**Unravelling food thermal reactivity by an original methodology to analyze and model reactions during baking of a cake model**

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**Highlights**

* Thermal reactions were followed in an inert cake model added with targeted precursors
* A wide range of markers were quantified fulfilling an observable reaction scheme
* Reactions were simulated by coupling stoechio-kinetics to heat and mass transfer models.

**1. Introduction**

In baked foods, process and formulation steps lead to the generation of a multitude of compounds responsible for quality: aroma, flavor, color and safety, through the activation of thermal reactions. However the link between composition, reactivity and quality determinants is not an easy task because of the interdependency of physical and chemical parameters and the complexity of real ingredients. Therefore, studying complex transformations in a food matrix under strictly controlled physical, structural and chemical conditions is of paramount help to verify the hypotheses formulated by many decades of results obtained in simple model systems (far from real foods) or in real products (with limited understanding on specific reaction pathways).

**2. Methods**

An inert model imitative of a sponge cake was developed in order to master the nature and the quantity of reaction precursors [1]. The cake model was added with targeted precursors to activate thermal reactions in a controlled way (caramelization in model G - glucose containing model; both caramelization and Maillard reactions in model G+L - glucose and leucine containing model). G and G+L models were submitted to controlled process conditions (140°C, 170°C or 200°C baking temperatures; high and low convection levels). Ten reaction markers (precursors, intermediates and products), were quantitatively analyzed during the course of baking (8 kinetic points) by a complementary sampling approach. Volatile markers (e.g. furanic compounds, pyrazines, Strecker’s aldehydes, acids) were sampled from baking vapors by on-line sampling device and TD-GC-MS analysis while nonvolatile and water-soluble markers were extracted from the cake matrices and quantified as follows: reducing sugars by UHPLC-CAD, free amino groups by Sørensen formol titration, dicarbonyl intermediates by UHPLC-DAD/MS, furfural and 5-hydroxymethylfurfural by UHPLC-DAD. These markers were thus selected to fulfil the requirements for an observable reaction scheme and a stoechio-kinetic modeling.

Synchronous experimental data on heat and mass transfers and reactions were acquired under perfectly controlled conditions of thermal treatment (temperature and convective transfer coefficient) and used for the modelling of coupled transfers and reactions in the cake using Comsol™ and Matlab™.

**3. Results and discussion**

The only presence of glucose in the G model was sufficient to activate caramelization reaction with the production of high levels of furfural, 5-methylfurfural, 5-hydroxymethylfurfural, and acetic acid. These compounds showed a typical final product behaviour (exponential production) except from furfuryl alcohol (bell-shaped behaviour) and a dependency to baking temperatures and convection speed. These markers were also found in the G+L model where caramelisation and Maillard reaction could jointly occur. Interestingly, specific pathways were activated by the presence in the system of leucine and glucose: the quantification of 3-methylbutanal in high amounts showed the activation of the Strecker’s degradation in model G+L. Moreover, when comparing the amounts of dicarbonyl intermediates, the higher generation rate of the 3-deoxyosone relatively 1-deoxyosone model suggested that the 1,2-enolisation pathway was favored compared to the 2,3-enolisation in the G+L model and showed that the higher the temperature and the convection level, the faster their degradation.

The stoechio-kinetic model was coupled with a mass and heat transfer model in order to predict markers content in the cake models during baking. Hence this joint approach provided an excellent opportunity to understand, model and control the kinetics of thermal reactions contributing to the generation of process-induced compounds in solid food.

**4. Conclusions**

An original methodology coupling chemical and physical on-line measurements was developed in order to follow a broad range of reaction markers and unravel Maillard and caramelization reactions under realistic but controlled processing conditions. Thanks to a solid food model (cake model) having a complex structure and technological history but only containing known amounts of one or two reactive precursors, two observable reaction schemes could be built and modelled into a stoechio-kinetic model, taking into account mass and heat transfer in the cake model. This model is helpful for capitalizing on knowledge about the impact of formulation and process on quality of baked products.

**References**

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