibration must be adjusted to include some samples of this formulation and further enhance the robustness of the model. Samples that are atypical or exceeding the %crystallinity range spanned by the pre-loaded model will be automatically flagged.

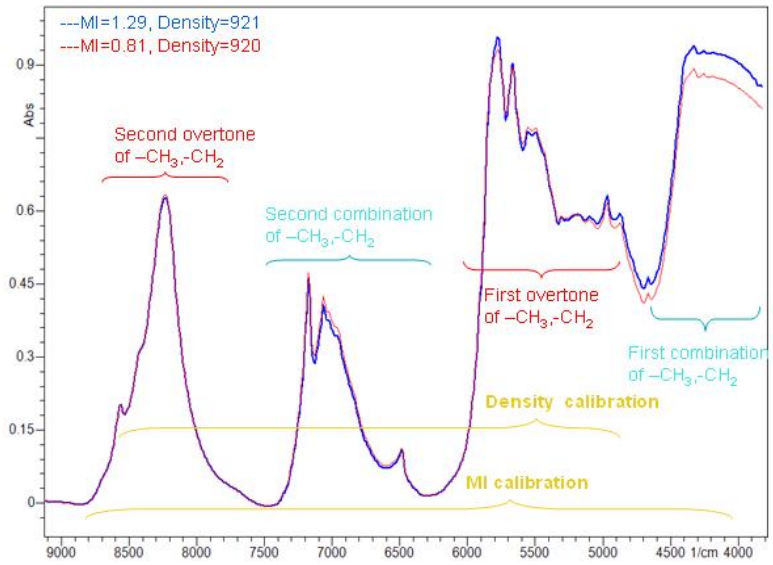


MB3600-CH80 PET Packaging Analyzer - Flexibility

- The MB3600-CH80 is a flexible analyzer that can also be used for measurements in powders, pellets or liquids, using a set of swappable sampling accessories:
  - The “Powder Sampl*ir*” is dedicated to analysis of solids like powders, pellets or small pieces of opaque packaging.
  - The “Universal Heatable Vial Holder” is dedicated to analysis of liquids or melted plastics in disposable scintillation vials.
- They accessories are positioned in the sampling compartment of the MB3600-CH80 and connected to the analyzer via a USB port for automatic recognition.
- Installation and removal of each accessory is straightforward.

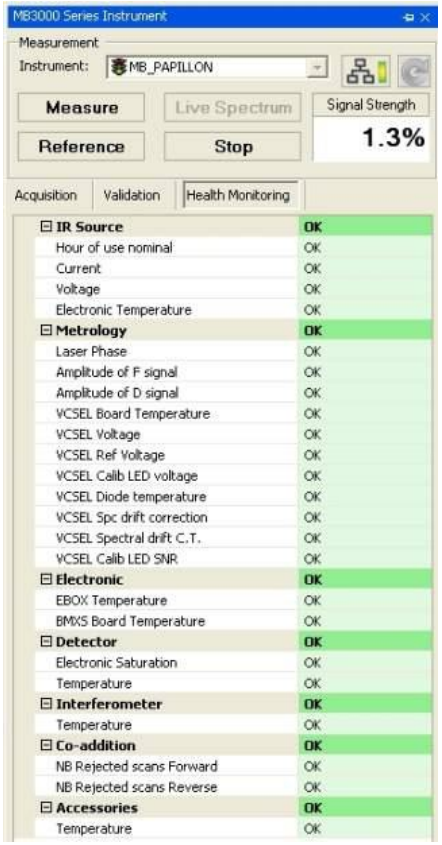
MB3600-CH80 PET Packaging Analyzer - Versatility

- In addition to %crystallinity, other important properties of PET can also be determined with the MB3600-CH80, for instance:
  - Moisture content
  - Bottle wall thickness
  - Density
  - OH value
  - Acid value
  - Viscosity
- Those properties are based on custom built calibration models that can either be supplied by ABB, or developed by the end-user.



MB3600-CH80 PET Packaging Analyzer - Robustness

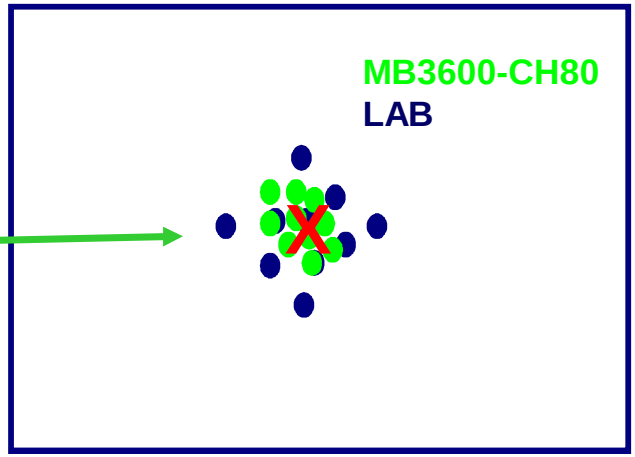
- The MB3600-CH80 is virtually maintenance-free and therefore allows end-user to significantly reduce maintenance and consumbale costs compared to traditional laboratory
- The pre-aligned source module with electronic stabilization is designed to operate for 10 years without replacement, and the solid state laser-based metrology module has a 20 year lifespan. All MB3600-CH80 optics are non-hygroscopic so that no instrument purging is necessary for optical protection. The MB3600-CH80 enables to significantly reduce laboratory analyses costs while improving product consistency and laboratory throughput.



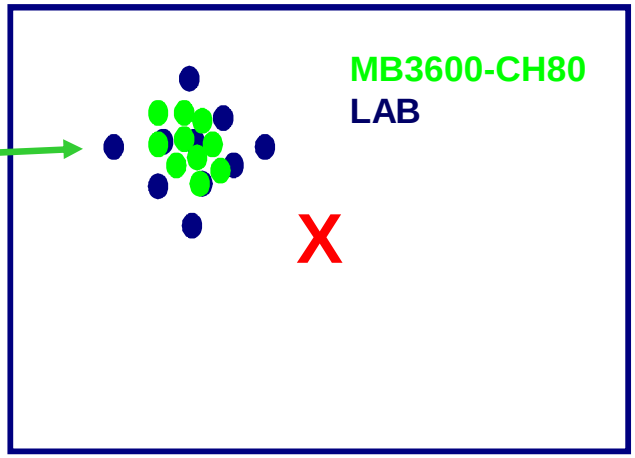
MB3600-CH80 PET Packaging Analyzer - Precision

- Compared to traditional laboratory methods, the MB3600-CH80 will exhibit similar accuracy (correlative technique) but superior precision (repeatability) due to the absence of sources of human errors and the calibration against ultra-precise laser.

Example of repeatability tests for a laboratory FT-NIR instrument calibrated against an un-biased laboratory method



Example of repeatability tests for a laboratory FT-NIR instrument calibrated against a laboratory method with systematic bias



PET Crystallinity Determination – Example 1

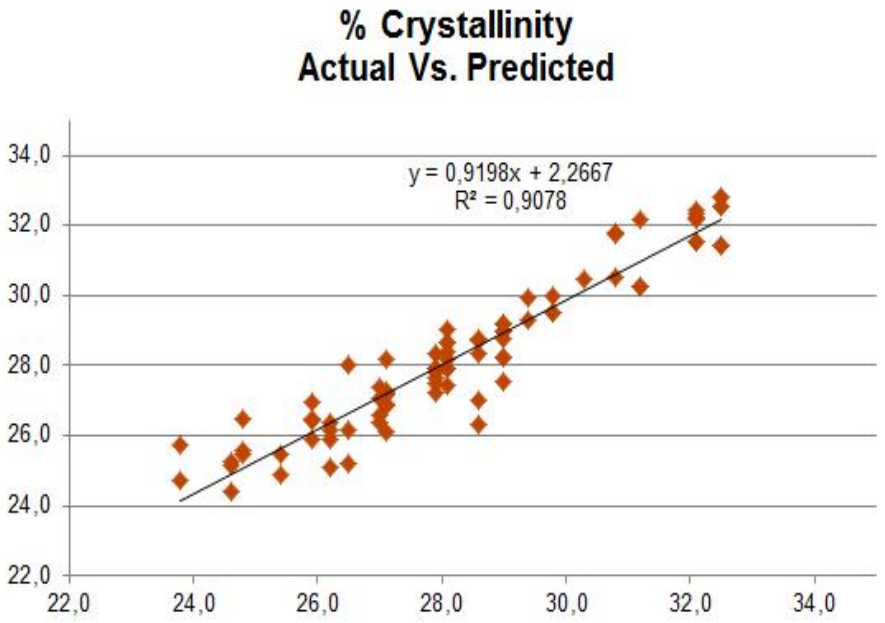
Summary

- Fast determination of crystallinity of 88 polyethylene intact bottles with a custom calibration.
- The instrument was also used for quantification of water content and bottle wall thickness, as alternative to Karl Fisher coulometer titration that takes 1 hour per sample.

Method

- Instrument: MB3600-CH80
- Sampling technique: intact bottles placed on sampling port.
- Analysis temperature: Room T
- Resolution: 8 cm^{-1}
- Number of scans: 16 (12s /sample)
- Chemometrics model: Partial Least Squares (Software Horizon MB Quantify)

Calibration Performance

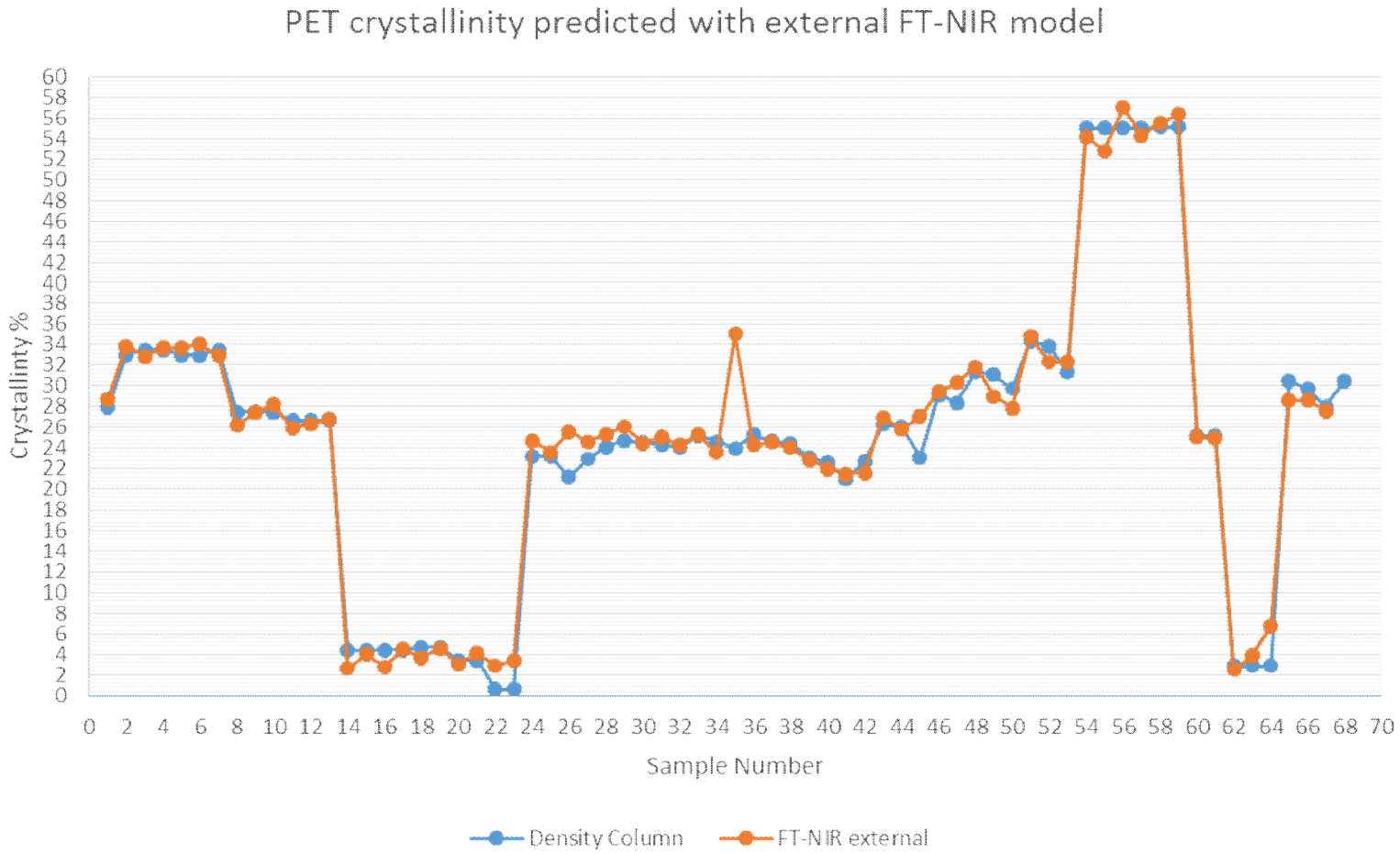


Property	Range (%)	R^2	SECV (%)
Crystallinity	23.8 – 32.1	0.91	0.7

PET Crystallinity Determination – Example 2

Use of MB3600-CH80 pre-loaded global calibration

- Une of MB3600-CH80 global calibration model for %crystallinity on customer samples that are not included in the global calibration.
- The FT-NIR crystallinity predictions on 67 samples are tested against density column values.



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