Arrived: April 2022 – Accepted: May 2022

News of the MTA Working Committee of Food Analysis and Classification

Short summaries of the presentations of 2nd quarter of 2022

Analysis and classification of carbohydrates.

Characterization of fiber and small molecule carbohydrate composition of cereals *opportunities and challenges from the perspective of separation techniques*

Eszter Schall, Marietta Klaudia Juhászné Szentmiklóssy, Sándor Tömösközi
(Budapest University of Technology and Economics, Department of Applied Biotechnology and Food Science, Research Group of Cereal Science and Food Quality):

In our plant-based foods, carbohydrates play an important role not only in terms of nutrition (energy source, food safety), but also in sensory and technological sense (structure, texture, stocking, way of production, etc.). In our research group we deal intensively with the composition of dietary fibre in cereals. But more detailed information about its quantitative and qualitative characterization, variability, and role in technological properties is only available in the case of common wheat. In addition, the characterization of FODMAPs (fermentable oligo-, di-, monosaccharides and polyols) among short-chain carbohydrates is gaining more and more attention in research due to their role in gastrointestinal disorders (irritable bowel syndrome). The analysis of both fibres and small molecular weight carbohydrates is a serious challenge, partly due to their diverse structure and their small amount. In the recent years, our research group has focused on the quantitative and qualitative characterization of arabinoxylans, the quantification of β-glucans, their quantitative and qualitative variability in cereals and understanding of their technological role. In addition, we have successfully adapted chromatographic and enzymatic methods for the quantitative characterization of FODMAP components. They can be used to obtain information about the typical amount in cereals, their variability between varieties and species, and any changes during processing. In the future, we intend to expand our equipment by adapting and developing chromatographic methods for the quantitative and qualitative characterization of β-glucans and arabinogalactan peptides.

Recent applications and possibilities of VIS, NIR and MIR spectroscopy in carbohydrate analysis

János Slezsák, András Salgó, Szilveszter Gergely
(Budapest University of Technology and Economics, Department of Applied Biotechnology and Food Science, Research Group of Cereal Science and Food Quality):

Vibration spectroscopy provides a fast, non-destructive way to study food industrial raw materials, as well as intermediates and end products. The first analytical applications of infrared spectroscopy were based primarily on the mid infrared (MIR) range. **[1]** However in recent decades, the near infrared (NIR) range was dominant in the study of food analysis (almost the entire agricultural and food vertical), as it has higher energy, so it can be used better than MIR in case of complex matrices of biological origin, and in contrast to the visible (Vis) range, significant chemical information can be obtained from the NIR spectra. Following the traditions of our research group **[2]**, we have recently carried out comparative studies in the field of carbohydrate analysis with respect to different electromagnetic ranges (Vis, NIR, MIR) and optical configurations. This included the construction of spectral libraries, in which the spectra of several pure mono-, di- and polysaccharides were recorded with dispersive (DS), Fourier transform (FT) and diode-array (DA) NIR spectrophotometers to obtain information on the absorption characteristics of different carbohydrates. Based on the results, NIR techniques provide a good opportunity to identify pure carbohydrates, in several cases it is possible to distinguish highly similar compounds (e.g. identification of anhydrous or hydrated carbohydrates, determination of botanical origin in the case of starch). In addition to the study of pure systems, we have

developed mathematical models for the qualification of various powder mixtures, including the quantification of carriers for commercially available flavorings (e.g. maltodextrin). One of the unusual segments of our research is the qualification of powdered samples (either in homogeneous or mixed form) through different packaging materials, either for identification or quantification. Based on the results of these experiments, in several cases it seems possible to develop NIR based techniques that allows the qualitative or quantitative determination of different carbohydrates without breaking the packaging. **[3-4]** Based on international trends, the Vis and MIR ranges are also receiving increasing attention due to advances in spectrum processing and evaluation. The implementation of advances in computer science (artificial intelligence based techniques, machine learning, data fusion) in the evaluation of analytical results will be an important task in the coming years. In addition, our objectives include a comparative study of miniaturized infrared devices, which are becoming more widespread today but have questionable reproducibility.

References

[1] Yakov M. Rabkin (1987): Technological Innovation in Science The Adoption of Infrared Spectroscopy by Chemists. Isis 78:1, pp. 31-54.

[2] Tömösközi S., Lásztity R, Salgó A., Vértessy G. B (2021): 100+10 év a felsőfokú élelmiszertudományi oktatás és a kutatás szolgálatában. Magyar Kémikusok Lapja 76: 10, pp. 286-292.

[3] Slezsák J., Szabó É., Gergely S., Salgó A. (2018): Measuring of food industrial raw materials via polyethylene packages by NIR spectrophotometers using different optical arrangements. Acta Alimentaria: An International Journal Of Food Science 47:1 pp. 104-112.

[4] Slezsák J., Szabó É., Besenyő G., Salgó A., Gergely S. (2019): Developing a model system for NIR based identification and quantitative analysis of food additives measured via polyethylene foils [konferencia-előadás]. NIR 2019, Gold Coast, Ausztrália.

Identification of the role of carbohydrates in the development of techno-functional and organoleptic properties of cereal-based food matrices

Renáta Németh, Edina Jaksics, Alexandra Farkas, Dávid Fekete, Sándor Tömösközi
(Budapest University of Technology and Economics, Department of Applied Biotechnology and Food Science, Research Group of Cereal Science and Food Quality)

Since ancient times, cereal grains have been the main source of energy in our diet, due to their high carbohydrate content (60-80%). The main constituents of carbohydrates in cereals are polysaccharides (70-80%), of which starch is of primary importance as a primary nutrient reserve. In addition, cell wall-forming polysaccharides such as arabinoxylans, beta-glucan, cellulose, etc., which are collectively referred to as non-starch polysaccharides, are present in significant amounts and function as dietary fibre. From a technological point of view, starch and non-starch polysaccharides are considered to be the most significant, as their molecular size and structure largely determine their solubility, hydration, gelling properties and thus the properties and quality of the intermediate and final products. Cereals also contain 1-2% of smaller carbohydrates, oligo-, di- and monosaccharides, which can also affect processing to some extent (e.g., fermentation). Several specific instruments can be applied to study the technological (e.g. mixing, stretching, gelling) behavior of grain flours, especially wheat. Examples include the rapid visco analyzer (RVA) and Mixolab techniques, as well as amylographic analysis and falling number measurement, which can be applied well to study the role of carbohydrate components. The mentioned instruments test the gelatinisation and gelling properties in a dilute flour-water suspension. An exception is Mixolab, by which mixing and viscous behavior together in a complex dough matrix can be investigated.

Our research on starch properties also confirms that the composition of starch (e.g., amylose-amylopectin ratio) fundamentally influences the gelatinisation properties (gelatinisation temperature, peak viscosity, degree of liquefaction) and gel formation (final viscosity). It can also be noted that isolated starches behave slightly different than flours, which may suggest interactions between flour constituents. The properties of non-starch polysaccharides, primarily arabinoxylans (AX), have also been investigated in our research works several times. Due to their structure, crosslinks can occur or decompose between arabinoxylan molecules through ferulic acid groups under redox conditions. Our results showed that using an appropriate oxidative enzyme (e.g., peroxidase, pyranose oxidase) crosslinks can form between AXs, increasing the consistency and viscosity of the matrix (suspension, dough). All this has proved to be suitable, for example, for improving the consistency of gluten-free dough matrices. In contrast, hydroxyl radical oxidation led to depolymerization of AXs, deteriorating the technological properties of the dough system. The study of the role of each constituents in a model system (fractioned into constituents and then reconstituted) provides an opportunity to identify deeper relationships. Our experiments in wheat-based model dough have shown

that the reduction and re-oxidation of gluten network suggest the incorporation of added AX into the gluten structure, which is an important information for understanding the structural role of AXs in the dough and end product matrices.

There are still many unanswered questions about the compositional and structural variability of carbohydrates in cereals and their understanding of their closely related nutritional and technological role. All this will require further research and methodological improvements in order to promote conscious food development and the provision of scientifically sound, credible information to consumers.