Opinion

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From fingerprinting to kinetics in evaluating food quality changes

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Historically, the study of food quality changes during processing, preservation, and storage has evolved from targeted, single-response studies towards studies relying on both targeted and untargeted approaches analyzing multiple responses. In our opinion, future studies should be based on a zoom-in approach in which fingerprinting is used as a multivariate, hypothesis-free starting point to screen for key quality differences in food extracts of differently processed, preserved, and stored foods. By interpreting the identity of selected fingerprint markers in terms of their relevance and consequences for application or connecting the markers to particular food reactions, in a subsequent kinetic study mechanistic as well as quantitative insight into the effect of extrinsic processing variables on quality changes can be obtained.

The food processing and preservation reactor

The concept of a food reactor model (Figure 1) can be applied to a single food unit operation and/or to a series of unit operations, including shelf-life. Independent of the technique under consideration, the main goal of food processing and preservation is the creation of a desired effect (e.g., increased safety, stability, and digestibility). However, when selecting processing conditions for this targeted effect, a balance needs to be made for possibly linked undesirable food quality changes (e.g., nutrient degradation, texture loss, and formation of process-induced contaminants) [1,2]. The way the quality characteristics of the food change in the processing reactor is influenced by intrinsic food properties such as pH, water activity, the food structure, etc., and by extrinsic processing factors such as treatment time, temperature, pressure, packaging material, etc. (Figure 1). By selecting and combining the intrinsic and extrinsic factors in a particular way, the final quality of the processed product can be optimized in order to meet consumer expectations and respond to commercial trends [3].

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Historical evolution of studying food quality changes

For decades already food scientists have been studying food quality changes during processing and preservation. Many studies evaluated quality aspects after a particular treatment. The residual quality was compared to its fresh counterpart and/or other types of treatment (using different intensities and/or unit operations). In fact, the integrated effect of all processing variables was studied [4–8]. Others studied the evolution of change of a specific quality characteristic, typically in a kinetic study in which the extrinsic processing variables were completely controlled and monitored [9–14]. Using kinetic modelling, insight into the effect of individual extrinsic processing variables on the quality change could be quantified, which has been an essential step towards model-based process design and optimization [15,16]. However, kinetic parameters (e.g., rate constant, activation energy) obtained through a single-response kinetic study (see Glossary) must be handled with caution because the parameters are empirical in nature and apparent and thus linked to the inherent reaction environment for which they were established

Glossary

Food matrix: the nutrient and non-nutrient components of foods, their molecular relation, and interaction.
Headspace: the space above a sample held in a sealed container. Headspace analysis is used to investigate the volatile constituents of a sample. Because the concentration of compounds in the sample headspace depends on the temperature and time of sampling, the headspace should be studied under equilibrium conditions at a particular temperature.
Multiresponse kinetic study: study of the evolution of change of multiple selected food characteristics (e.g., glucose concentration, asparagine concentration) under a range of extrinsic processing variables (e.g., time, temperature). The selected responses are linked to each other in a complex reaction network (e.g., maillard reaction). In a kinetic study, the extrinsic processing variables should be completely known.
Single-response kinetic study: study of the evolution of change of a single selected food characteristic (e.g., color, vitamin C content) under a range of extrinsic processing variables (e.g., time, temperature). In a kinetic study, the extrinsic processing variables should be completely known.
Targeted analytical approach: in a targeted analytical approach, one or more food characteristics of interest are known *a priori* and thus selected as a starting point. The food characteristics can be a food attribute (e.g., color, texture) or a chemical compound (e.g., vitamin C). The analytical methods applied are specifically optimized for the full quantitative expression of the characteristics (e.g., concentration).
Untargeted analytical approach: the aim of an untargeted analytical approach is to detect as many chemical compounds as possible present in the particular food matrix. Decisions on extraction, separation, and detection methods to be applied define the particular range of compounds studied in the food extract. Before analysis, the identity of the detected compounds is not known. Quantification is relative to other (control/treated) samples (e.g., relative concentration) and the initial goal is generally sample comparison and discrimination analysis.

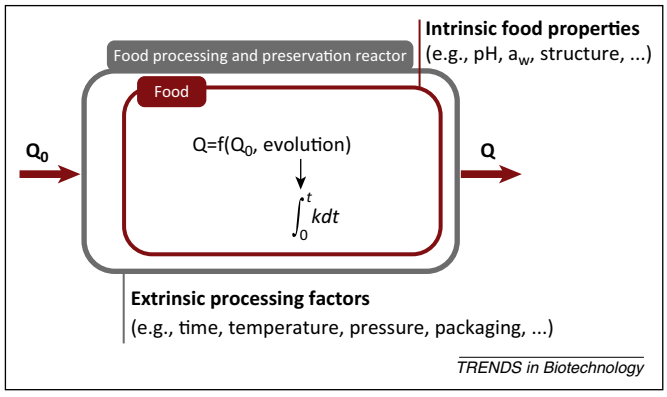

Figure 1. Schematic representation of a food processing and preservation reactor model. Depending on the intrinsic food properties as well as the extrinsic processing factors, food quality aspects might change as a function of time, resulting in the final quality after processing. Q_0, food quality characteristic at initial conditions; *k*, reaction rate constant; *t*, time; a_w, water activity; Q, food quality characteristic at the end of processing.

[15,16]. In general, these early studies, and still many studies today, focused on a particular (set of) quality response(s) (e.g., vitamin C, texture, color) selected at the start of the experiments, which can be identified as a 'targeted approach'. Following this approach, many researchers evaluated only a single response that related to a specific food characteristic or reaction [17,18].

In recent years, relying on multiresponse kinetic studies and modelling approaches, progress has been made on mechanistic insight into complex food quality-related reactions [15,19]. In this targeted analytical approach, 'multiple' selected responses, rather than a single response, of a particular food quality-related reaction are evaluated as a function of the extrinsic processing variables. By forcing the modeler to build reaction schemes behind the model, the understanding of the reaction pathway is increased. Multiresponse kinetic models are often more generically applicable than single-response models and can be more easily applied to other products or processes, although parameter re-estimation and even model reformulation might be necessary to take into account the complex reaction environment the food system offers [15,19].

Fingerprinting is a new approach to study food quality-related changes and food characteristics are studied at the molecular level. However, molecular targets to be studied are not *a priori* selected as a starting point. Fingerprinting is an -omics approach that was adopted from the world of metabolomics [17] and transposed to food systems; it has only recently proven its use for unbiased insight in quality changes during processing, preservation, and subsequent storage [20–22]. By definition, it is an 'untargeted, multivariate approach' in which as many compounds as possible of a particular food extract are detected [17,18]. At the first instance, compounds are unknowns. Fingerprinting techniques are intended to perform comparative analysis to find differences among samples [17]. Using appropriate multivariate data analysis (MVDA; chemometrics), chemical fingerprinting should lead to the selection of markers: compounds of which detected quantities are clearly different when compared to other sample conditions [18,23]. These markers are identified and can be linked to reaction pathways or particular food characteristics for more insight.

In summary, progress in analytical methods and data analysis techniques made it feasible to obtain more information from a particular food matrix analyzing multiple responses or, even more convenient, from a single analytical run analyzing multiple variables in a particular food extract. Besides the evolution from single- to multiple-response studies and from targeted to untargeted food quality evaluation, kinetic studies have evolved from an experimental and modelling point of view. By performing experiments under static processing conditions, modelling has evolved from a two-step to a one-step modelling approach. Finally, by including the full sample processing history (dynamic conditions), one-step statistical approaches for estimating kinetic parameters have been successfully applied [15,16,24].

Integrating fingerprinting and kinetics: a state of the art approach for studying food quality changes

Using state of the art analytical techniques, advanced MVDA, and the current knowledge of the design of kinetic experiments and associated data analysis techniques, it is now feasible to study food quality changes using a hypothesis-free approach. Starting from a fingerprint, markers can be selected from which enhanced mechanistic and quantitative insight can be obtained in a targeted, kinetic study. Integrating fingerprinting with kinetics is presented schematically (Figure 2) and elucidated step by step below. The approach requires the concerted action of food technologists, analytical experts, and engineering approaches for advanced data analysis.

Step 1. Fingerprinting of a particular food extract

The ultimate analytical goal of a food scientist might be the injection of the solubilized food part to the analytical equipment rendering the molecular separation, quantification, and identification of all compounds in the food system. This unique chemical fingerprint would be the basis of discriminating the food matrix under study from all chemically different food matrices [25,26]. Despite the large progress made in increasing the resolution and identification power of advanced analytical methods such as gas chromatography (GC) and liquid chromatography (LC) coupled to a mass spectrometry (MS)- or nuclear magnetic resonance (NMR)-based detector, food fingerprinting can today only be performed on one or more particular sets of extracts [18,25,26]. The fact that chemical fingerprinting considers all compounds detected in the investigated food fraction makes it a comprehensive, unbiased methodology. In contrast to a targeted analytical approach, in which focus is given to predetermined particular compounds of interest, fingerprinting opens the possibility to uncover unexpected compound changes [18,23]. In our opinion, fingerprinting should be the first choice starting point for hypothesis-free screening for key food quality changes and differences. Recent studies from our group have proven the potential of fingerprinting the food headspace to compare the integrated impact of particular processing/preservation technologies or to obtain insight in quality changes during storage after preservation [20–22]. In addition, by screening different food matrices under the same sets of processing/preservation conditions, fast insight can

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