Food Analysis

● FT-NIR Spectroscopy for QC in the Lab and Production

Innovation with Integrity

Bruker Optics Solutions for the Food Industry

Near Infrared Spectroscopy is a well-established technique and today an important element of quality control in the food industry. Bruker Optics modern FT-NIR spectrometers can analyze both, liquid and solid samples and are the ideal tool for the non-destructive and rapid analysis of raw materials, intermediate and finished products throughout the entire manufacturing process.

FT-NIR Analyzers for the Food Industry

Quality control

Questions and concerns regarding food quality are endless, and the demand for easy-to-use tools to monitor and ensure the integrity of foodstuffs is growing around the world. FT-NIR is a powerful and effective technology for control of raw materials, intermediates and finished products. Common tasks in food processing are:

- Identification of raw materials
- Conformity testing
- Composition analysis
- Process control

FT-NIR advantage

In contrast to most wet-chemistry and other reference methods the FT-NIR technology is quick, cost-effective, non-destructive and safe, since it does not use chemicals, solvents or gases. It simply measures the absorption of near-infrared light of the sample at different wavelengths recording molecular vibrations of all molecules containing C-H, N-H or O-H groups. By this NIR spectroscopy is the first choice for the analysis of all kind of organic materials, making it ideal for a wide variety of foodstuffs.

The key benefits of FT-NIR spectroscopy are:

- no sample preparation, no waste
- no special skills required, easy sample presentation
- no typical errors of classical lab methods
- analysis of multiple components in less than one minute
- suitable for any solid, semi-solid or liquid sample

Bruker - your partner for lab and process analysis

For more than 50 years, Bruker has been driven by the idea to always provide the best technological solution for each analytical task. Bruker Optics is the world leading manufacturer of FT-NIR instruments for a wide range of industries including the agricultural sector and food manufacturing. Bruker Optics' portfolio ranges from small footprint, touch screen operated analyzers to fully automated in-process systems for closed loop control.

Our analyzers combine an unrivaled flexibility and easy operation with state-of-the-art spectrometer technology. Software controlled optical modules, optimized sampling accessories for numerous applications and user friendly operator interfaces guarantee excellent results from day one.

• Flour & Milling: The base of all good things.

Cereals are the cornerstone of the daily nutrition for most people around the world. The Flour & Milling industry plays an essential part in turning cereals into flours for a wide variety of baked goods from bread to cake.

The specifications for wheat and flour often require specialized and time consuming testing to determine how flour will perform during processing. Bruker offers solutions for the Flour & Milling industry for the analysis of wheat, various flour types as well as co-products based on FT-NIR Spectroscopy - from small, easy-to-use benchtop spectrometers to complete online monitoring systems.

Ready to use calibration packages give you results in seconds and are a highly cost-effective solution compared to conventional testing methods.

Wheat Intake: Know what you get

It is essential to verify the grade as well as the quality of wheat before forwarding it to the milling process. This way, the maximum yield and the correct quality of flour can be achieved. Parameters like moisture, protein, ash and wet gluten content can be monitored with FT-NIR spectroscopy within seconds.

Knowing the moisture content is essential for millers in order to adjust the wheat to a standard level before milling. The protein content is a key specification for flour producers as it influences many processing properties, like water absorption or gluten strength. The ash content in wheat is an indication of the yield to be expected during the milling process.

Flour & Milling

Products:
- Wheat grains
- Wheat flour
- Semolina
- By-products
- Other types
  of flour
- ...

Parameters:
- Moisture
- Protein
- Ash
- Wet gluten

additional for Flour:
- Alveograph
  (L, P, P/L, W)
- Resistance
- Extensibility
- Water absorption

Tempering: Maximize the yield

Adding water to wheat before milling helps producing consistent, high quality finished flours. Utilizing FT-NIR spectroscopy helps you to monitor the moisture content of the wheat in order to optimize the conditioning step and addition of water.

Flour Milling: Optimize the process

The analysis of ash content is essential during the milling phase. Monitoring the ash concentration serves as a benchmark for the production process. Moreover, parameters like protein content or wet gluten content can be utilized in order to optimize the blending process for increased profitability. These parameters can easily be assessed on-line or at-line with FT-NIR.

Flour Quality: Monitor the final product

If a wheat flour is suitable for baking purposes and which process adjustments need to be made, is traditionally assessed by an array of rheological and physical/chemical testing. Most of these labor intensive tests like protein content, Alveograph or Extensograph testing can be substituted by FT-NIR leading to substantial cost reductions and process improvements. Moreover, due to the speed of FT-NIR, a high sample throughput can be achieved.

Measurement of flour in a
quartz glass cup on the integrating sphere of
of the TANGO-R FT-NIR spectrometer

• Dairy: All the good from milk.

Bruker Optics' dairy portfolio ranges from small footprint, touch screen accessible, dedicated analyzers to multiple channel analyzers for the full range of samples from raw milk to the various dairy products as well as fully automated in-process systems for closed loop control.

Bruker's Dairy Analyzer MPA-D II with the software controlled Liquid Sampling Module (LSM) sets a new standard in routine QC for the analysis of liquid and solid samples. The LSM has a dual module with homogenizer and peristaltic pump including automated cleaning cycles and visible tubing for easy inspection. The modular concept is based on Brukers' FT-NIR instrument MPA II:

- Transmission measurement through a thermostatted quartz flow cell with 1mm (1,000µm) path length for all liquids. The robust design shows no cuvette wear over time. Viscous samples can be pumped through easily, even with small particles or sugar crystals.

- Reflection analysis for all solid and semi-solid samples with the integrating sphere in sample cups for powder samples and for semi-solids in Petri dishes. The sample is rotated during analysis to obtain the average result from a larger sample volume.

Raw milk and liquid milk products

The homogenizer of the LSM secures excellent precision and repeatability of raw milk analysis and the flow cell is analyzing a 20x larger sample volume compared to FTIR analyzers. Results of tests with certified standard milk samples sets from the dairy laboratory services show excellent accuracy and linearity for fat and protein. Using the peristaltic pump only, even viscous milk products and intermediates such as cream, milk drinks and condensed milk can be analyzed.

Alternatively, Bruker offers the pre-calibrated MIRA liquid milk analyzer, based on infrared spectroscopy – a stand-alone system for the quality control of raw milk, and liquid milk products.

Whey and whey protein products

Using whey as a liquid side-product of the cheese making process adds value to cheese producers. The

production capacity for whey protein concentrates (WPC) to be used as an ingredient has increased significantly and thus the need to analyze liquid whey and whey proteins. Samples from different phases of production are covering a broad range of concentrations for protein and total solids which can be analyzed with the LSM.

Milk and whey protein powders

The analysis of powders is fast and easy for moisture, fat and protein as well as ash or lactose content where required. Producers in the dairy industry monitor these parameters to:

- Optimize the moisture content
- Increase product consistency
- More efficiently utilize energy
  (e.g. optimization of the drying process)
- Reduce final product testing in the laboratory

Cheese and butter

A simple reflectance measurement analyzes important quality parameters such as moisture in butter and fat, protein and total solids in a large variety of cheeses from hard-, slicing-, cream-, to soft and processed cheese. Grated cheese is typically sprinkled, whereas softer cheese varieties are spread into the disposable polystyrene Petri dish.

Yoghurt and desserts

Many companies produce a wide range of recipes with many different flavors and textures, from plain yoghurt and desserts to fruit and chocolate flavored products. With NIR spectroscopy, the typical quality parameters such as fat, protein and dry matter can be determined very quickly in the lab or at-line in the production area. Only one calibration model per parameter is required, no matter what flavors or ingredients are being added.

MPA-D II with LSM module
for the analysis of milk and
milk products in a 1mm flow cell

• Meat: King of the grill.

Within the meat industry the continuous analysis of fresh meat and other ingredients is necessary in order to adapt the recipes to ensure a constant batch to batch quality of sausages, salami and various other types of meat products.

FT-NIR Spectroscopy offers a lot of advantages over classical wet-chemical and chromatographic analyses. It is very fast with analysis times below 30 seconds, cost-effective and safe, since no hazardous chemicals are used. Today it is widely used in the food industry for non-destructive qualitative and quantitative analysis of raw materials, in-process materials, and finished products throughout the entire manufacturing process:

- produce a consistently high product quality
- make the most efficient use of valuable raw materials
- improve product efficiency and reduce downtime

With the growing global demand for meat and meat products it can be a challenge to keep the standard quality requested by the customers. FT-NIR technology being able to provide analysis results in less than a minute has the potential to complement or even substitute a wide range of classical test methods for the quality assessment of meat and meat products in the laboratory as well as on-line.

Analyzing raw meat

Meat can be a very complex raw material where small changes in external impacts like animal nutrition can lead to large variation in the final meat quality. Fluctuating fat content in the supplied meat can e.g. be a large problem for a sausage producer if he is not aware of it. Measuring the fat content of carcasses is also often a criterion for the value-based payment of the suppliers. FT-NIR Spectroscopy offers here a valuable tool for assessing the incoming material. The parameters fat, protein and moisture can be determined simultaneously with only one measurement.

Measurement of minced meat in a polystyrene Petri dish on the integrating spere of an MPA II spectrometer

Products:
- Raw meat
- Sausage meat
- Boiled sausages
- Raw sausages
- Meat products
  (e.g. corned, dried
  or smoked)
- Ham
- Hamburger patties
- and many more...

Parameters:
- Fat
- Water
- Protein
- Collagen
- Ash
- Salt
- pH-Value
- a_w
- ...

With the results, decisions can be taken on how to proceed with the production.

Monitoring the final product quality

In Germany alone, there are more than 1500 different types of sausages available in the shops, including fresh or fresh smoked, dry and cooked sausages, as well as a wide variation of hams. The regulating bodies require the determination of the amount of water, protein and fat in every type of sausage. Moreover, the salt content is of interest for the producer as well as for the customer. FT-NIR has proven to be an efficient analysis method for the determination of moisture, fat, protein and salt content in various types of sausages. Furthermore the water activity (a_w) can be analyzed for the optimization of product shelf life.

Compositional analysis of rendering products

Approximately 40-50% of the weight of any slaughtered animal is not fit for human consumption. This material is mostly transformed by the rendering industry into highly nutritional ingredients for the animal feed and pet food production. These include sources of energy like tallow or lard as well as protein rich material like meat and bone meal or poultry meal. FT-NIR is well established for the analysis of edible fats of animal origin where parameters like free fatty acids and iodine value can be analyzed simultaneously. For animal meals the classical constituents like moisture, fat, protein, fiber and ash can be determined as well as more specialized parameters like energy values or amino acid profiles.

Edible Oils: The essence of taste.

Oils and fats are recognized as essential nutrients of our daily diet and contribute significantly to the regulation of different body functions. Numerous parameters are used to assess their quality. Bruker's dedicated FT-NIR solutions enable a rapid analysis of edible oils and fats.

Analysis of edible oils

Different parameters are used to assess the quality of edible fats and oils, including fatty acid composition, iodine value (IV), free fatty acids (FFA), trans fatty acids (TFA), anisidine value (AnV), and various other parameters.

The traditional analyses are generally carried out using standardized chemical and physical methods, which tend to be time-consuming and produce high running costs, e.g. GC analysis. Moreover, they often require hazardous solvents and reagents, which create a potential health risk and add disposal costs.

Rapid quality control for edible oils can be achieved by Bruker's dedicated FT-NIR solutions. The analysis is quick, cost-effective and safe to use, even for untrained staff, since no sample preparation is required. The oil is simply filled into an 8mm glass vial and measured in the sample compartment of the spectrometer.

Olive oil analysis

An acidity value below 0.8% is the main criterion for the classification of the olive oil as "extra virgin". Other quality parameters include the peroxide value, an indication for the rancidity of the oil as well as K-values (UV absorption) and many others. The amount of 1,2-diglycerides as well as the pyropheophytin content in the oil reveals if a an olive oil was stored for too long or even adulterated with refined (olive) oils to obtain lower acidity values.

All these critical parameters can be tested with a 30 second FT-NIR measurement, enabling a thorough quality control along the production chain of the olive oil.

Edible Fats & Oils

Products:
- Vegetable oils
- Animal fats
- Olive oil
- Frying oils
- Marine oils
- ...

Parameters:
- Free fatty acids
- Trans fatty acids
- Iodine value
- Peroxide value
- Anisidine value
- Fatty acid profile
- Omega-3s
- Triglycerides
- Solid Fat Content
- more specialized parameters...

Frying oil analysis

Frying is a well established, cost effective and fast method of food preparation. However, frying oils, used continuously and repeatedly at high temperatures, are subject to a series of degradation processes. Increasing amounts of free fatty acids and total polar components indicate oil degradation leading to a deterioration of the sensory quality and to potential health issues.

FT-NIR spectroscopy is a proven method to assess the quality of deep-frying oil with regards to its key parameters describing all aspects of the fat degradation. This was acknowledged by the DGF who issued the Standard Method „FT-NIR Spectroscopy: Screening analysis of used frying fats and oils for rapid determination of polar compounds, polymerized triacylglycerols, acid value and anisidine value [DGF C VI 21a (13)]."

Analysis of marine oils

Marine oils are the main source of polyunsaturated omega-3 fatty acids. Especially EPA (Eicosapentaenoic Acid) and DHA (Docosahexaenoic Acid) are known to be highly beneficial to human health. FT-NIR spectroscopy can analyze the level of the individual omega-3s of the sample, as well as the oxidation status like anisidine or peroxide value in less than a minute.

To ensure that pharma-grade fish oils and omega-3 fatty acids meet the strict quality parameters before their release, it is essential to carry out a completely traceable analysis according to GLP. Bruker Optics spectrometers can be fully validated according to US Pharmacopeia and PhEur. The operating software supports Operational Qualification (OQ) and Performance Qualification (PQ) as well as full traceability according to 21 CFR Part 11.

Measurement of edible oils in an 8mm vial in the sample compartment of the TANGO-T FT-NIR spectrometer

Condiments: Adding spice to your life.

The vast number of types and preparations of condiments offer a sensational experience of taste and flavors but is very demanding in terms of quality control. FT-NIR analysis is a key tool to ensure easily the quality of the various raw materials and finished products.

There is a broad variety of condiments to choose from for industrial or home cooking and to complement the dish during the meal. The products and their ingredients being liquid, semi-solid or solid can all be analyzed using FT-NIR spectroscopy, but require choosing the right sample presentation and measurement setup.

Especially for creamy or paste-like products accurate and reproducible measurements can be a challenge. Bruker offers with transflection measurements a technology, which collects scattered as well as transmitted light and is therefore providing excellent repeatability.

Ketchup and table sauces

For ketchup, the most important parameters such as Brix, salt content, pH and acidity can easily be analyzed with just one measurement in transflection using ready-to-use calibrations. For more complex table sauces which sometimes show regional variations, the calibration methods can be easily adapted by implementing a limited number of customer samples.

Mustard

Prepared mustards are one of the most popular condiments with a wide range of strengths and flavors, from sweet to spicy. The finished product can be analyzed in reflection for parameters like dry matter, acidity, salt and pH. As guidance even viscosity and density can be analyzed by NIR within the same analysis. The quality of seeds which is dominating the properties and taste of the final product can be also controlled using FT-NIR spectroscopy.

Products:
- Ketchup
- Table sauces
- Mustard
- Mayonnaise
- Dressings
- Vinegar
- Soy sauce
- ...

Parameters:
- Fat
- Dry matter
- Salt
- Acidity
- pH
- Brix
- Density
- Viscosity
- Ash
- Alcohol
- Total titratable acid (TTA)

Condiments

Mayonnaise

A base mayonnaise is an emulsion of edible oil, egg yolk and vinegar in water. The quality control for the raw materials by FT-NIR is the first step for a high quality product. The fat content in a standard mayonnaise varies from 50 to over 80 %, with some low fat variations having less than 15% of fat. The texture can reach from a light cream to a thick gel with different optical properties. For the common parameters fat, dry matter, acidity and salt ready to use methods are available for a quick start.

Vinegar & dressings

Vinegar is used on its own in food preparation, but is also a valuable ingredient for other condiments. With a simple NIR measurement in a flow cell, the analysis of dry matter, acidity, ash, pH and citric acid is easy to do.

Derived from vinegar, there are many different recipes for vinaigrettes and creamy dressings with ingredients like yoghurt, sour cream or mayonnaise. Due to the high water content and low reflectivity of such samples the NIR analysis on most of the parameters is performed in transflection.

Soy sauce

Soy sauce is a fermented food with a high salt concentration. Due to the high water content the NIR transmission measurement and the analysis on nitrogen, salt and alcohol content must be performed under tight temperature control. The analysis is performed in a 1mm water-cooled flow cell and an optional autosampler can be attached to the MPA II FT-NIR spectrometer.

Transflection measurement of ketchup in a 22mm vial on the integrating sphere of the MPA II

• Confectionary: Chocoholics under control.

A tight quality control along the production steps is critical for
valuable ingredients like cocoa as well as the final chocolate products.
FT-NIR provides accurate analysis results of multiple components
within seconds for fast decisions to maintain highest quality.

Cocoa

The chemical composition of cocoa beans as well as cocoa products is complex and will change depending on the processing. The seeds are fermented which causes many chemical changes helping the chocolate flavour to develop and the seeds to change colour. The dried seeds are the raw material for the production of cocoa mass, cocoa powder and cocoa butter.

The qualitative heterogeneity and increasing value and consumption of cocoa products require fast and efficient methods for quality assessment of fermented cocoa beans and cocoa powders. Besides the fat and moisture control, more specific parameters like theobromine, organic acids and phenols are nowadays analyzed by NIR for fermentation quality to decide fast what cocoa batch is useful at a certain time and where to use it.

Chocolate

Chocolate contains valuable ingredients like cocoa powder, cocoa butter, lecithin, milk powders and sugars. The art of chocolate making is the careful mixing of these ingredients to achieve an constant product at optimized cost. A tight quality control along the production steps is therefore critical. FT-NIR provides accurate analysis results of multiple components within seconds.

One example is the determination of fat content in chocolate. The standard reference lab method is Soxhlet extraction which takes at least 2 hours - too slow to react on deviations in the production process. Here, NIR spectroscopy is the preferred method. All ingredients can be analyzed in less than a minute with MPA II or TANGO spectrometers. Alternatively, fiber optic probes can be used in conjunction with the on-line

Products:
- Raw sugar
- White sugar
- Syrups
- Molasses
- Cocoa products
- Chocolate
- Pastries
- Cookies & biscuits
- Cakes
- ...

Parameters:
- Brix
- Pol
- Color (ICUMSA)
- Ash
- Fat
- Moisture
- Protein
- Lactose
- Sucrose
- Reducing sugars
- Theobromine
- ...

spectrometer MATRIX-F. An ideal position for sampling is e.g. at the Conche, before the chocolate is brought into its final form.

Moreover the chocolate can be analyzed as liquor or as the final product. The sample measurement is carried out in seconds using easy to fill disposable polystyrene or glass Petri dishes.

Bakers' confectionery

Many kinds of sweet baked products are made from ingredients such as flour, sugar, milk, oils, butter; ideal for the analysis with FT-NIR. Moreover, the finished products can be tested for nutritional values. Examples are sweet pastry products, cakes, cookies or biscuits with many different recipes. A challenge can be the sample preparation and presentation which are often not as homogeneous as a plain cookie or biscuit.

Pastries for example can be quite heterogeneous with chocolate coatings, fruits and added nuts, confectionery often have cream fillings. Here the sample must be homogenized to derive reliable average values e.g. for checking of labeling claims.

In addition ingredients such as honey, nuts, caramel and marzipan can be analyzed with the same instrument to secure the requested quality and adjust recipes if required.

• Sugar: Sweet by nature.

Producing sugar from sugar cane or beet is a complex process requiring a tight quality control along the production chain to ensure optimized yield and quality. FT-NIR offers a fast and effective tool for controlling the critical QC parameters of raw materials, products and by-products in all production steps.

Near infrared spectroscopy provides accurate analysis results of multiple components within seconds. It is a non-destructive method without any sample preparation and does not require the use of any solvents or reagents. Operators can easily perform the real time measurements resulting in huge time and cost savings. FT-NIR can be implemented in the lab of a sugar mill, at-line in the production area or even on-line in order to control products and by-products.

Cane reception and milling
The samples of incoming cane taken by a core sampler from the trucks are shredded for further analysis. Instead of pressing out the cane juice for payment analysis the cane can be directly analyzed with the CPS (Cane Processing System) which allows an analysis of 3 to 15 kg in one run. The cane is automatically settled on a small conveyor belt and passes the NIR sensor head which can be installed for an on-line cane analysis directly in the mill as well. On cane the parameters Brix in juice, POL, fiber and moisture can be analyzed simultaneously and within a minute.

Sugar factory operations
During the different steps of processing the cleared juice to raw sugar a lot of intermediate products are of interest to be analyzed quickly for process monitoring and control. With a lab or at-line FT-NIR bench top analyzer all kind of samples of different juices, molasses, magma, seed, pan feeds and massecuites can be analyzed on Brix, POL, ash, sucrose, glucose and fructose directly by filling a sample vial. If the samples are diluted the analysis is

Products:
- Sugar cane
- Bagasse
- Filter cake (mud)
- Juices
- Molasses
- Massequite
- Syrup
- Raw sugar
- White sugar
- Bioethanol
...

Parameters:
- Brix
- Pol
- Dry matter
- Moisture
- Ash
- Sucrose
- Glucose
- Fructose
- Reducing sugars
- Purity
- Color
- Ethanol
...

performed in transmission flow cell with temperature control which ensures higher accuracy.

Sugar refinery process

In the refinery process first the raw sugar can be analyzed on many parameters: POL, moisture, reducing sugars, ash and color (ICUMSA). During processing again intermediate products like molasses and other can be checked for process optimization. Final products like crystal sugar and syrups can be analyzed for quality control.

Bioethanol process

Fermentation of molasses and other sugar process by-products is a straight forward and widely used production process for bioethanol. With FT-NIR each of the steps can be controlled starting from the raw materials over the fermentation and distillation/rectification to the final bioethanol. Especially for the fermentation and the distillation NIR in-line technology is an option which provides best opportunities for real time process control to optimize yield and processing time.

Measurement of raw sugar in a Quartz cup on the integrating spere of an MPA II spectrometer

• Beverages: Here's to quality control!

High-quality raw materials are the base of prime beverages. FT-NIR can help to evaluate incoming goods and assist production by monitoring and controlling processes, e.g. the fermentation of must or wort. Also, ensuring a tight specification for a wide product variety can be easily achieved with such fast analyzers.

Many of the raw materials used for producing beverages can be analyzed by NIR. From solid samples like wheat, barley, malt, hops and yeasts to liquids like concentrates. A special raw material is grapes which can be measured with the right sample preparation.

Most intermediates and products are liquids and analyzed in transmission through a maintenance free quartz flow cell with 1mm (1,000µm) path length that does not show cuvette wear over time. Adding the Liquids Sampling Module (LSM) to a MPA II or TANGO-T spectrometer automates the whole process of analyzing and cleaning for highest reproducibility and accuracy.

Must & wine
Must, must under fermentation and finished wine are analyzed in transmission and even more viscous liquids like sweet wine can easily be pumped through the flow cell for analysis. Since no reagents or consumables are needed the method is very cost effective. Numerous quality related must and wine parameters such as alcohol, acids, sugars, density, extract content and more can be monitored.

Spirits
Distillery and other spirit production processes are ideal for NIR analysis since most compounds are organic and at sufficiently high concentration. From unloading the grains off the truck, to the final bottling, NIR analysis can provide useful information for process control. Especially fermentation optimization can be complex to reach the targeted alcohol content and optimum yield. Here and during distillation NIR is fast tool to gain required information and allow correction of potential problems.

Beverages

Products:	Parameters:
- Cereals	- Protein
- Malt	- Fat
- Hops	- Moisture
- Spirits	- Alcohol
- Grapes	- Density
- Wine	- Sugars
- Must	- Brix
- Coffee	- Total acids
- Tea	- Caffeine
- Fruit juices	- Extract content
- ...	- ...

Soft drinks and fruit juices

These popular beverages cover a wide range from a liquid up to smoothies or even a fruit puree texture. Depending on the viscosity and insoluble dry matter content, e.g. pulp in fresh juices, a measurement is done temperature controlled in transmission or alternatively in transflectance. Common parameters of interest are e.g. Brix, density, acidity, citric acid and vitamin C content.

Non-dairy milk and beverages

Milk alternatives are today very important for several reasons like avoiding animal products or lactose intolerances. From the analytical point of view milk made from soya, almonds, rice, hemp, cashew, oat or coconut can be analyzed like cow milk in terms of handling using different calibrations. Main parameters are protein, fat, total sugars and density. The transmission analysis in the 1mm flow cell is independent of fat content and globule size distribution.

Coffee & tea

Coffee beans are analyzed by NIR as green beans and finally roasted to varying degrees, depending on the desired flavor. Protein and fat content as well as more relevant parameters like total acidity, moisture and caffeine can be determined. Low caffeine content can be analyzed accurate enough to control the de-caffeinated coffee to ensure that a certain minimum content guaranteed. Similar applications are used to control the caffeine content in de-caffeinated tea which is moreover tested for moisture and parameters like polyphenols to monitor the fermentation process.

Labelling: Look what's inside.

All food products for sale, marketing and distribution in countries of the European Union as well as in the US need to comply with regulations on the labelling of nutritional and health claims. Here FT-NIR spectroscopy can offer a fast solution for the screening of the main constituents.

From 13 December 2016, a nutrition declaration became mandatory for prepackaged foods in the EU (Regulation 1169/2011) and must include the following:

- Energy Value
- Fat Content
- Saturated Fat
- Protein
- Carbohydrates
- Sugar
- Salt

In the US, the FDA regulates the nutrition labeling of food in guideline "21 CFR part 101.9" which also requires the declaration of trans fats, cholesterol and dietary fibers.
The analysis of these parameters is a time consuming procedure, sometimes taking days. Screening the sample with FT-NIR in less than a minute can reduce the amount of samples that need to be analyzed with the traditional methods dramatically. This will not only help to reduce the running costs of the laboratory, but will also take workload off the existing staff, who can then carry out more specialized tasks.

FT-NIR offers a valuable tool for the screening of food products. The high information content of NIR spectra provides a finger print of the complete sample. This makes it applicable not only for the analysis of food composition, but also for quality control of raw materials and finished products in general. It is already widely used in all areas of the food industry, like dairy, meat and edible oil manufacturing with an excellent cost-benefit ratio and unrivaled ease-of-use.
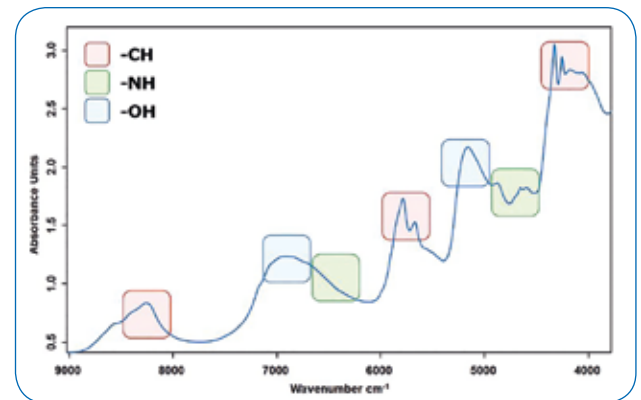
FT-NIR spectrum of a biscuit showing the distict absorption bands of -CH, -NH and -OH functional groups. From this fingerprint, the main constituents can be evaluated.

Food Fraud: The real thing?
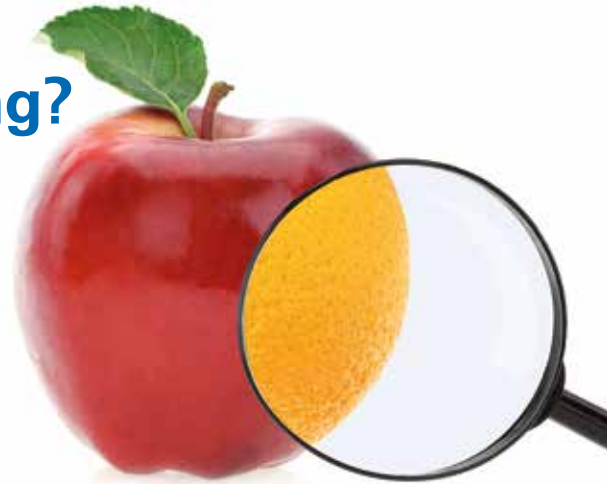
Maintaining brand reputation and product quality has led to increased focus on qualifying raw materials and ingredients used in food production. In addition to traditional quality parameters like moisture, fat, and protein, detection of adulterants plays a critical role in ensuring food safety and quality. The USP (US Pharmacopeial Convention) Food Fraud Database currently lists hundreds of incidents of economically motivated adulteration (EMA), substitution, counterfeiting or mislabeling of food products, such as olive oil and milk powder and some prominent adulterants e.g. melamine.

FT-NIR offers a valuable tool for screening almost any raw material with an excellent cost-benefit ratio and unrivaled ease-of-use. The high information content of NIR spectra provides a finger print of the complete sample. Comparing the spectra of the incoming raw materials with those measured using samples of known quality permits a non-targeted screening of adulterants or contaminants within the detection limits. If a material is tested positive on adulteration by FT-NIR, further investigations with complementary analytical methods can be carried out to determine the exact identity of the adulterant.
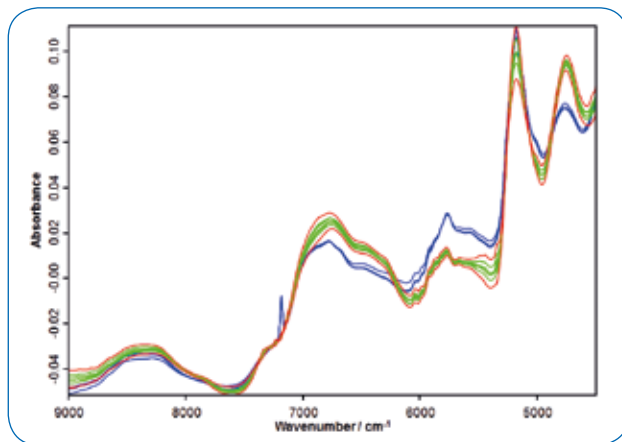
Display of reference spectra in a conformity test method (green) with spectra detected as outliers (blue).

Bruker FT-NIR spectrometers offer a fast and effective tool for quality control of raw materials, intermediate products and final products. As a non-destructive method without any sample preparation it is already extensively used in the food industry for analyzing main constituents such as protein, moisture, fat, lactose, ash, and fiber.

With the measurement of a single spectrum the sample can be evaluated in a three-step process:
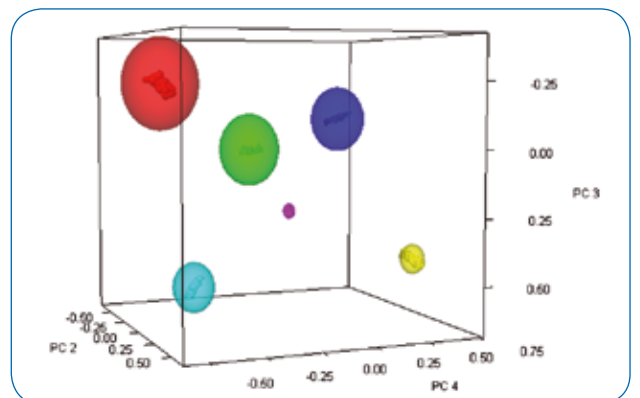
1. Identification

Identification of a sample is carried out to determine if the spectrum of an incoming raw material fits within the statistical population of authentic and previously accepted batches. With this first step it can be checked if the correct raw material was delivered and properly labeled to avoid usage of the wrong ingredient in production.

2. Conformity

In the next step the sample is further qualified using conformity test, which is a more specific evaluation of the spectrum. Each data point of the NIR spectrum is subject to a dedicated test with an individual threshold. This check for conformity at each data point allows a real fingerprinting of the material with adjustable sensitivity.

3. Quantification

During the quantification of the different constituents an outlier test based on the Mahalanobis Distance is performed. Again the analysis spectrum is compared to the sample population in the individual quantification models.

3D scores plots showing different material groups in an identification library.

Technology

State-of-the-art technology for RockSolid results

The Bruker Optics FT-NIR technology incorporates state-of-the-art optics for outstanding performance and stability. The heart of the instrument is Bruker´s permanently aligned RockSolid interferometer with cube corner mirrors, providing consistent high quality results, less downtime and highest stability.

Unlike flat mirrors, cube corners are practically immune to mirror tilt (i.e. angular movement of the mirror). This is an important consideration in FT technology since for the modulation the light returning to the beam splitter must be precisely recombined for interference to avoid a reduction in stability, resolution, and spectral quality.

The RockSolid interferometer design therefore leads to a superior resistance to vibration and thermal effects, ensuring exceptional robustness and reliability even in harsh environments, making it ideal for the laboratory as well as the factory floor.

Moreover, the instrument maintains the wavelength accuracy over time - a precondition for a successful calibration transfer.

All analyzers are designed to be easily maintained by the user, and to minimize downtime and maintenance costs. Consumables such as the light source are pre-aligned modules which can be easily and quickly changed by the user.
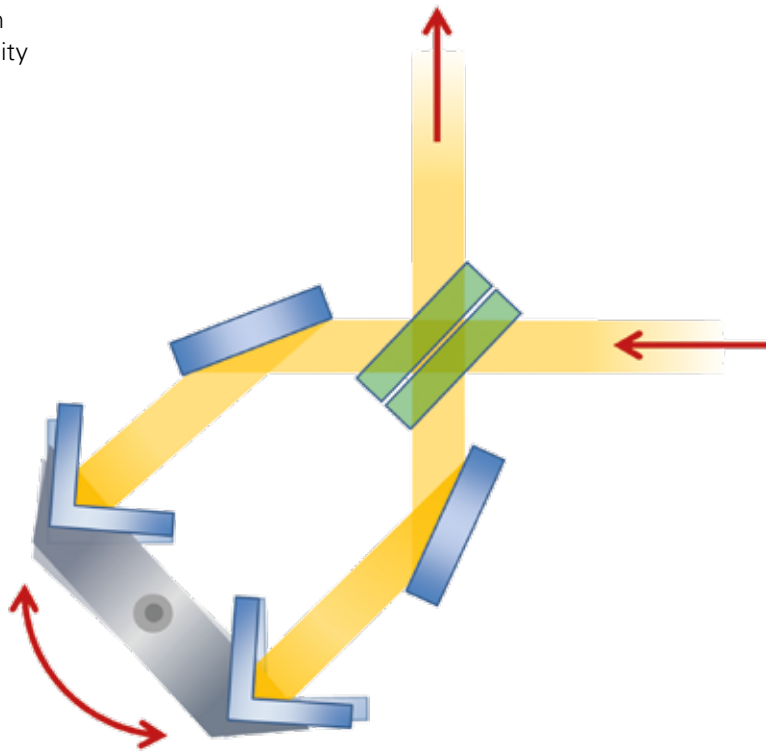
Bruker's well-proven RockSolid interferometer with Cube Corner Mirrors.
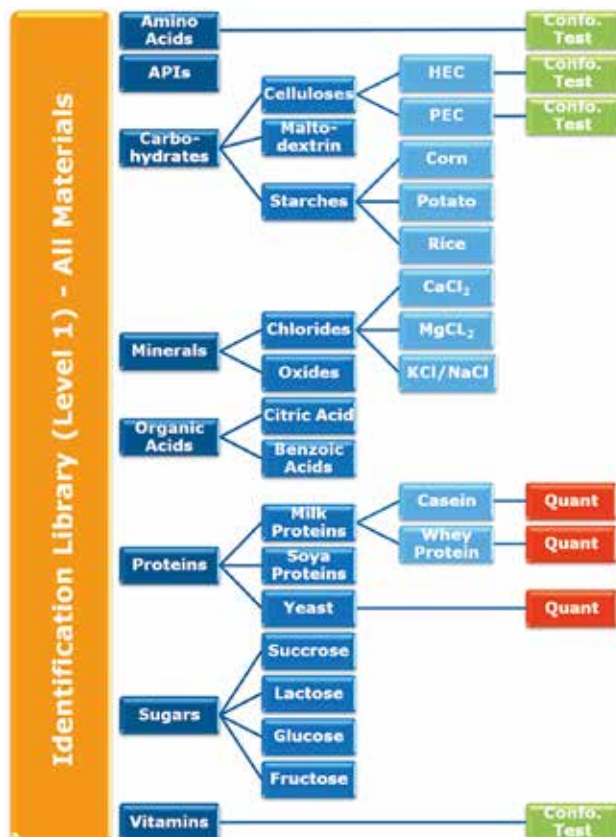
• Software

OPUS - Optics User Software

Bruker Optics' OPUS is an easy-to-use and a powerful all-in-one spectroscopy software package. It includes the most comprehensive collection of data acquisition, processing, and evaluation functions and can be completely configured to meet your needs including extended user management and access features.

For method setup there are three main functions for

- Calibration development for quantification of components and properties
- Library setup for identification of raw materials
- Conformity test for quality control

Multi Evaluation

Using the unique OPUS Multi Evaluation (ME) function, users can set up hierarchical methods to automate different evaluation and decision steps or to perform additional calculations. With ME, an identification step can be followed by a quantification step and a conformity test; or a quantification step can be followed by an additional quantification step depending on the results of the first step. The results are displayed, and customizable reports are stored and printed.

Example scheme of a Multi Evaluation method with Hierarchical Identification followed by Conformity Testing or Quantitative Evaluations.

In the laboratory

The OPUS/LAB package is an intuitive and easy-to-use software interface for routine analysis tasks. It can be used by routine operators who can quickly be trained to perform analyses. The operator just selects the product to be analyzed and enters the sample ID and optional sample information. The results are visualized on screen and stored in PDF and log files readable by LIMS.

In the process

OPUS/PROCESS is a software package used to easily set up scenarios for automated process control and visual display of results. The scenarios can be configured with many optional settings for cyclic measurements or analysis triggered by process control systems. Triggers and results can be exchanged with PCS using Profibus DP, Modbus, 4-20mA connections or OPC.

Data security

OPUS ensures the safety and integrity of your data.

- No loss of data or overwriting of raw data
- Fully GMP/GLP compatible, 21 CFR Part 11 conform
- Automatically generated data history (audit trail)
- All relevant data (measurement parameters, manipulations, evaluation results, reports, etc.) are stored in one data file

Spectrometer diagnostics

Only a permanently monitored spectrometer can ensure the acquisition of reliable data.

OPUS includes:

- Permanent online diagnostics
- Real-time display of instrument status
- Instrument status reports
- Integrated automatic instrument tests (OQ, PQ)

Service and Support

Bruker Optics is staffed by expert scientists and engineers with an in-depth knowledge of instrumentation and applications in the food and agricultural industry. Our product specialists are available to assist you with method development either remotely or in your lab. FT-NIR application scientists will assist you in the selection and use of sampling accessories, choice of optical components and software operation. We offer customized instruction and support packages to fit your needs.

Bruker Optics spectrometers are designed to provide years of trouble-free operation, but should a problem occur, a large network of Bruker companies and representatives throughout the world are ready to promptly respond to your needs. Professional installations, comprehensive applications support as well as high standard of post-delivery service are commitments Bruker Optics makes to each of its customers.

www.bruker.com/optics

Bruker Optics Inc.	**Bruker Optik GmbH**	**Bruker Shanghai Ltd.**
Billerica, MA · USA	Ettlingen · Germany	Shanghai · China
Phone +1 (978) 439-9899	Phone +49 (7243) 504-2000	Phone +86 21 51720-890
Fax +1 (978) 663-9177	Fax +49 (7243) 504-2050	Fax +86 21 51720-899
info.bopt.us@bruker.com	info.bopt.de@bruker.com	info.bopt.cn@bruker.com