PRODUCT QUALITY DRIVEN FOOD PROCESS DESIGN

Promotoren:

Prof. dr. ir. G. van Straten
Hoogleraar in de Meet-, Regel- en Systeemtechniek, Wageningen Universiteit

Prof. dr. ir. R.M. Boom
Hoogleraar in de Levensmiddelenprocesskunde, Wageningen Universiteit

Co-promotor:

Dr.ir. A.J.B. van Boxtel
Universitair docent, leerstoelgroep Meet-, Regel- en Systeemtechniek, Wageningen Universiteit

Promotie-commissie:

Prof. ir. J. Grievink
Technische Universiteit Delft

Prof. dr. ir. M.A.J.S. van Boekel
Wageningen Universiteit

Prof. dr. ir. B. M. Nicolai
Katholieke Universiteit Leuven

Dr. A. Friis
Biocentrum Technical University of Denmark

Dit onderzoek is uitgevoerd binnen de onderzoekschool VLAG

PRODUCT QUALITY DRIVEN FOOD PROCESS DESIGN

H A D I Y A N T O

PROEFSCHRIFT
ter verkrijging van de graad van doctor
op gezag van de rector magnificus
van Wageningen Universiteit,
Prof. dr. M. J. Kropff
in het openbaar te verdedigen
op Dinsdag, 27 November 2007
des namiddags te vier uur in de Aula

Hadiyanto. (2007). Product Quality Driven Food Process Design

PhD Thesis Wageningen University, the Netherlands
with summary in English, Dutch and Indonesian.

Key words: Conceptual Process Design, Delft Design Matrix, Food design, Baking, Modelling, Bakery Production, Dynamic Optimization, Multi Objective Optimization.

ISBN : 978-90-8504-803-9

Preface and Dedications

This thesis is the final work of my PhD study at the Systems and Control Group cooperating with Food Process Engineering Group, Wageningen University, the Netherlands. It provides documentation of my four year work during the study from summer 2003 until summer 2007. The research has been financially supported by the Graduate School VLAG. Besides numerous people have contributed substantially to the research on which this thesis is based, I am deeply indebted to **drs D.C. Esveld** for his creative ideas and help that give significant value for this thesis. As matter a fact, you acted as co-supervisor since the initial phase till the end of the work and therefore, I would like dedicate this thesis to you.

The thesis consists of eight chapters including introduction and conclusion chapters covering aspect of food process design driven by final product quality. The five chapters contain papers that are accepted by or submitted for an international journal. These chapters describe various views of process design methodology, food modelling, food process optimization, multi-objective optimization and baking processes.

Wageningen, November 2007

Hadiyanto

This thesis is also dedicated to my beloved wife Adian Khoironi and daughter Adhelia Intan Sabhira

….The products we design are going to be ridden in, sat upon, looked at, talked into, activated, operated, or in some way used by people individually or in masse. If the point of contact between the product and the people becomes a point of friction, then the industrial designer has failed. If, on the other hand, people are made safer, more comfortable, more eager to purchase, more efficient—or just plain happier—the industrial designer has succeeded.

HENRY DREYFUSS

Content

CHAPTER 1

State of the Art and Challenges

Hadiyanto

1. Developments in the food industry

The last decade has shown a continuous growing interest in product and process development within the food industry. Major drivers for this interest are the introduction of new products to the market and the wish to increase the added value of the current products in order to stay in the competitive market. This situation requests for concurrent product and process design, especially for food products where changes of process conditions will affect the final product quality. Furthermore, quick changes in the market request flexible production units which can follow the rapid developments.

Traditionally, food industries have organized their production systems such that large quantities can be produced (van Donk, 2000). However, the current rapid changes in the consumer market (greater variety of products, demand for high quality products and new products) request for lower production quantities and a larger diversity of products.

These developments make that advancing food process design concepts is of strategic importance for the food industry in the endeavor to rethink, reconsider and redevelop their current processes.

2. The potential of conceptual food process design

Process design has a significant tradition in the chemical industry. It encompasses the broad range of creative activities in generating ideas to develop production processes that give improvement to existing processes or products or to develop new processing systems (Douglas, 1988; Diefes, Okos and Morgan, 2000). The main goal of process design is to identify the optimum processing equipment, the arrangement of the equipment, and the operation conditions that deliver the desired products for the best yield, the lowest cost, the highest efficiency in the use of the production line and minimal loss of quality (Bruin and Jongen, 2003). Normally, process design begins at a conceptual level (initial phase), where the basic ideas are generated, and from this point the design continues in several advanced steps such as validation experiments, engineering and construction, pilot scale experiments, etcetera.

King (1972) distinguishes two complementary activities in process design (see Figure 1): process analysis and process synthesis. Process analysis involves for example the calculation of the outputs of a known process for given input conditions. Process synthesis, on the other hand, concerns the configuration of a new process which transforms the given inputs into specified outputs.

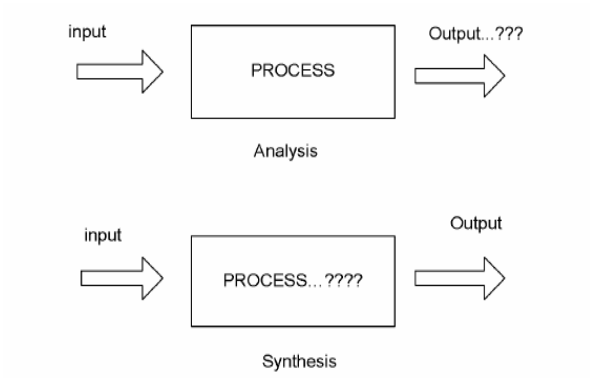


Figure 1. Two complementary types of activities to characterize process design: Process analysis with the outputs as result and process synthesis with the process definition as result (King, 1972).

Process synthesis is frequently used in the chemical industry to extend or improve existing processes. Between 1970 and 2001 the chemical industry has put a great amount of effort into the implementation of systematic approaches for process synthesis. Examples are superstructure optimization (Grossman, 1996), hierarchical decomposition (Douglas, 1988), property difference elimination (Siirola, 1996), and the Delft Design Matrix (Grievink, 2001). Some of these methodologies are discussed in Chapter 2.

In recent years the food industry starts to show interest in the translation of the process synthesis concept from the chemical domain to the food processing domain. As a result, the idea of a systematic approach to food process and product design is developing in food research. Various approaches and techniques have been suggested, each with its own perspective and aim. With regard to production systems the Delft Design Matrix was extended with food specific features (Jadhav *et al.,* 2002). The group of Fito *et al.* (Universidad Politecnica, Valencia) works on the SAFES (Systematic Approach to Food Engineering Systems) methodology to recognize the complexity of food system and to allow coordinating the information about food structure, composition, thermodynamic, and quality in adequate tools to develop real food product and processes (Fito *et al.*, 2007).

A major point in food process design is that the design is not mainly focused on process improvement but that it has a strong link to product quality and product development. Methods as Quality Function Deployment and Chain information models (Brenner *et al.*, 2005) are specially focused on the product design, but are only weakly coupled to the actual processing system. An open challenge for process synthesis in food process design is to develop processes which can adapt adequately to the changes in consumers' and market demand. This requires a high degree of flexibility but most and for all the ability to understand and control the crucial product transformations that occur during the process. Only in this way a tailored process can be designed through synthesis with the requested product properties as starting point.

2. Food quality in relation to food process design

Product quality is a key parameter for the food industry as it is the basis for success in today's dynamic and highly competitive market (Du and Sun, 2006). Much research has been done to understand and to improve product quality. However, it is remarkable that developments for process design or process synthesis, in which product quality has a central role, are still limited. Most design procedures start from a specified problem, which is solved by forward reasoning. If the goal is not achieved, the design is iteratively adjusted. This procedure can be regarded as a process analysis approach and that is technology driven: product quality is considered to be a constraint.

Food product attributes are qualified by three categories: quantitative, sensory and hidden attributes (Quirijns, 2006). Quantitative attributes comprise the simplest group for process design as they can be evaluated directly (for example weight, moisture content, and etcetera). Sensory attributes depend on the perception of consumers. They are related to questions as 'Is the colour good', 'do I prefer this texture and shape?', or 'Does it taste good?'. These attributes depend heavily on consumer inspection and perception which are easily influenced by external and psychological factors that can induce subjective and inconsistent evaluation results (Brosnan and Sun, 2004). The third category is the group of hidden attributes. These attributes cannot be evaluated by our senses or be fully quantified by measurements. Examples of these attributes are nutrient value and toxicity of the product.

Final product quality is the result of the properties of the starting materials, process and storage conditions and their interactions (not necessarily in this order, as many products are also processed by the consumer just before consumption). During processing and storage, products undergo physical, chemical and/or biological changes which are called transformations. Understanding the mechanisms of these transformations is important for food process design because they form the basis for process synthesis to select appropriate process equipment and conditions. For example, toxicity of products can be caused by microbial growth during storage; extending the products' shelf life as a design objective may be realised by adjusting the conditions for storage, or by changing the pasteurization step in the production process. Crispness of bakery products is a complex sensory attribute that results from a combination of physical parameters, such as structural and molecular properties and fracture behaviour (Luyten *et al.*, 2004; Vincent, 1998). These characteristics are affected by both the production process and storage conditions.

For food production systems, it has to be realised that products are often not homogeneous; consequently quality has a spatial distribution in the product. Product quality is, therefore, also evaluated on its size and internal qualities. For bread products not only the crust is important but also the internal water content and the quality of the crumb (soft inner part). Spatial quality differences arise from the temperature and water distribution which occur during processing. Food process design therefore also has to be directed to the creation of spatially varying properties. Stigter *et al.* (2001) showed that a specific heating strategy, derived through an optimal control strategy, makes its possible to heat lasagne to a uniform temperature in a convection oven. Banga *et al.* (1994) reported that for sterilization the toxicity of the product depends on the position of the product in the container. These examples show that the spatial quality distribution is an important aspect which affects decisions during design.

3. Modelling for design

A model is considered here as a mathematical representation of transport phenomena and product transformations in a real system. Models have crucial roles in process design methods. Banga *et al.* (2003) distinguishes three model categories:

- White box or first-principles models which are derived from known physical and chemical relationships. Laws of conservation for mass and energy, kinetic models and physical property transitions are part of this category.
- Data driven or black box models which are normally derived from qualitative information or sets of quantitative experimental data, for example response surface models.
- Combination of two given categories and which are named “grey box” models. Here white box parts are complemented with data based information. A special position in this group can be given to fuzzy models which are based on expert knowledge in qualitative rules.

Process design requires mathematical models to simulate, to optimize and to predict quality formation during processing. As they basically describe changes in space and time due to process conditions which may be dynamic as well, they may be written as partial differential equations (PDE) for spatially distributed and time dependent systems, ordinary differential equations (ODE) for time or position dependent systems and additional algebraic equations for stationary phenomena or extremely fast (instantaneous) transformations, and as representation for the interconnection between several variables. Heating of wet porous products (such as bakery products), for example, involves heat and mass transfer which is represented in the form of PDE equations, while the kinetics for textural changes are captured with ODE and algebraic equations.

As stated in section 2, the quality of food products is, almost by definition, subjective and therefore difficult to quantify. However, if the quality is required for design purposes then it must be defined and related to the process. This is a very challenging task, for which one should strive to grasp the most dominant mechanisms, with inevitable ignorance of subtleties. After all, the changes in quality are a direct manifestation of the changes in chemical and physical properties of food materials during processing. In bakery products, the Maillard reaction, caramelization and carbonization are involved in brown colouring of products. These transformations are driven by kinetic reactions between sugar and water that produce the browning compounds. The formation of the texture in bakery products is also strongly influenced by starch gelatinization and retrogradation. Here the physical states of starch changes due to the process conditions. For design purposes these relationships must be quantified. Literature search shows that ready-to-use first-principle relationships on food quality and their transformations are scarce. The major part of the available information is data driven and translated into expert knowledge based on rules or translated into (statistical) correlations.

Literature on food quality research is mostly focussed on single phenomena and properties. The interconnection with other variables is subject of investigation as well, but it is not often fully used for quality prediction. An integral prediction of all phenomena in food products requires a systems approach. With a systems approach we mean here investigating how a multitude of external variables affect a single phenomenon, and subsequently predicting quality by connecting all relevant variables and phenomena in mathematical (quantitative or semi-quantitative) models.

4. Optimization in Food Process Design

Optimization is the procedure to find the optimal solutions among process alternatives and to find the best process conditions and processing routes. For optimization, two classes of problems are distinguished. The first group concerns steady-state problems which can be solved as an instantaneous optimization problem. This type of optimization problem normally searches the most effective design parameter, without considering the transient properties of physical or chemical transformations. An example of this category is optimization by using response surface methodology (RSM). Here process conditions are optimized from a meta-model obtained from a set of experimental data (Gan *et al.*, 2007; Sumnu *et al.*, 2004; Demirekler *et al.*, 2004).

Table 1. The application of optimization in food process design

Process	Objective function/problem	References
Membrane fouling	Find input trajectories (pressure and velocity) to improve gross cash-flow	Van Boxtel *et al.*(1992), van Boxtel *et al.*(1993)
Thermal processing (sterilization of canned food)	Find optimal trajectory (heating temperature) which maximize the final nutrient retention	Holdsworth,(1997); Chalabi *et al.*(1999); Kleis and Sachs(2000); Garcia *et al.* (2006); Balsa Canto *et al.*(2002)
Drying process	Find the drying input trajectory to maximize product quality of potato slab, minimization of processing time and maximize energy efficiency, maintaining bacterial activity during drying	Karel (1988); Mishkin *et al.* (1983); Banga and Singh (1994); van Boxtel and Knol (1996); Quirijins (2006)
Fouling of heat exchangers	Find design of heat exchangers with minimal fouling precipitation	van Boxtel (1994)
Contact cooking	Find the optimal operating procedures for contact-cooking of non-homogenous foods	Banga *et al.* (2001)
Convection ovens	Find the oven temperature trajectory to obtain uniform temperature throughout the product	Stigter *et al.*(2001)
Pasteurization	Find the pasteurization temperature to minimize the volume average cook value (C_{av}) and to maximize the multi-factor objective function	Ghazala and Aucoin (1996)
Microwave heating	Find the microwave heating strategy for bioproduct	Banga *et al.* (1999)
Freeze-Drying	To decrease the processing time and reduce energy	Boss *et al.*(2004)

The second group concerns transient processes, for which dynamic optimization has to be applied. In contrast to instantaneous optimization, in dynamic optimization one takes the future consequences of a current design/control decision into account. Food products are in a transient phase during processing, with duration given by the time of residence and the momentary position in the process. For such problems dynamic optimization is a suitable tool, since it allows to find an optimal route starting from the aimed final properties. From the optimization results the trajectories can be translated in a realization of the production system and the feasibility and limitations in the product design can be understood.

In the area of process design, optimization has been used to solve problems such as (Balsa-Canto *et al.,* 2002; Banga *et al.*, 2003; Garcia *et al.*, 2006):

- determination of optimal operation policies for the control input,
- calibration of process models (parameter estimation)
- searching for the optimal values of design variables
- arranging process units in an optimal network.

Process optimization is thus a proven technique to improve the efficiency of existing processes. It can however also be used in process design (synthesis). After specification, the design issue has to be translated into an objective function. By using the food process model as a constraint, the optimization problem can be solved as a minimization or maximization problem. Table 1 gives an overview of examples for food process optimization where this approach is applied.

A main barrier in optimization of food production systems is the complexity and non-linearity of the transformations and the spatially distributed character of the systems that often leads to non-convexity and large computational costs. Therefore, the choice of an appropriate method of optimization is required before starting the actual optimization.

5. Multi-objective Optimization for food process design

The consumers' demand for integrally good food products usually means that several product quality attributes are important at the same time. In other words, we have to deal with multiple objectives. Full realization of all individual specifications simultaneously is often not possible, and one can only try to come close to the combination of targets. For such problems a multi-objective optimization approach must be used.

Multi-objective optimization is defined as the simultaneous optimization of several conflicting objectives (more than two), which produces a set of alternative solutions called the Pareto front (Halsall-Whitney and Thibault, 2006). These solutions are optimal in the sense that no one solution is better than any other in the domain when compared on all criteria. The decision-maker's experience and knowledge is then incorporated into the optimization procedure in order to classify the available alternatives in terms of his or her preference (Doumpos and Zopounidis, 2002).

In recent years, the use of multi-objective optimization techniques for simultaneous optimization of multiple and sometimes even conflicting objectives has received wide attention in chemical engineering, but the information on food applications is still minimal. In food process optimization the problems are typically solved by single-objective functions. Here the objectives are summarized into one objective function by using chosen weight factors for each individual objective.

Although the single-objective optimization algorithms are sufficient in many cases, there are serious drawbacks to their use especially when the objectives are conflicting or can not all be satisfied simultaneously (Halsall-Whitney and Thibault, 2006). Banga *et al.* (2003) state that multi-objective optimization is a particularly interesting approach to ensure that the problem formulation and the solutions are more realistic for such problems. Here optimization with multi-objectives is required to find a set of solutions representing the trade-offs between the different individual objectives instead of trying to find one single best result for a combined objective function (Kiranoudis and Marakatos, 2000). Halsall-Whitney and Thibault, (2006) listed the following advantages of multi-objective optimization compared to single-objective optimization:

- Single-objective optimization does not provide information about the trade-off amongst the various objectives or about alternative solutions.
- Single-objective optimization relies on a single objective function which is based on the chosen weights for the individual objectives. Thus the solution is dependent on the application of the different weights. Obtaining a good and relevant set of weights is not a trivial task.
- Single objective optimization techniques give only one optimal operating solution even if there may be other possible solutions.

The ability to identify a set of optimum solutions for a problem with conflicting objectives can be extremely useful in food processes design. It clarifies the trade-offs between several objectives and therefore it helps the decision maker to select different conditions suitable for the process. Different sets of optimal solutions might also indicate different process designs suitable for the product. It is therefore important in the optimization for food process design to consider a search for the Pareto front to obtain information about the trade-offs among objectives and possible range of operation strategies.

6. Thesis challenges and outline

Although food process design has a long history, product quality is still not often taken as the starting point for design. Most of the design procedures start with a given problem and by forward reasoning (process analysis approach) the design problem is solved in an iterative cycle. This thesis is dedicated to the development of procedures which allow to start the process design explicitly from the defined product qualities (process synthesis approach). The work concerns the following research questions:

1. Are the current conceptual design methodologies applicable for food process design?
2. How should one combine quantitative and qualitative knowledge on product qualities in a model?
3. Which contribution does dynamic optimization of transient processes give to quality driven food process design?
4. How should one deal with conflicting objectives in the process optimization and design?

For a motivated development of the methodology, we review first the applicability of the current process design methodologies for food production applications. **Chapter 2** contains a general description of relevant process design methodologies. The necessity and criteria of process design for food production systems are discussed. This chapter also provides the potential applicability of the Delft Design Matrix as framework of food process design

The central application in this thesis is a bakery production. **Chapter 3** concerns the development of a mathematical model to describe the transformations and quality development that occur during baking. It illustrates that white-box models on bakery production are only partly available in the literature and it investigates how this problem can be solved by using grey-box models. The purpose of the model is to describe the dominant mechanisms during the process, how the product changes with varying input variables, and it allows to rank different production methods with respect to the final product quality.

Once a model is available, it can be used to improve current processing routes and for finding possible solutions. **Chapter 4** studies the role of dynamic optimization to generate process alternatives. It explores the idea that once the final quality is set, the operation strategy can be determined by tools of process optimization. Furthermore, the optimization also reveals how a different product quality can be obtained by changing the operational procedures and properties of the starting material. The numerical solution method is a relevant component in optimization based process design. Therefore, as a side step, **Chapter 5** introduces an alternative method to the standard control vector parameterization method for dynamic optimization based on a stepwise refinement. To reduce the high computational effort for optimization, a refinement method can be useful. The proposed refinement method is based on sensitivity functions.

Chapter 6 explores the problem of multiple conflicting objectives. The application of multi-objective optimization helps to improve the range of operational strategies. The domain of conceivable product quality combinations is scanned by a single-objective function optimization to find a feasibility region, where operational conditions can be found that fully satisfy the quality criteria. It will also be shown that an alternative and more efficient method to obtain the edge of the feasibility domain is to use multi-objective optimization with varying weights. It is also investigated how a designer can extend the feasibility region by changing the properties of the starting materials and by changing the operational procedures.

Chapter 7 describes the parameter adjustment of the model prediction developed in Chapter 3. Some selected parameters in the heat - mass transfer and the quality models are tuned to match experimental findings. Baking experiments with constant and dynamic operations are performed to test the model, and it will turn out that the model gives good prediction of quality.

The last **Chapter 8** provides the conclusions and a view on future perspectives in this field

References

Balsa-Canto, E., Alonso, A.A. and Banga, J.R.(2002).A novel, efficient and reliable method for thermal process design and optimization. Part I: theory. *Journal of Food Engineering*, 52, 227–234

Banga,J.R. and Singh, R.P.(1994). Optimization of air drying of foods. *Journal of Food Engineering, 23*,189.

Banga, J.R., Saa,J. and Alonso, A.A. (1999). Model-Based Optimization of Microwave Heating of Bioproducts. *7th International Conference On Microwave And High Frequency Heating, Valencia, Spain.*

Banga, J. R., Pan. Z. and Singh, R. P. (2001). On the optimal control of contact-cooking processes. *Food and Bioproducts Processing* ,79(3),145-151

Banga, J.R., Balsa-Canto, E., Moles, C.G and Alonso, A.A. (2003). Improving Processing Using modern Optimization Methods. *Trends in Food Science and Technology,* 14, 131-144

Brenner, M. (2005). The Chain Information Model :A Systematic Approach for Food Product Development . *Thesis Wageningen University*, the Netherlands

Boss, E.A., Filho, R.M and de Toledo, E.C.V.(2004). Freeze drying process: real time model and optimization. *Chemical Engineering and Processing, 43(12),1475-1485*

Boxtel, A.J.B. van. (1994). Optimal operation policies in food processing. Developments in food Science 36: *Automatic Control of Food and Biological Processes*. Ed. J.J. Bimbenet, E. Dumoulin, G. Trystram. Elsevier 1994, 449-456.

Boxtel, A.J.B van , Otten, Z.E.H and Linden, H. J. L. J. van der. (1992).Dynamic optimization of a one-stage reverse-osmosis installation with respect to membrane fouling. *Journal of Membrane Science,* 65(3), 89-111.

Boxtel, A.J.B van, and Otten, Z.E.H. (1993). New strategies for economic optimal membrane fouling control based on dynamic optimization. *Desalination,* 90 (1-3), 363-377

Boxtel, A.J.B. van, and Knol, L. (1996). A preliminary study on strategies for optimal fluid-bed drying. *Drying Technology*, 14(3 and 4), 481-500.

Brosnan,T. and Sun, D.W. (2004). Improving quality inspection of food products by computer vision—a review. *Journal of Food Engineering*, 61 (1), 3–16.

Bruin,S. and Jongen, T.(2003). Food process engineering: the last 25 years and challenges ahead. *Compr. Rev. Food Sci. Food Saf.,* 2 , 42–81

Chalabi,Z.S., Van Willigenburg, L.G. and van Straten, G.(1999). Robust optimal Receding horizon of the thermal sterilization of canned foods. *Journal of Food Engineering*,40,207-218

Demirekler, P., Sumnu, G., and Sahin, S.(2004). Optimization of bread baking in a halogen lamp–microwave combination oven by response surface methodology. *European Food Research Technology*, 219,341-347

Diefes, H.A., Okos, M.R., and Morgan, M.T. (2000). Computer-aided process design using Food Operations Oriented Design System Block Library. *Journal of Food Engineering,* 46(2), 99-108

Doumpos, M., and Zopounidis, C.(2002). Multicriteria decision aid classification methods. *Applied Optimization*, 73, Kluwer Academic

Du, C.J. and Sun, D.W. (2006). Learning techniques used in computer vision for food quality evaluation: a review. *Journal of Food Engineering,* 72, 39-55

Fito, P., LeMaguer, M.L, Betoret, N. and Fito, P.J. (2007). Advanced food process engineering to model real foods and processes: The "SAFES" methodology. *Journal of Food Engineering*, 83(2), 173-185.

Gan, H.E., Karim,R., Muhammad, S.K.S., Bakar,J.A., Hashim, D.M., and Rahman,A.R. (2007). Optimization of the basic formulation of a traditional baked cassava cake using response surface methodology. *LWT - Food Science and Technology*, 40(4),611-618

García, M.-S. G., Balsa-Canto, E., Alonso , A. A. and Banga, J. R. (2006). Computing optimal operating policies for the food industry. *Journal of Food Engineering*, 74(1),13-23.

Ghazala, S and Aucoin, E.J. (1996). Optimization of pasteurization processes for a *sous vide* product in rectangular thin profile forms. *Journal of food quality* , 19 (3), 203–215.

Grievink, J. (2001). Delft Design Matrix for Conceptual Process Design. Delft University of Technology, Delft Internal Report

Grossman, I.E. (1996). Mixed-integer optimization techniques for algorithmic process synthesis. *Advances in Chemical Engineering,* 23, 171-246

Halsall-Whitney, H. and Thibault, J. (2006). Multi-objective optimization for chemical processes and controller design: Approximating and classifying the Pareto domain. *Computers and Chemical Engineering,* 30(6-7), 1155.

Holdsworth, S.D. (1997). Thermal processing of packaged foods. *Blakie Academic and Professional Publishers*, London.

Jadhav, N.Y., Stappen, M.L.M., Boom, R.M, Bierman, G., and Grievink, J. (2002). Mass Balance and Capacity Optimization in The Conceptual Design of Processes for Structured Products. *European symposium on Computer Aided Process Engineering-12,* 85-90

Karel,M. (1988). Optimizing the heat sensitive materials in concentration and drying. In S.Bruin(Ed), Pre-concentration and drying of food materials (pp 217-233). Amsterdam-Elsevier

King, C. J., Gantz, D. W and Barnes F. J. (1972). Systematic Evolutionary Process Synthesis. *Ind. Eng. Chem. Process Des. Develop.*,11 (2).

Kiranoudis,C.T. and Markatos,N.C.(2000). Pareto design of Conveyor-belt dryers. *Journal of food engineering,46,145-155*

Kleis ,D., and Sachs,E.W.(2000). Optimal Control of the sterilization of pre-packed foods. *SIAM journal on optimization*,10,1180-1195

Lewicki, P.P.(2006). Design of hot air drying for better foods. *Trends in Food Science and Technology* 17(4), 153-163

Luyten, H., Plijter, J.J, Van Vliet,T. (2004).Crispy/Crunchy Crusts Of Cellular Solid Foods: A Literature Review With Discussion. *Journal of Texture Studies*, 35 (5), 445-492

Miskhin, M., Saguy, I., and Karel, M. (1983). Dynamic Optimization of Dehydration Processes: Minimizing Browning in Dehydration of Potatoes. *Journal of Food Science*, 48, 1617-1621

Quirijns, E.J. (2006). Modeling and dynamic optimization of quality indicator profiles during drying. *PhD Dissertation Wageningen University*, *the Netherlands*

Siirola, J.J. (1996). Strategic Process Synthesis: Advances in the Hierarchical Approach. *Computer Chem Engineering,* 20, 1637-1643

Şumnu, G., Ndife, M.K, and Bayindirli,L.(2004). Optimization of microwave baking of model layer cakes. *European Food Research Technology,* 211(3), 169-174

Stigter, J.D., Scheerlinck, N., Nicolaï, B., Van Impe, J.F.(2001).Optimal heating strategies for a convection oven. *Journal of Food Engineering*, 48(4), 335-344

Van Donk, D.P.(2000).Customer-driven manufacturing in the food processing industry. *British Food Journal*, 102(10),739-747

Vincent, J.F.V. (1998). The quantification of crispness. *Journal of Science of Food and Agriculture,* 78, 162–168.

CHAPTER 2

Potential of Conceptual Design Methodology for Food Process Innovations

This Chapter has been accepted for publication as: Hadiyanto, G. van Straten, R.M. Boom, A.J.B van Boxtel and D.C. Esveld.(2007). Potenttial of Conceptual Design Methodology for Food Process Innovation. *Journal Food Science and Technology International*

Abstract

The available time span for food product and process innovation is steadily decreasing, and to increase the efficacy of the development cycles, systematic design procedures can to be used to redesign existing processes and to develop new processes. The Conceptual Process Design (CPD) methodologies used in chemical industry could also be meaningful in the food industry to rethink their systems and to break down the complexity of problems into several hierarchical levels. The Delft Design Matrix, a combination of the iterative design procedure, hierarchical decomposition and task driven methods, is a promising tool which can cover the different objectives and criteria of food design. This paper analyzes the potential applicability of Delft Design Matrix as a conceptual process design methodology for food process design and illustrates its functionality with the design of a bakery production system.

Keywords: Conceptual design, process design, bakery, Delft Design Matrix, baking.

1. Introduction

Innovation in process development is an essential instrument for the food industry to stand out from competitors and to fulfill market expectations (Menrad, 2004). Hutcheson and Ball (1995) pointed out that an industry can only be successful if it can readily translate market opportunities into process and product development. Once an industry has defined a new product based on an identified market opportunity, it comes down to the process designer to translate the processing and production needs of this specific product quickly into a tailored and efficient solution. This is the concept of market driven design (*top-down approach*) where consumer preferences in terms of product quality are considered as the starting point of design. On the other hand, process design is often based on the opportunities created by new technologies or changes in existing lines, which are explored to create new products. This is known as technology driven design (*bottom-up approach*). Meanwhile, the time frame available for process innovation in food industries has steadily decreased over last decades. Boom, Dekker and Esveld (2005) stated that to accomplish an innovation in a short time span, the development activities will increasingly rely on the use of current design methodologies. Next to new processes, it applies equally strong for the re-designing and rethinking of existing processes.

For design problems, a design framework is needed that helps i) to organize the information, ii) to break down the problem iii) and to aid the selection from different alternative solutions. Conceptual process design (CPD) is a methodology applicable in the early stage of (re-) design of production systems (Boom *et al.*, 2005) and to organize process development based on specified external needs (Li and Kraslawski, 2004). It has been reported that streamlining the design according a CPD approach could result in total cost savings of about 20-60% (Harmsen, 2004). The idea of CPD was initially developed in chemical engineering area from the basic design procedure which iterates over a synthesis and analysis phase to meet the specified criteria. Douglas (1988) introduced a way to decompose the overall layout of a process in a hierarchical organization, to find new configurations for series of unit operations. The classic iterative design cycle and decomposition methods are typically used in forward design fashion, driven by the experience with available technology. Siirola (1996) proposed a CPD- approach based on property differences between input and output streams. Product transformations which reduce the differences are defined to specify the operational units. This method is more inline with product oriented process design (market driven approach). Inspired on Douglas's (1988) and Siirola's (1996) approaches, the Delft Design Matrix (DDM) approach was developed to deal with complex design problems and to break it down into several levels (Grievink, 2001). With combination of iterative design cycle, decomposition and task driven methodologies, the Delft Design Matrix (DDM) gives more flexibility for food process innovation as either driven by technology or by market opportunity.

Even though design methodologies have been well established in chemical industries, the application of such methodologies is still limited in the food industries. The design of a food process has different challenges as compared to chemical processes. This is for a part due to the inherent complexity of foods and the limited detail understanding, but it also deals with the other criteria and the different design objectives that have to be realized. These aspects will be discussed in section 2.2 and 2.3. The objective of this paper is to present Delft Design Matrix (DDM) as a generic conceptual process design methodology and to analyze its potential applicability to food process design. The features of the methodology are illustrated with a design case for bakery production system.

2. Food Process Design

2.1. Overview of design methodology

A design methodology provides a framework for a systematic approach to the design problem. Despite the fact that use of conceptual process design methodologies have spread in chemical industries only a few studies deal with the conceptual process design in food industries. In fact, the design methods available at the moment are not directly useable for food design due to several aspect differences between chemical and food processes (see Table 1).

Table 1. Main discrepancies between chemical and food process design

Aspects	Chemical industry	Food industry
Model information	Mass and energy balances,	Mass and energy balances have no central position
	Product kinetics; quantitative relationships	Product transformation; qualitative knowledge
Objective for design	Product composition (*purity*), efficiency, energy and water savings etc	Product properties and quality (taste, texture, safety, appearance etc)
Flexibility requirements	Product diversity is low	Many products at one site
Product and process interaction	Separation of product and process knowledge possible	Integration is essential
Process structure	Recycle loops	Minimal recycle loops; typical one line production

The basic design activity which widely used in chemical engineering describes the activities in the reasoning process to find a suitable form from the required function (Roozenburg and Eekels, 1995). The main activities are to generate alternatives and to evaluate these to the specified criteria. The alternative generation activities are iterated when the configurations do not meet the criteria. However, such an overall iteration loop does not help to encompass the full complexity of the overall processes. Hence, extra selection criteria are required to deal with the complexity of the problem.

The hierarchical decomposition of process has been proposed by Douglas (1988). This approach concerns the arrangement of a series of unit operations (synthesis of flowsheets) and to find a recycle structure from specified input-output structure. Shortcut calculations (e.g. overall balances) to evaluate economic criteria are carried out at every stage of design (Li and Kraslawski, 2004). This design method has been well experienced in the industrial environment despite of its disadvantages that safety, health and environmental aspects are not considered and the method focuses mainly on economic improvement (Harmsen, 2004). The usefulness of the method is however limited when applied to food production, especially when final product properties are required as design criteria and when dealing with multi product lines (Meeuse, Grievink, Verheijen and Stappen, 1999; Jadhav, Stappen, Boom, Bierman and Grievink, 2002). In addition, Li and Kraslawaski (2004) pointed out that this methodology has a major limitation in a systematic handling of multi-objective issues.

Alternatively, Siirola (1996) introduced a task driven method. The method is based on property differences between initial state (raw materials) and the goal state (desired product). After defining the input-output structure the property differences between input and output are specified and tasks are determined based on heuristic rules to eliminate the property differences and to perform transformations. Harmsen (2004) pointed out that this method has advantages in a large of number of applications and the method encourages creativity, which results in an increased number of processes alternatives. However, this methodology is not applicable if the initial and goal states are ill-defined (Korevaar, 2004) and hence it is not suitable for an overall design framework.

A promising methodology has been proposed by Grievink (2001) who combines basic cycle, the hierarchical decomposition and the task driven method in one design framework: the Delft Design Matrix (Table 2a and 2b). The first horizontal level in the design matrix starts with gathering all information about the process by considering input and output properties as a black box model in level 1. The design boundary and all external information have to be identified during this first level. Subsequently in level 2, the process is decomposed into sub process blocks based on design criteria such as the product microstructure. At level 3, the required tasks and transformations of each block have to be determined. The operational units needed to fulfill these tasks and transformations are determined in level 4. Level 5 concentrates on the process integration with respect to energy consumption and effective use of materials by a proper combination of operational units. The design ends with equipment selection and design at level 6. Jadhav *et al.* (2002) partly employed this method to design a production line for structured products and stated that the disadvantage of Douglas's method to consider the product structure could be overcome. Each level has now a hierarchically limited design scope and can be accomplished by means of a seven step design cycle, for which the generic activities are summarized in table 2a (Grievink, 2001; van der Stappen, 2005). Step 2 and 6 are explicitly added to stimulate the information management during the design cycle, such that it is possible to trace back the assumptions and arguments that were used for the decision to either abandon or continue a certain approach.

Table 2a. Delft Design Matrix (Grievink, 2001)

Level \ Step	Scope of design	Knowledge of objects	Synthesis	Analysis	Evaluation	Reporting	Go/no go
I/O structure							
Generation of structure blocks,							
Transformations and tasks							
Operational unit							
Integration							
Equipment selection and design							

2. 2. Specific criteria in conceptual food process design

Criteria are essential to screen design alternatives in the conceptual design phase. The work can only progress to a higher level of design if the proposed solution meets design criteria; otherwise another route has to be considered. Unfortunately, some of the relevant criteria for food production system are difficult to predict and to apply which are notably: i) consumer appreciation, (ii) micro structure, (iii) food safety, and (iv) process flexibility.

Producing food with high quality is an obvious objective for food process design. The success of a design depends on the degree to which a product fits to the design specifications (Gilmore, 1974), and therefore product quality must be regarded as the starting point for process design. Therefore it is essential that the qualities are measurable and predictable. Food quality, however, is intrinsically linked to the appreciation of quality by the consumer and as such subjective. Quantification in descriptive quality attributes is only useful for design purpose if one has a notion how these attributes can be influenced. Therefore, it is essential to make links between quality experience and physical and/or chemical properties, while still experimental work is required to confirm the quality specification. The use of quality criteria can be more complicated if the consumer plays a role by finishing the product at home (*e.g* bake-off bread, dried soups).

Table 2b. Design steps in Delft Design Matrix

Step	Task	Description of activity
1	Scope of design	– Define system boundary – Identify constraints and criteria of system – Evaluate economic aspects – Evaluate the existing process and product
2	Knowledge of object	– identify all information for design space – identify the possibilities to manipulate design object
3	Synthesis.	– generate design alternatives
4	Analysis.	– analyze the alternatives – generate models for product transformations
5	Evaluation.	– Evaluate design alternatives with respect to external constraints and requirements like safety, process hygienic, environmental issues.
6	Reporting	– Report all information and use it for next level
7	Decision	– The propagated alternatives are selected for next design level. Constraints, targets and other information are also transferred to next level

Food products are not merely determined by their composition, which only gives limited information on physical state, but must be characterized also by its microstructure properties. Villadsen (1997) and Aguilera (2005) stated that the micro structure is a dominating feature when improving existing or designing new products. This important design criterion can be cumbersome to quantify and to specify. The detailed mechanism of structure generation is only sufficiently understood for a limited range of products, and the design will therefore heavily rely on heuristics of exiting unit processes.

Food safety and process hygiene are main issues in food process design. The product must be microbiologically safe and stable during the shelf life. Another aspect is the process hygiene and clean ability, which must minimize the risk of product contamination during production. Practical lay-out of food factories is highly determined by food safety concerns that put stringent restrictions on the order and type of operations that can be applied. Recycles are for instance not common in the food industry.

Large process facilities for (semi-final) bulk foods are just as dedicated and optimized as their chemical counterparts. In contrast, fast moving consumer foods are produced in smaller quantities and larger diversity. An important design criterion for those production systems is therefore the flexibility of the process to produce multiple final products with minimal switch-over procedures. Furthermore the process should incorporate enough flexibility to counteract the variability of the starting materials.

2.3 Different objectives in Food Process Design

The drive behind new developments in food process design is often a combination of market pull and technology push. Market pull urges the producer to provide desired products and consequently the redesign of process or products is started. This results in a product oriented process design. Technology push is the reverse of the previous principle in which the producer applies a technology concept and to ultimately introduce a new product into the market. There are considerable differences in starting point. Process development might be based on the existing process, which is modified to satisfy the changed design objectives. In other cases, a new production line is aimed for an existing product, or starts with both a new production process for a new class of products. These differences in objectives are important for the work flow in the design. Based on the different demands, the challenge or objective for the design strategy is categorized in Table 3.

Designs of category A are based on the re-evaluation of existing systems. The design objective is to improve the performance of an existing process while the product is retained. The current system is analyzed and optimized with respect to well known criteria. For such well-defined design problems, formal optimization strategies can be applied. Balsa-Canto, Alonso and Banga, (2002) showed this for a thermal (sterilization) process design and Stigter, Scheerlinck, Nicolaï, and Impe (2001) demonstrated a case for optimal heating of convection ovens. However, due to their mathematical formulation, these design technologies are rarely applied by food process designers.

Category B designs deal with the production of new products in an existing production system. The challenge for the designer is to manipulate the ingredients and process conditions in such a way that the new quality attribute is obtained. An example is the design of low-calorie syrup (Manzocco and Nicoli, 2003). Once the main attributes of the target product are known, the potential ingredients are selected from the specific criteria. Due to ingredient change, the processing conditions are adapted to cope with the colour, texture, and taste.

Table 3. Objectives and requirements for food process design

		Reference		Drive			
Category	**Objective**	**Product**	**Process**	**Technology push**	**Market driven**	**Reduction of processing costs**	**Product improvement**
A	Optimizing efficiency of production	Existing	Existing	••	•	•••	•
B	Adaptation for product diversity	Variation	Existing	•	•••	•	•••
C	Change of unit operation	Existing	Existing	••	•	••	•••
D	New process for existing product	Existing	New	••	••	•	•••
E	New process to enable new product	New	New	•••	••	•	•

The number of dots (•) indicates the relative weight of different arguments that drive the design.

The objective of category C designs is to redesign of unit operations in existing systems. The main goal is to produce an existing product in a more efficient way (e.g. shorter production time) by introducing new technology. The work of Ferrari *et al.* (2003) on the redesign of Mozarella cheese production is typical example for this category. The aimed reduction of water used and processing time formed a well defined problem and the scope of design was limited to a bounded part of the production. Rethinking of the primary process tasks and integrating several unit processes resulted in a new extrusion process. A problem with radical new processes for existing products is that the product quality criteria are frequently based on the old process, and cannot be exactly mimicked by the new process. This is especially true for artisan type products and less a problem for half and bulk products such as pizza cheese as in the fore mentioned case.

The fourth category (D) concerns the development of a whole new production line for an existing product. Diefes, Okos, and Morgan (2000) reported a process development in milk powder production with minimal energy use and high vitamin content as criteria. To realize the aimed product, alternative process configurations are introduced and then evaluated with respect to the specified criteria. The work of Jadhav *et al.* (2002) and Meeuse *et al.* (1999) follows this line as well. Here, for dressing and mayonnaise products, several alternative mixing configurations were introduced and evaluated on flowability and cleanability. The design criteria were furthermore extended to production scheduling and overall plant performance.

The most complex design category (E) requires a new processing concept to produce a new class of products, for example, the production of structured vegetable proteins as a meat alternative. The design faces many open questions due the lack of prior process and product experience and must go for a sequence of trial productions and up-scaling steps. If the production route is not yet available from previous experiences, the use of make-ends-meet design methodology can be very helpful to unravel the problem at hand in terms of transformations and process tasks. From such a level of abstraction it is only possible to proceed further if one has prior knowledge about a mechanism that can fulfil the crucial step, e.g. for protein fibrilization this could for instance be freeze alignment. Therefore, such developments are often triggered by a technological break-trough and are very difficult to enforce from a perceived market need. An example is the development of Danish feta. A new cheese making technique by ultrafiltration, instead of coagulation and pressing, could produce a white, neutral and fairly structure-less cheese. It was only later developed as a kind of feta cheese, and not the other way around in the sense that the quality criteria of feta cheese stood at the basis of the technology development.

3. Delft Design Matrix for bakery production system

The basic implementation of the Delft Design Matrix (DDM) relies in the decomposition of the design problem in hierarchical levels. Its generic nature does practically imply that the level with main focus during the design can vary widely, depending on the previously categorized design objectives. This section discusses these levels of DDM methodology and their interpretation illustrated with the design of a bakery production system.

Illustration example: The design aims a single baking facility near the point of sale. It should be able to produce different kind of bakery products, such as bread, biscuit, cake etc, in a short sequential order on the same line (Figure 1). Traditionally, baking technology is optimized to specific product ranges, which however show great similarity in ingredients. The differences in size and final product attributes (structure, volume, crispness, softness and colour) are reflected in the different optimal handling and process conditions. Since different products are now aimed to reside simultaneously in the same process, it requires an extra flexibility beyond the conventional hot air oven. The objective is an example of design category D, since it initially considers the whole line, but will be reduced to single unit process design problem (C), after decomposition in level 2, where it is argued to separately design the dough preparation and shaping step.

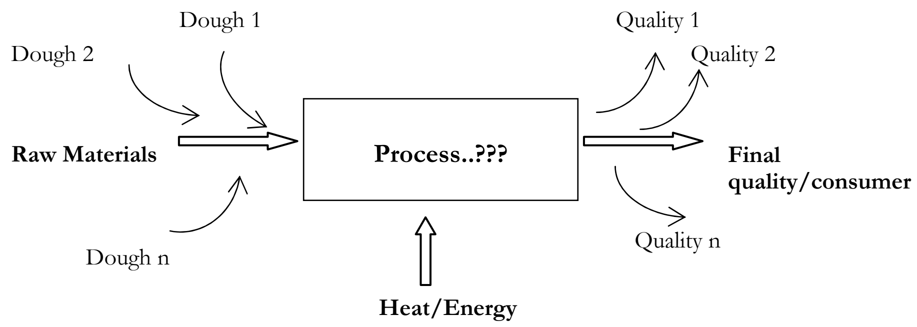


Figure 1. Illustration of bakery design problem. Design is purposed to find the operation strategy to handle multi products.

Level 1: Input-Output definition

This level is essential for all design categories A-E as it concerns the embedment and relevance of the process for the whole plant or business performance (van der Stappen, 2005). The design problem is considered with respect to the overall process performance (process efficiency, effective time, flows), product formulation (quality, safety, stability) and external boundary (market opportunity, life time span). At this level, the details of the actual process are not relevant, since we focus on the boundary of the system and the interaction with the environment. Despite its obvious character, this level is easily taken for granted by technical specialists, assuming that the constraints which play such a steering role in the design are thoroughly analyzed.

The central activity in this level is to determine the overall scope of design and hence it determines also what should be and be not considered. Depending on the requirements, many food process designs start from an existing process with a well-defined problem. A pragmatic approach is to focus and limit the design directly on the key unit operations where the problem arises; it also limits the degree of freedom to generate process alternatives. When the scope of the design is broadened, more opportunities arise which inevitably also increases the complexity of the overall design task.

Illustration: In this level, the scope of design is decided only for production system (Figure 1). The external boundary that we considered is only consumer which gives criteria for final goal of product quality.

Table 4. Key design parameters in Level 1.

Design decisions	Description
Input	
- Raw Materials	Water, Flour, Sugar, Protein, Fat
- Possible Energy	-Convection oven
	-Radiation
	-Microwave
Output :	
- Product Quality	- Crispness
	- Softness
	- Volume (size)
	- Crumb
	- Brownness
	- Staled product
- Type of products	*Crumb*: cake, croissant, wholemeal rusk, toast, wholemeal bread, rye bread, eqq cake, luxury white bun, *knackebrod*, wheat bread, white water bread, ginger bread, cake, white milk bread.
	No crumb: biscuit, cookie, cracker, spiced biscuit, *krakeling*, bastogne cookie
- Single production line	No recycle stream
- Temperature of product	25^{o}C

For this design, 18 local Dutch bakery products are taken as design examples. The design requires information of raw materials and product specification in terms of functionality, quality and composition. We considered that each product is composed from similarity ingredients: water, flour, sugars, fat, and protein, and the data of composition of each ingredient can be observed from literature study. The role of each ingredient in the product formation has been intensively described (see description of Giannou, Kessoglou and Tzia**,** 2003). In addition, most of bakery products are valuated based on quality: colour, texture, softness, crispness, and size as product specification. Products are also characterized by structure properties i.e. products with crumb properties as bread, cake, toast, croissant, etc, and products without crumb properties as biscuits, crackers, cookies, etc. Quality is the most important design criterion since it determines the value of the product and also as indication of consumer preferences.

Table 4 depicts the example of design decision of Level 1. The input of bakery system is specified as energy and raw materials. The raw materials of bakery products are water, flour as source of starch and gluten protein, fat and sugar. The potential heating sources are convection, microwave and radiation. The convection oven has been widely used in bakery production to induce browning and crust formation. Microwave and radiation energy will be adapted to increase the process flexibilities, i.e. saving processing time. The combination of these heating inputs may give better operation.

Level 2 Generating block structure

In level 2 the I/O structure from level 1 is decomposed into sub-blocks. The objective of the decomposition is to simplify the design problem, to systematically develop a list of process configurations and to reduce the complexity during calculations (Douglas, 1988; Jadhav *et al.,* 2002). Douglas (1988) suggested that the decomposition should not be directly on the level of a small subsystem, i.e. unit operations, since that would hamper the formulation of process alternatives which are not based on these unit processes. Optimization of small subsystems will yield a sub optimal solution for the design, while on the other hand too large blocks, can not be handled efficiently in a design. We propose several criteria, listed in Table 5, which can be used to mediate the decomposition of the design space.

The design space seems obviously limited to that part of the production chain that is under the control of the designer. In the broader context of the total food production system, different actors will play different roles. For example, actor's chain can be divided into: raw materials supplier, multiple producers which converts the raw materials into (half) products, retailers and consumer, who takes the final decision in the quality examination. These actors have links and influence each other in the overall production system.

For processes with different product flows, the decomposition can be further guided by the process topology. For example to produce a filled product, there are two streams i.e. the filling stream and the main product stream. A single production line can be decomposed into different blocks based on process time. It is obvious to split for instance a fast heating process and long storage process into two different blocks.

Table 5. Criteria for structure block decomposition

Criteria	**Description and example for bakery cases**
Actor in chain	The production process is decomposed into blocks that have an independent role in the product development.
Topology (branch)	The process is decomposed into distinct material streams
Time of process	Blocks are based on the time scale of the process
Quality specification	Decomposition is driven by distinct quality blocks.
Structure and phase	The structure of product either micro or macro is considered as different design block. Phases as solid, liquids and gas are also considered as criteria in the decomposition.

Product quality can function as a criterion for decomposition, in the sense that it is not meaningful to split a process into individual blocks when quality criteria at intermediate points are not clearly defined. For example, for bakery products, quality criteria brownness, texture, crumb formation, volume expansion and microbial growth can only be assessed at the end of the cooling process.

Structure and phase decomposition are important criteria for the block decomposition of structured products (Meeuse *et al.,* 1999; Jadhav *et al.,* 2002). The decomposition follows not only from the phases in the product: solid, liquid and gas, but notably from the changes microstructure, such as powders, emulsions, foams, gels etc. Formation and break-down of product structure are transformations and they are often irreversible and put large constrains on the admissible order of the process blocks.

Illustration: An example of this level regarding to bakery products is shown by Figure 2. The total production chain can be seen as an obvious sequence of steps: ingredient manufacturing, dough preparation, product shaping, heating, cooling, retail and consumption. The baking and subsequent retail must be within the owner actor space, given the ‘fresh made at point of sale’ concept. The process topology is a single line, except that the shaping is very product specific, which forms a suitable break point.

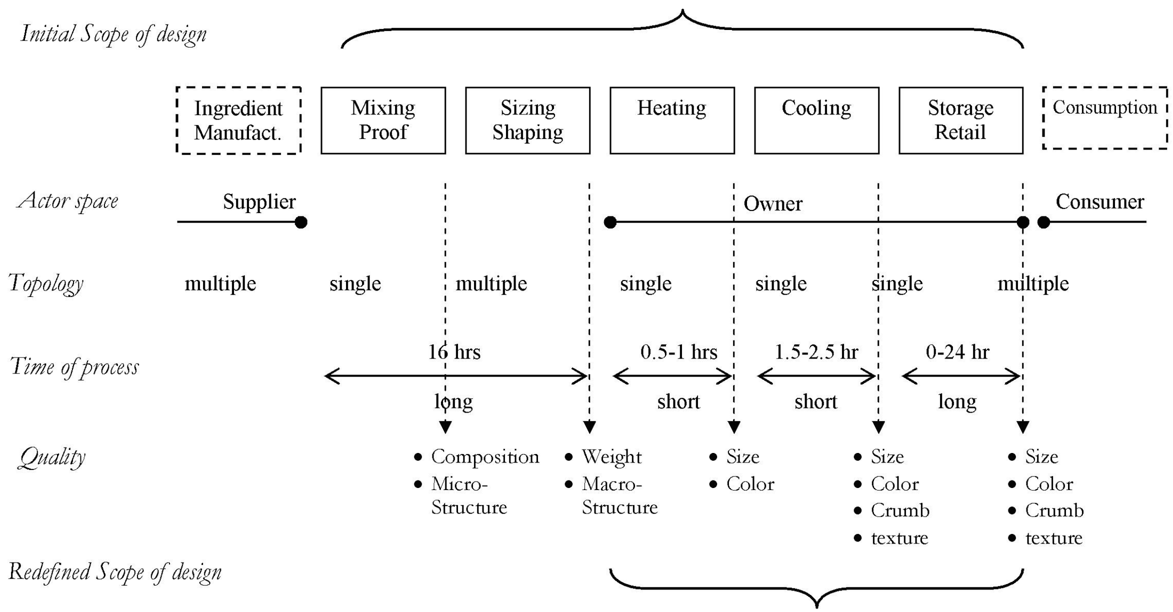


Figure 2. Process decomposition from input-output of total supply chain into small blocks based on criteria specified in Table 5.

Based on the criteria time of process, preparation which consists of kneading, proofing and fermentation require at least 16 hrs (Kannan and Boei, 2003), while time of heating and cooling is about 2.5-3 hrs, and intended retail within a day. The decomposition based on quality shows that the most quality are formed in the heating and cooling. Quality as result of preparation block: size and initial structure; heating and cooling block: colour, size, crumb, softness and crispness. Quality of softness, crispness, and crumb is difficult to be determined after heating block and it should be evaluated after product temperature reach room temperature. In the storage block, it is observed that only small changes occur. From these decompositions, we further decide that the design is focused in the heating and cooling as the most important for quality formation, and that the activities before heating are outside now reduced design scope.

Level 3. Define transformations and tasks for each design block

The activity of this level is to identify the transformations involved in the conversion from input to output properties for each specified product quality. This level involves rethinking of the system via the reverse engineering concept (Boom *et al.*, 2005) were questions like: "how relate the structural compounds to the required attributes?" and "what is the relationship between the composition and the structure?" etc., have to be encountered. Product changes must be analyzed and understood in terms of physical and chemical transformations. Often, there are multiple ways to achieve a transformation, which can be translated into alternative designs and process conditions.

The list of transformations must be augmented with the factors that influence their occurrence and kinetics. Water transport or enthalpy changes highly influence other transformations that occur in foods (coloring, microbial, texture formation). Structure compounds as carbohydrates, proteins and fats appear in several phases or states depending on the temperature and water content. State diagrams of relevant compounds can be versatile tools to map the transformation routes as a function of temperature and composition, and are becoming increasingly important in food technology (Bruin, 1999).

To analyze the time dependency of the transformations, quantitative kinetic and process models are required. For food products it is generally not feasible to construct models with a level of detail as encountered in chemical engineering. Published models are mostly very product specific and valid for a limited range of process conditions. Moreover, they tend to concentrate on either mass and heat transfer or on models on the product transformations without the complication of transport phenomena. The translation of the mechanistic understanding obtained in this level to a quantitative concept design as is done in chemical engineering is only partly possible. However, the achieved understanding and analysis will create a solid basis for a targeted experimental program.

Table 6 Summary of quality related transformations and tasks in Level 3

Design decision	Description/transformation	Task	Required function
1. Scope	Determining physical and chemical task/transformation for specified quality in each design block		
2. Main parameter	Starch is most dominant factor for texture formation		
3. Quality			
- Brownness	Caused by Maillard Reaction($T<150^oC$) and Caramelization ($T>150^oC$)	Heating	$f(a_w,T)$
- Volume	Increased dough size (Gas expansion) Structure change	Heating	$f(\Delta P)$
- Structure (crumb or crust)	Change of moisture content, changing phase of starch (*gelatinization*)	Heating	$f(W,T_g, Z, \alpha)$
- Texture (Softness, crispiness)	Change of moisture content, changing phase of starch (*recrystallization*)	Cooling Heating	$f(W,T_g, \alpha)$
- Staling	Starch recrystallization	Cooling	$f(W,T_m,T_g, \alpha)$
4. Model	To predict quality and dynamic changes of quality and transformation	Heat and Mass transfer, Model of transformation	

Note: W is water content, Z starch composition, T_g glass transition temperature, T_m melting temperature, ΔP pressure differences, a_w water activity, α degree of gelatinization

Figure 3 shows the output for level 3 in a quality mapping for the texture of bakery products as function of gelatinization degree (α) and glass transition temperature (T_g). Crispness and softness are a function of glass transition temperature and degree of starch gelatinization during the process. The diagram shows that a product is soft when the degree of gelatinization is higher than 0.3 where it is in the rubbery state. In contrast, crispy products are achieved when below glass transition temperature, which means that the products are in the glass state. These products are more stable than soft products. Another region (stale) concerns products with low degree of starch gelatinization while and above glass transition temperature. This situation arises when baked product are stored at temperatures where starch recrystallizes due to retrogradation.

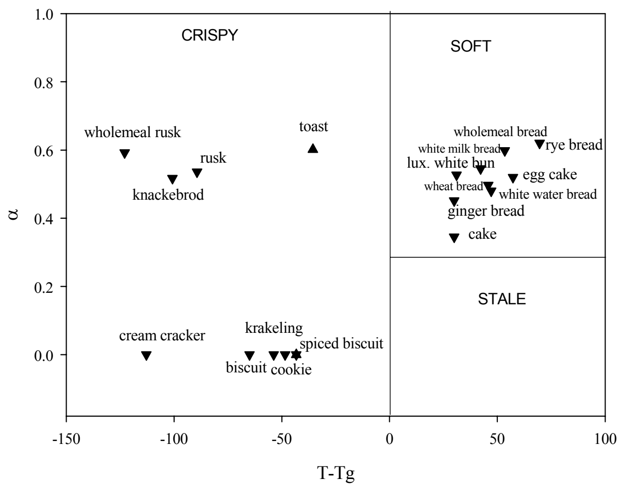


Figure 3. Texture quality of bakery products is represented as a function of the degree of starch gelatinization (α) and the difference between product temperature (T) and glass temperature (T_g).

Level 4: Unit Operations

Here the information of design decisions in level 3 is used to translate tasks and transformations into unit operations. From the models (heat and mass balances, state transformation and quality model) obtained in previous level, the design objective should be achieved by using optimization tools to choose the optimum operational unit. In this level the mode of operation (batch or continuous) is also defined. In conceptual food process design, the actual arrangement of unit operations ideally follows from the determined overall optimal operation strategy. The optimization procedure is performed to search design alternative and to determine optimum operation strategy in the unit operation. From optimal input trajectories, the decision of selecting type of unit operation and processing time can be realized.

Illustration: In this case, we considered production of 3 different types of products: bread type, biscuit type and cake type for 2.5 hrs of processing time. These products are different in terms of composition and quality attributes. Bread type products are soft and higher brownness, cake type are soft and less brownness, while biscuit type products are crispy and higher brownness.

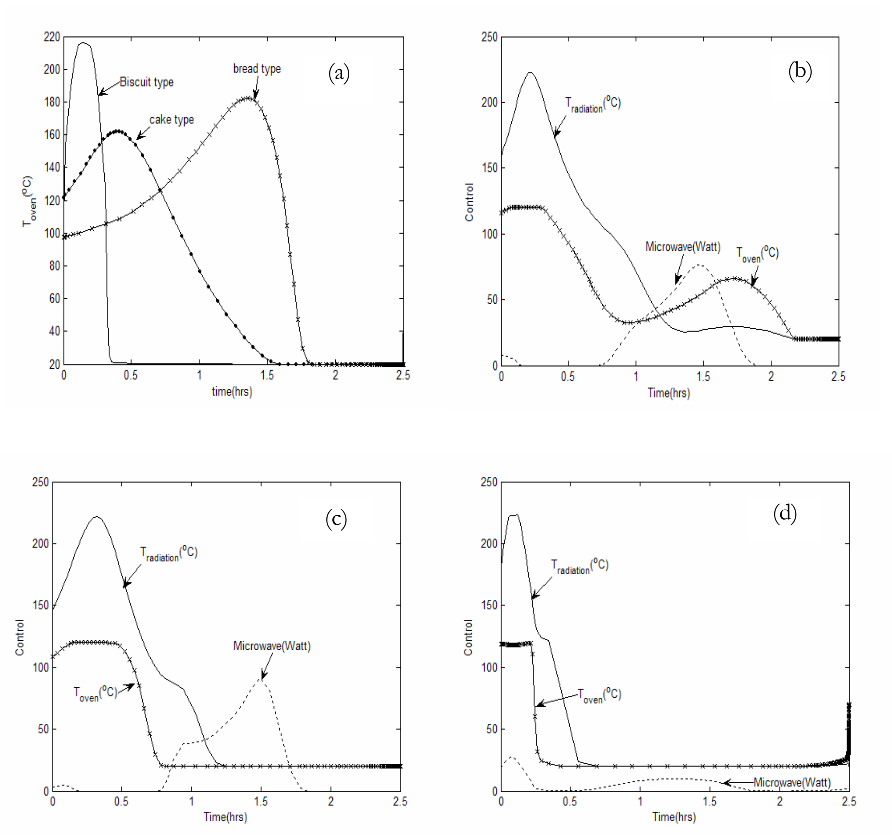


Figure 4. Optimization result for three different product qualities. (a) Input trajectories of external temperature, (b) Optimal multi-heating inputs for bread-type products, (c) Optimal multi-heating inputs for cake-type products, and (d) Optimal multi-heating inputs for biscuit-type products

Figure 4a shows the convective heating trajectories for the three products. The figure shows that the heating procedures strongly differ for the distinct final product quality criteria. For bread products a longer period of heating is required, while the biscuits products need shorter time of heating due to low water content and smaller size of products.

Combined heating inputs increase the process flexibility and improve the process with respect to the interior quality. Figure 4b, c, d show the optimal heating inputs for a combination of convective, radiation and microwave heating for three different products. To reduce the intensity of convective heating upper bounds of convective heating were set at 120°C, while radiation and microwave heating are applied to increase the flexibility. Figure 4b shows that bread type products can be successfully produced by combining the heating inputs. It suggests that there are two heating phases: i) 1 hour with radiation and convective heating ii) then 1.2 hour for convective and microwave heating. The similar heating profiles were found for cake products (Fig 4c). For the biscuit-type of products (Figure 4d), the process has a heating phase with convective and radiation heating only, which originates from the lower water content of the dough and the smaller size of products.

Level 5: Integration.

This level concerns the integration of unit operations for heat and water streams. For the chemical industry the objective of this level is to minimize the use of water and energy and in this level the recycle structure is developed. Most food production systems are sequential processes where product recycling has a minor role or is avoided to limit contamination risks. Recycles for utility flows (energy, water) recycles can be relevant. For conceptual design of bakery systems, we concluded that the integration of heat and water streams is not very crucial and therefore we did not pay further attention for this level.

Level 6: Equipment selection and design

The design proceeds with the details of equipment selection and design. As a matter of fact this step is central in process engineering where draft sketches are made and the way how to produce is fixed. However, the activities in this phase gradually shift away from the conceptual design of a production system. Nevertheless, it is often required, even in a conceptual phase, to proceed up to here in order to judge the feasibility of the concept.

Illustration: On basis of the optimal input trajectories of Level 4, we can make a translation to equipment design (Figure 5). It is possible to process the different products in a single 2 zones continuous oven with residence time of the zones of 1 hrs and 1.2 hour respectively. After zone 2, the cooling period is applied for 0.5 hrs. Each zone has a fixed air temperature, while the product specific local heating conditions are controlled by IR radiation in the first, and microwave energy in the second stage.

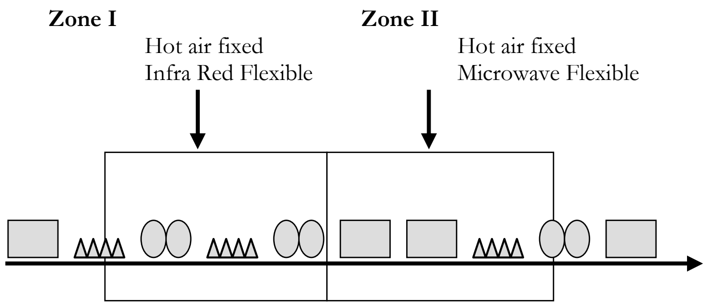


Figure 5. Translation of heating strategies into possible process equipment. The different shapes represent different bakery products

4. Conclusion and remarks

The changing tendency from a steady to opportunity driven market has reduced the life cycle of food products and forces the food industry to introduce more frequently new products. Therefore food production systems must be improved to follow rapid changes in product specifications. Conceptual process design as design framework is considered to be the main step in the generation of new solutions.

From the approaches for conceptual process design that are emerging in chemical engineering, notably the Delft Design Matrix is more preferably for food production systems (shown by bakery illustration). It allows the decomposition of the problem in blocks and reduces the complexity. It has a potential strong point for food production design by a reverse engineering step to find the logical transformations to form the aimed product properties.

Further development of the DDM can be helpful in creative mapping of potential design solutions. Reverse-engineering attempts to transform product quality to the required variables and transformations. Product quality as the main criterion for food process design is important as it can ultimately represent the consumer satisfaction and thus the success of design.

A systematic procedure organizes the workflow during process design and is essential to make the design process more efficient and less time consuming. The design procedure can be started from different points; existing processes and products or for really new products and processes. Depending on the design objective and the starting point, the focus is concentrated on different levels in the DDM methodology.

Acknowledgment

This research has been financially supported by VLAG Graduate School, The Netherlands. The authors would like to acknowledge the efforts of Prof J Grievink from Process System Engineering Group, Delft Technology University who gave valuable suggestion during personal communication and discussion.

References

Aguilera, J.M. (2005). Why food microstructure?. *Journal of Food Engineering ,67, 3–11*

Balsa-Canto, E., Alonso, A. A., and Banga, J.R. (2002). A novel, efficient and reliable method for thermal process design and optimization. Part I: Theory. *Journal of Food Engineering,* 52(3), 227-234

Boom, R.M., Dekker, M., and Esveld, D.C. (2005). Food production: trends in system innovation. In W.M.F. Jongen and M.T.G. Meulenberg (Eds.), *Innovation in Agri-Food systems. Product quality and consumer acceptance* (pp. 173-202). Wageningen: Wageningen Academic Publishers.

Bruin, S. (1999). Phase Equilibria for food product and process design. *Fluid Phase Equilibria, 158,* 657-671

Cuq, B., Abecassis,J. and Guilbert,S. (2003). State diagrams to help describe wheat bread processing. *International Journal of Food Science and Technology,* 28(7),759

Diefes, H.A., Okos, M.R., and Morgan, M.T. (2000). Computer-aided process design using Food Operations Oriented Design System Block Library. *Journal of Food Engineering,* 46(2), 99-108

Douglas,J.M. (1988). Conceptual Design of Chemical Processes, Mc *Graw Hill, New York*

Ferrari, E., Gamberi, M., Manzini, R., Pareschi, A., Persona, A., and Regattieri, A. (2003). Redesign of the Mozzarella cheese production process through development of a micro-forming and stretching extruder system. *Journal of Food Engineering*, *59(1),* 13-23.

Fryer, P. (1994). Mathematical Models in Food Processing. *Chem Ind-London, 13,* 515-518.

Gilmore, H.L. (1974). Product Conformance Cost. *Quality progress June* 1974

Giannou, V., Kessoglou,V., and Tzia, C. (2003). Quality and safety characteristics of bread made from frozen dough. *Trends in Food Science and Technology,* 14 (3), 99–108

Grievink, J., (2001). Delft Design Matrix for Conceptual Process Design. Delft University of Technology, Delft Internal Report

Hadiyanto, Asselman, A., van Straten, G., Boom, R.M., Esveld, D.C. and Boxtel, A.J.B. van. (2007). Quality Prediction of bakery products in the initial phase of process design. *Innovative Food Science and Emerging Technologies*, 8(2), 285-298

Harmsen, G.J. (2004). Industrial best practices of conceptual process design. *Chemical Engineering and Processing*, 43(5), 671-675

Hutcheson, P., and Ball, D.F. (1995). Innovation in process plant: A case study of ethylene. *Journal of Product Innovation Management,* 12(5), 415-430

Jadhav, N.Y., Stappen, M.L.M., Boom, R.M, Bierman, G., and Grievink, J. (2002). Mass Balance and Capacity Optimisation in The Conceptual Design of Processes for Structured Products. *European symposium on Computer Aided Process Engineering-12,* p. 85-90

Kannan, R., and Boie, W. (2003). Energy management practices in SME: case study of a bakery in Germany. *Energy Conversion Management*, 44, 945–959.

Korevaar, G. (2004). Sustainable Chemical Process and Products: New Design Methodology and Design Tools, Eburon, Delft

Li, X., and Kraslawski, A. (2004). Conceptual process synthesis: past and future. *Chemical Engineering and Processing,* 43(5), 583-594

Manzocco, L., and Nicolai, M.C. (2002). Food design: from the methodological approach to the case study of low-calorie syrups. *Trends in Food Science and Technology.* 13, 422-429

Meeuse, F.M., Grievink, J., Verheijen, P.J.T., and Stappen, M.L.M. van der. (1999). Conceptual Design of Processes for Structured Products, *Conference Foundations of Computer Aided Process Design*, Breckenridge

Menrad, K. (2004). Innovations in the food industry in Germany. *Research Policy.* 33, 845-878

Nishida, N., Stephanopoulos, G., and Westerberg, A. (198l). A Review of Process Synthesis. *AIChE Journal,* 27(3), 321-350.

Otto, K.N., and Wood K.L. (1998). Product Evolution: A Reverse Engineering and Redesign Methodology. *Research in Engineering Design,* 10,226-243

Roozenburg, H.J.H, and Eekels,J.(1995). Product Design-Fundamentals and Methods. Wiley and Sons, Chichester, England.

Siirola, J.J. (1996). Strategic Process Synthesis: Advances in the Hierarchical Approach. *Computer Chem Engineering*, 20, 1637-1643

Stappen, M. van der. (2005). Process Synthesis Methodology for Structured (Food) Products. *NPT Processtechnologie 6,* pp: 22-24

Stigter, J.D., Scheerlinck, N., Nicolai, B., and Impe, J.F. van. (2001). Optimal heating strategies for a convection oven. *Journal of Food Engineering*, 48(4) , 335-344

Ternstrom, A., Lindberg, A.M., and Molin, G. (1993). Classification of the spoilage flora of raw and pasteurized bovine milk with special reference to Pseudomonas and Bacillus. *Journal of Applied Bacteriology*, 75, 25–34.

Villadsen, J. (1997). Putting structure into chemical engineering. *Chemical Engineering Science,* 17, 2857–2864

Zhang, J. and Datta, A.K. (2006). Mathematical modeling of bread baking process. *Journal of Food Engineering*, 75(1), 78-89

CHAPTER 3

Quality Prediction of Bakery Products in the Initial Phase of Process Design

This Chapter has been published as: Hadiyanto, A. Asselman, G. van Straten, R.M. Boom, D.C. Esveld and A.J.B van Boxtel. (2007). Quality Prediction of Bakery Poducts in the Initial Phase of Process Design. *Journal Innovative Food Science and Emerging Technology, 8(2),285-298*

Abstract

The development of food production processes is facilitated by tools which explore the interaction between process design, operation conditions and product characteristics. In this work an approach how to set-up a simulation model is presented for the phenomena and transformations which occur during baking and which fix the product quality. The simulation model has three consecutive parts: mass and heat transport in the product, transformations concerning starch state transition and color, and the formation of quality attributes (color, softness, crispness and staling). The model for mass and heat transfer is based on laws of conservation and expressed in partial differential equations for spatial products. The starch state transition and color formation are a mixture of qualitative and quantitative information, while the product quality model is mainly based on qualitative information. The model is applied to three bakery products: bread, biscuit and a cake-type. The results show that the model estimates the product quality and its transformations as a function of dough composition, baking and storage condition. The results fit well to observed changes of properties and product quality during baking.

Keywords: baking; heat mass transfer; product quality prediction

1. Introduction

Nowadays, the life cycle of products in the food industry decreases and new or modified products are more frequently introduced to the market. As a consequence, the period for product and process development becomes shorter. Modification of old products or introduction of new products starts by making an inventory of desired product quality. Next, a feasibility study defines the main concept of the product and a global design for the production system. The feasibility phase allows creativity to explore several directions and searching for different alternative solutions. To be efficient in the feasibility phase a systematic working procedure is necessary. In the chemical industry the working procedures are supported by conceptual process design methodologies (CPD). This methodology is used in the chemical industry to find a description for the production plant through the following activities: arrangement of unit operations, routings of product and energy, the estimation of required process conditions, the composition of the streams and the required energy (Douglas, 1988, Siirola, 1996 and Wibowo and Ng Ka, 2001). These procedures extensively rely on process models for the analysis, evaluation and prediction of the physical state of the product.

There are some examples of the use of models in the food equivalent of conceptual process design. Bruin (1999) showed the importance of the phase diagram for food product and process design and Diefes, Okos, and Morgan (2000) performed the design of a milk powder production plant by ranking of process alternatives based on flow sheet calculations in order to achieve high product quality (safety) with low energy costs. In this case, besides mass and energy balances, the kinetics for microbial growth and vitamin degradation were used to predict quality. Wibowo and Ng Ka (2001) used properties of the most important ingredients as a starting point of designing creams and paste products. Here models were used to evaluate the rheological properties of the products. Meeuse, Grievienk, Verheijen, and vander Stappen (2001) and Jadhav, van der Stappen, Boom, Bierman, and Grievink (2002) worked on a mixing process for mayonnaise. The final product is composed of three different components, and models are used to estimate the final composition after the mixing process.

The requirements for models used in the initial phase of process design for the food examples above, however, differ from chemical industry. The difference is that the information about formation of food products is based on the knowledge domain of the designer and mostly not defined in quantitative relations. Fryer (1994) emphasizes that lack of information and the qualitative character complicates product and process design for foods. Other reasons for the complexity are the simultaneous occurrence of product transformations and the subjectivity of food product quality due to consumer preferences. Therefore, specifying product quality attributes, translating these into a quantitative model and making a link with the process are the main challenges for food process design.

The bakery industry is considered as an example of a strongly experience based sector where the products have a long history but modification of existing products is still important. Due to the experience-based character of the industry only limited information is captured in models. So, for this sector, it is paramount to have a solution dealing with limited information for quick product and process design. For example during baking gelatinization which is essential for crumb and crust formation, occurs simultaneously with volume changes due to gas expansion. Part of the available knowledge of these transformations is given in well defined models as heat and mass transfer relations; the others appear as qualitative descriptions (for example softness and crispness of product). Bakery products are also judged on their colour, which is result of reactions that occur during baking due to heating. The components involved in these reactions are known, but the correlations of these reactions with temperature and water activity are not yet fully described. Furthermore, bakery products are spatial products in which temperature and water gradients arise during baking. As a consequence texture and colour properties depend on the position in the product. Because in product valuation consumers make distinction between parts of the product (e.g. crisp on the edge and soft in the center) spatial temperature and water models are needed for prediction of local texture and colour.

The objective of this paper is to present a systematic approach, which captures the most dominant physical phenomena and product transformation during baking. In this approach modelling the interconnection between input, heat and mass transfer, product transformation and product quality attributes represents the total behaviour of the product. The final model is used to simulate and to explore product quality in the early phase of process design. The simulation shows how product attributes are modified by changing the initial composition and process variables during baking and allows the ranking of different processing alternatives.

2. System description of baking

Bakery production concerns a series of processing steps such as mixing, baking, cooling and storage during which a number of product transformations take place. Baking is the central process in bakery production and here quality such as size extension, brownness; texture and flavor are formed due to consequence of physical and chemical changes in the product (Sablani, Marcotte, Baik and Castaigne, 1998). During baking, transformations, which depend on the course of water content and temperature, are decisive for the final product quality (Thorvaldson and Janestad, 1999). These transformations are coupled and influence each other (Zhang and Datta, 2006).

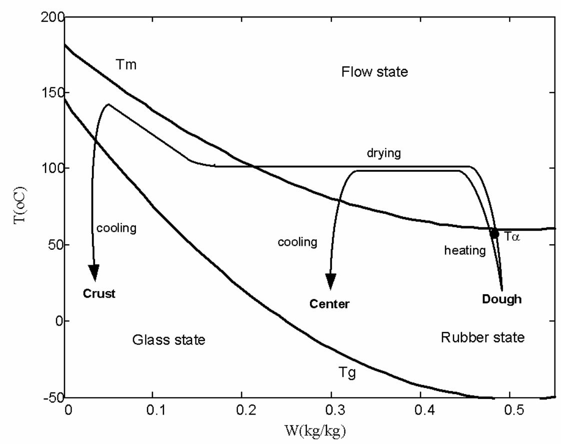


Figure 1. Schematic state diagram during bread baking. T_m is melting temperature for starch. The glass transition temperatures (T_g) for protein and starch. T_α is the gelatinization temperature for starch. The arrows present the courses of the center and crust of a product during baking

The most dominant phase transitions in bakery product are the starch gelatinization, protein denaturation, the water evaporation, starch retrogradation, water crystallization and glass transition. The phase transition temperatures are dependent on the composition; especially on the water content but are also influenced by other small molecules which significantly alter the water activity. However, they are relatively insensitive to changes in protein and lipid composition as long as they form minor components. Figure 1 shows the several transition temperatures for starch as a function the water content (derived from Farhat, Blanchard, Descamps and Mitchell (2000) with sugar content as in wheat bread). Such state diagrams, as introduced by Levine and Slade (1990), are increasingly used in structured product design as a way to comprehend the transformations that occur along the process path for a given location in the product (Cuq *et al.*, 2003).

The process paths for the bread center and surface in figure 1 reflect the three stages of baking which occur after the dough is placed in the oven.

1. Heating phase where dough is gradually warmed up to evaporation temperature (~100°C). Yeast or baking powder produce CO_2 inside the dough at temperatures between 40-60°C (Zhang and Datta, 2006). During the heating the pressure in the dough increases due to presence of CO_2 gas and water vapor.

During the heating phase the proteins will denaturize and form a solidified network at the thermosetting temperature. Around the gelatinization temperature T_α, part of the crystalline starch will swell into an amorphous rubbery state. In presence of enough water the gelatinization of starch occurs at temperatures between 60-80°C (Zanoni, Schiraldi and Simonetta, 1995) and is required to form the characteristic sponge network. Because the protein thermosetting and starch gelatinization temperature are within the same range, both phenomena are simultaneously observed and frequently lumped to a single transformation in baking heuristics. Within the model we therefore choose to track only the state change of starch.

2. The drying phase is the following step. Now, water evaporates and the surface of the product, which is in direct contact with the heated air, will be dehydrated first. Several studies indicate that during the drying period not only the evaporation but also the condensation in the product is an important mechanism ruling the heat and mass transfer. This phenomenon is known as the evaporation-condensation principle (see for example Zhang and Datta, 2006; Thorvaldson and Janestad, 1999). Here water evaporates and generates vapor near the surface, but because the temperature decreases towards the center of the product the vapor, which is transported into the product due to diffusion or Darcy flow (Zhang and Datta, 2006), will condensate towards the center.

   The increasing partial water pressure and the presence of CO_2 inside the dough cause product extension, which results in an increase of product size. The gelatinization and protein thermosetting reactions that occurred in the heating phase have altered the rheological properties such that the extension results in the bread crumb and crust formation (Zanoni *et al.*, 1995; Cuq *et al.*, 2003).

   Sugars together with protein will produce browning compounds, which give color to the product that lead to irreversible changes (Cuq *et al.*, 2003). The required relative high temperature for these reactions to occur will typically only be reached in the outer zones, once they are sufficiently dried to have a low water activity and corresponding high evaporation temperature.

   The duration of this phase depends on the initial water content of the dough and is ruled by the heat and mass transfer.

3. Cooling phase. The phase following on drying concerns cooling where the temperature of the product decreases together with a moderate change of water content. The remaining water content determines the state of the product after cooling. The cooled crust will be far below the high glass transition temperature (T_g) due to its low water content. Therefore it will transform during the cooling phase from a rubbery to the glassy state which is essential for the crust crispness (Cuq *et al.*, 2003). The crumb with a

high water content will remain soft (rubber state) after cooling to room temperature because it is above the corresponding T_g. However, the gelatinized part of the starch can slowly (re)crystallize in a process called retrogradation because it is below melting temperature of those crystallites (T_m). The effect of retrogradation is loss of firmness due to physical changes of the product (staling). The retrogradation rate diminishes near the glass transition temperature and therefore can long term storage of bread best be done under the corresponding T_g of the crumb.

3. Modeling approach and considerations

Since the intention of this work is to build a generic baking model suitable for an initial exploration of process alternatives with respect to the resulting quality attributes, the model should fulfill the following requirements:

– Being applicable to a broad range of bakery products.
– Cover the interconnections between sub processes
– Concern only the most critical variables involved in the transformations
– Provide a direct mapping from the state variables to quality related attributes

In the modeling approach only the dominant phenomena and transformations are modeled. Although the accuracy of the model predictions will be limited, it learns to understand the phenomena that occur in the product and how the phenomena are connected and will also help to find which additional experiments are required to improve the prediction.

Table 1 presents an inventory of relevant variables. It starts with quality as observed by the consumers in the left column. These qualities are characterized by the composition, mechanical and structural properties of the product. Water content and the state of starch, proteins and lipids characterize texture properties. Thermosetting reactions for protein solidify the crumb network in the product. As these reactions fall almost together with the gelatinization of starch (Cuq *et al.*, 2003) and because starch is the dominating component for the structural properties, the protein model is omitted in this work. Lipids are hardly transformed during baking, but they may affect the kinetic parameters in the relations for softness, crispness and staling. Information from literature is still too limited to get information on how lipids affect these parameters.

The formation of melanoidins by the Maillard reaction is important for the color. Baking of most products is finished before caramelisation and carbonization reactions at temperature above 150°C start. The degree of extension is responsible for the changes in volume.

Table 1. Analysis of interactions in the system

Quality	Composition	Structure	Mechanical properties	Required transformation	Model required	Model Input
Crumb	Water Starch Protein	Volume fraction Maintaining structure	Elasticity	Gelatinization Retrogradation Thermosetting	Thermodynamic properties: T_g, T_m, T_α Gelatinization and retrogradation kinetics Thermosetting kinetics	Composition (S,W,Z) Process temperature Process temperature
Softness	Water Starch Lipids	-	Elasticity Elasticity	Gelatinization Retrogradation	Thermodynamic properties: T_g, T_m, T_α Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
Crispness	Water Starch Lipids	-	Elasticity Elasticity	Gelatinization Retrogradation	Thermodynamic properties: T_g, T_m, T_α Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
Staled	Starch Water Lipids	-	Elasticity Elasticity	Gelatinization Retrogradation	Thermodynamic properties: T_g, T_m, T_α Gelatinization and retrogradation kinetics	Composition (S,W,Z) Process temperature
Size (Volume)		Extension (oven rise)	-	Gas extension	Kinetic of oven rise	Composition (W) Process temperature
Brownness	Melanoidin Caramel	-	-	Mailard reaction Caramelization	Kinetic of browning reaction	Composition (W) Process temperature

- Note: Initial composition of dough: (S) Sugar, (W) Water, (Z) starch.
- Protein maintains the structure. As the thermosetting reactions of protein fall together with the gelatinization reactions there is no separate model for the protein used.
- Lipids are hardly affected due to heating. There is no transformation reaction. Lipids may affect kinetic parameters but literature information is minimal.

These state variables are the result of a number of transformations that take place in the product. During baking the transformations change the state of components into the final quality. The transformations are driven by heat and mass transfer which depend on the energy input and initial composition of the dough. The changes of the physical and chemical properties may affect the mass and heat transfer in the system (e.g. heat conductivity depends on the water content, or permeability depends on gelatinization), but literature study showed that these effects are insufficiently known and therefore they are not yet included in this work.

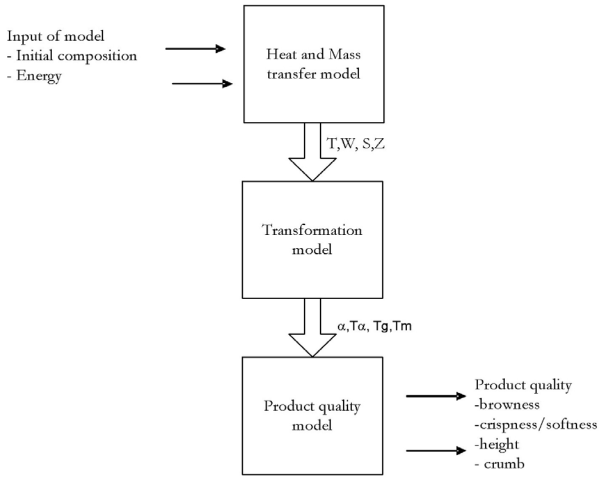


Figure 2. The model is developed in three sequential modeling steps. The model for transformations and product quality are the result of heat and mass transfer model.

Figure 2 gives an overview of the connection of these processes, the inputs and the resulting quality as outputs. The total model has three parts: the heat and mass transfer model, the state changes due to the heat treatment (transformation model) and the product quality model. Setting up a model for heat and mass transfer is rather straightforward by using laws of conservation and additional constitutive equations. The transformation model is more difficult to define, as well as the modeling of the product quality as a function of the transformations. Information given in the literature is a mixture of qualitative rules, experimentally observed correlations and (sometimes) well established relations; so a mixture of expert information, black-box and white box-models. For this work all qualitative descriptions are translated into quantitative information. The translation is expressed into a range between 0-1, which has the meaning of minimum to maximum values.

4. Heat and mass transfer of product during baking

The mass balances

The mass balances for liquid water; water vapour and CO_2 gas are given in Eqs. 1-3. The changes of liquid water in the product are result of the diffusion and the evaporation rate (I_v). Water vapour is considered as an ideal gas which is in equilibrium with liquid water content. The vapour concentration is a function of diffusion and evaporation rate. The rate of extension (e) describes the change of size (height) correspond to initial height of product.

$$\rho_s \frac{\partial W}{\partial t} + \frac{\rho_s . W}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_w \text{ - } I_v \tag{1}$$

$$\rho_s \frac{\partial V_v}{\partial t} + \frac{\rho_s . V_v}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_v + I_v \tag{2}$$

$$\rho_s \frac{\partial V_c}{\partial t} + \frac{\rho_s . V_c}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_c + I_c \tag{3}$$

The energy balance

The energy balance concern conduction, evaporation-condensation, and the water vapour and CO_2 fluxes (eq. 4).

$$\rho_s c_p \frac{\partial T}{\partial t} = \nabla.(k\nabla T) - \lambda I_v - \nabla(m_v H_v) - \nabla(m_c H_c) \tag{4}$$

The flux equations

Flux equations for Eqs 1-3 are described as follows:

$$\phi_w = \rho_s D_w \nabla W \tag{5}$$

$$\phi_v = \rho_s D_{vc} \nabla V_v - m_v \tag{6}$$

$$\phi_c = \rho_s D_{vc} \nabla V_c - m_c \tag{7}$$

Constitutive relations and assumptions

The liquid water and water vapour are correlated by the water activity and partial water vapour relationship in the sorption isotherm. The evaporation rate (I_v) is solved by combining Eqs 1, 2 and-4 with Eq 8 and Eq. 9.

$$V_v = \frac{\varepsilon M_w}{\rho_s RT} a_w \cdot p_{v,sat} \quad (8)$$

$$a_w = \frac{1.05W}{0.09 + W} \quad (9)$$

Water vapour and CO_2 are considered as an ideal gas and balances are derived from Fick's law and by CO_2 production.

Zhang and Datta (2006) used a general term for production of CO_2 both for yeast or baking soda as:

$$I_c = R_{C0}\rho_s \exp(-\frac{(T - T_{ref})}{dT})^{\ 2} \quad (10)$$

With R_{CO} is the CO_2 production at T_{ref}.

Mass fluxes of CO_2 and water vapour depend on local pressure differences, kinematics viscosity and permeability of product.

$$m_v = -\frac{\kappa}{\nu}\frac{V_v}{V_v + V_c}\nabla P \quad (11)$$

$$m_c = -\frac{\kappa}{\nu}\frac{V_c}{V_v + V_c}\nabla P \quad (12)$$

The changes of size (extension) are caused by the increasing pressure inside the gas cells in dough due to the release of water vapor and CO_2 from baking powder or from yeast (Fan, Mitchell and Blanshard, 1999; Zhang and Datta, 2005). We considered bread as a Kelvin-Voigt visco-elastic material for which the rate of deformation is proportional to the pressure difference between the internal product pressure (*P*) and the ambient pressure (P_{atm}) minus the elastic strain (equation 13). A similar expression was proposed by Lostie *et al.* (2002). The two parameters involve in this expression are viscosity *(η)* and the elasticity *(E)* of product. The total pressure *(P)* is a sum of partial water vapor pressure and CO_2 pressure which can be derived from gas ideal law.

$$\eta \frac{de}{dt} + Ee = P - P_{atm} \quad (13)$$

Initial and boundary conditions

The initial values for heat and mass transfer are given by:

$$T(0) = T_0, W(0) = W_0; e(0) = 0; \quad and \quad p_c(0) = 1.10^5 - p_v(0)$$

The boundary conditions of model are given by Eq 14-17:

- Fluxes at the surface

$$k\nabla T = h_c(T_{oven} - T_s) - \lambda.\rho_s.D_w\nabla W \tag{14}$$

$$D_{vc}\nabla V_v = h_v(V_{ext} - V_{v,s}) \tag{15}$$

- Symmetry at the center of the product

$$k\nabla T = 0 \tag{16}$$

$$D_{vc}\nabla V_v = 0 \tag{17}$$

5. Product transformation model

5.1. Starch gelatinization and retrogradation

Starch gelatinization and retrogradation are starch state transition processes which largely determine the final product texture. If enough water is available the crystalline starch granules will transform into an amorphous rubbery state by adsorption of water; this transformation is named gelatinization (Eliason, 1993). Retrogradation is the process where the gelatinized starch turns to a non-native crystalline state. This occurs mainly during storage (Farhat, Blanshard and Mitchell, 1999). With respect to the amorphous-crystalline ratio, the gelatinization and retrogradation will be simply considered as reverse processes (see Figure 3).

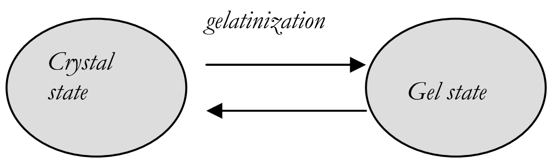


Figure 3. Changing starch state due to gelatinization and retrogradation

The change of the degree of gelatinization is given by equation 18. First order kinetics is adopted to describe the changes of gelatinization and retrogradation (Zanoni *et al.*, 1995;

Karapantsios, Sakondiou and Raphaelides, 2002; Chinachoti and Vodovotz, 2001, Farhat *et al.*, 1999).

$$\frac{d\alpha}{dt} = k_{gel}(T) f_g(\alpha) - k_{retro}(T) f_r(\alpha) \tag{18}$$

where α the degree of gelatinization which ranges from 0 to 1, $k_{gel}(T)f_g(\alpha)$ and $k_{retro}(T)f_r(\alpha)$ the conversion rates for gelatinization and retrogradation are respectively:

$$\begin{aligned} f_g(\alpha) &= (\alpha_{\max} - \alpha) \\ f_r(\alpha) &= \alpha \end{aligned} \tag{19}$$

α_{max} is the maximum attainable degree of gelatinization. Fessas and Schiraldi (2000) showed that the maximum degree of gelatinization α_{max} is a function of the water content in the product (see section 5.1.1).

The gelatinization rate constant $k_{gel}(T)$ and retrogradation rate constant $k_{retro}(T)$ are given in Eqs 20-21 and depend on temperature. Zanoni *et al.* (1995) found that $k_{gel}(T)$ follows an Arhenius equation

$$k_{gel}(T) = 2.8.10^{19} \exp\left(\frac{-139000}{RT}\right) \tag{20}$$

Retrogradation is significantly slower than gelatinization, and takes mainly place during storage. Farhat *et al.* (1999) reported that the Lauritzen-Hoffman model can be used to express the rate of starch retrogradation.

$$k_{retro}(T) = G_0 . \exp\left[\frac{-U^*}{R(T - T_\infty)}\right] \exp\left[\frac{-K_g}{f \cdot T \cdot \Delta T}\right] \quad \textit{if} \quad T < 298K \tag{21}$$

With additional information on this expression in Table 2.

Because of the limited validity range the retrogradation calculations are started in the cooling phase after baking when the product temperature falls below 25°C during the baking process and storage.

Table 2. Variables in retrogradation kinetics (Farhat *et al.*, 1999)

Variable	Expression	Unit
G0	$10^{-10.44W+5.75}$	1/s
*U**	-8140W+8464	J/mol
Kg	$-3.422.10^5W+3.2322.10^5$	K^2
f	$\frac{2T}{T_m+T}$	[-]
T_∞	T_g-30	K
ΔT	T_m-T	K

5.1.1. Calculation of α_{max}

The role of water for gelatinization of starch has been studied (Fessas and Schiraldi, 2000; Karapantsios *et al.*, 2002; Roos 1995). Roos (1992) states that for a starch-water system, the amount of water bound to starch is equal to 50% of total of starch, while the rest is available for gelatinization. In addition, for the same system, Roos (1995) reported that at least 60% of water (40% starch) is required to achieve complete gelatinization. In conclusion, 20% of water bound to starch and the rest (40% of water) will be available for gelatinization. This gives a as a rule that free water and starch require a ratio 1:1 for gelatinization.

For bakery dough which is not only composed of water (W) and starch(Z), other components such as sugar(S) and other water-binding components(C) should be taken into consideration for calculation of maximum gelatinization. Fat as hydrophobic material can be excluded as water binding component. We remark that gelatinization occurs only if the amount of water in dough exceeds 50% of the summed weight of starch and other water binding components. Otherwise there is no gelatinization (Roos, 1995). These findings are based on the composition of dough and in the following expressions the composition of dough is used to calculate α_{max}:

$$\alpha_{\max} = \begin{cases} 0 & if \quad W < 0.5(Z+C) \\ \dfrac{(W - 0.5Z - 0.5C)}{Z} & if \quad 0.5(Z+C) < W < 0.5(3Z+C) \\ 1 \quad if \quad 0.5(3Z+C) < W \end{cases} \tag{22}$$

5.1.2. Glass transition and melting temperature (T_g and T_m)

To calculate the retrogradation rate, glass transition (T_g) and melting temperature (T_m) have to be determined. Roos (1995) states that the effect of the product composition on the glass transition and melting temperatures is an important aspect in the design of food products which are subject to well-defined processing and storage conditions. The main components in bakery dough, sugar, starch and water, have effect on glass transition and melting temperature. The work of Farhat, Blanchard, Descamps and Mitchell, (2000) concerning the effect of sugar-starch solution on the glass transition and melting temperature of starch is used in this study. Farhat *et al.* (2000) performed experiments for the glass transition and melting temperature as a function of sugar/starch ratio (S/Z=0:100, 10:90 and 30:70) and for the water content range of 0-0.5 kg water/kg total. The expressions for T_g and T_m for bakery products as a function of water content (W) and sugar/starch ratio (S/Z) is extrapolated from the work of Farhat *et al.* (2000) by non-linear regression (Eq 23).

$$T_{g/m} = p_1 + p_2(S/Z) + p_3 W + p_4(S/Z)W + p_5(S/Z)^2 + p_6(W)^2 + p_7(S/Z)^2 W^2 \quad (23)$$

With p as the estimated parameters which are listed in Table 3.

Table 3. Estimated coefficients in the expression for glass transition and melting temperature as a function of composition.

Parameters	p_1	p_2	p_3	p_4	p_5	p_6	p_7
T_g	457.10	-396.32	-853.21	716.76	430.27	778.44	-1424.71
T_m	472.69	-180.90	-519.97	419.63	124.46	471.87	-749.88

5.2. Maillard reaction

The Maillard reaction is a non-enzymatic reaction which causes the formation of melanoidins. The melanoidins give an impression of brownness which increases with increasing concentration of melanoidins. The formation of melanoidins by the Maillard reaction follows a zero order kinetic (Eq 24) (Morales and van Boekel, 1998; Bates, Ames, Mac Dougall and Taylor, 1998; Martins and van Boekel, 2003).

$$\frac{dm_e}{dt} = k_{m_e} \quad (24)$$

$$k_{m_e} = k_o \cdot \exp\left[\frac{-E_a}{R}\left(\frac{1}{T}-\frac{1}{To}\right)\right] \tag{25}$$

Van Boekel (2001) reported that the activation energy for bakery products is about 100 kJ/mol. k0 is determined from a correlation between browning reaction rate and water activity, which shows a maximum rate for water activities between 0.7-0.8. This information is not yet sufficient, and to complete the model a reference value is introduced as a standard. This standard is that the level of melanoidins (m_e) equals 1 when a product is exposed for 30 minutes to a temperature of 90°C and water activity 0.93. This statement leads to the next expression for k_0 as function of water activity (Eq 26).

$$k_o = 4.9.10^{-3}\frac{\exp(9a_w)}{2.10^3+\exp(11.3a_w)} \qquad \text{for } T\text{=363 K} \tag{26}$$

The water activity (a_w) is taken from Eq. 9

6. Quality attributes

6.1 Crumb formation

During baking the elastic dough transfers into a fixed structure due to starch gelatinization. At this moment crumb, which is a major texture quality, is formed. The degree of gelatinization depends on the actual temperature and water content and is used as a measure for the final level of crumb formation. Examination of Dutch bakery products, with product compositions given in table 4, by a small panel learned that the degree of crumb increases with degree of gelatinization (α); (see Fig 4) and reaches a maximum value for α>0.5. Between these levels a linear relation between crumb and gelatinization is used (Eq 27).

$$crumb = \begin{cases} 0 \quad if \quad \alpha = 0 \quad (no\ crumb) \\ 2\alpha \quad if \quad 0 < \alpha < 0.5 \quad (moderate\ crumb) \\ 1 \quad if \quad 0.5 < \alpha < 1 \quad (crumb) \end{cases} \tag{27}$$

Table 4. The composition of Dutch bakery products.

Products	Water	Sugar	Starch	Fat	Protein	Other
Krakeling	0.15	0.30	0.26	0.02	0.04	0.22
Wholemal rusk	0.45	0.02	0.33	0.04	0.09	0.07
Bastogne cookie	0.17	0.31	0.29	0.18	0.04	0.00
Knackebrod	0.43	0.04	0.31	0.04	0.08	0.10
Cream cracker	0.20	0.04	0.54	0.14	0.07	0.01
Rusk	0.45	0.05	0.36	0.03	0.09	0.02
Biscuit	0.19	0.15	0.49	0.08	0.07	0.02
Toast	0.45	0.09	0.31	0.02	0.08	0.04
Cookie	0.20	0.24	0.31	0.17	0.06	0.02
Speculas	0.21	0.24	0.31	0.17	0.05	0.02
Cake	0.30	0.23	0.16	0.21	0.06	0.04
Ginger bread	0.40	0.23	0.23	0.01	0.02	0.11
Luxury white bun	0.45	0.04	0.37	0.04	0.07	0.03
White milk bread	0.46	0.05	0.37	0.02	0.08	0.02
Wheat bread	0.45	0.02	0.37	0.02	0.09	0.06
White water bread	0.46	0.03	0.41	0.02	0.07	0.01
Wholemeal bread	0.45	0.04	0.31	0.03	0.08	0.09
Egg cake	0.40	0.28	0.22	0.03	0.06	0.01
Rye bread	0.46	0.05	0.31	0.01	0.06	0.11

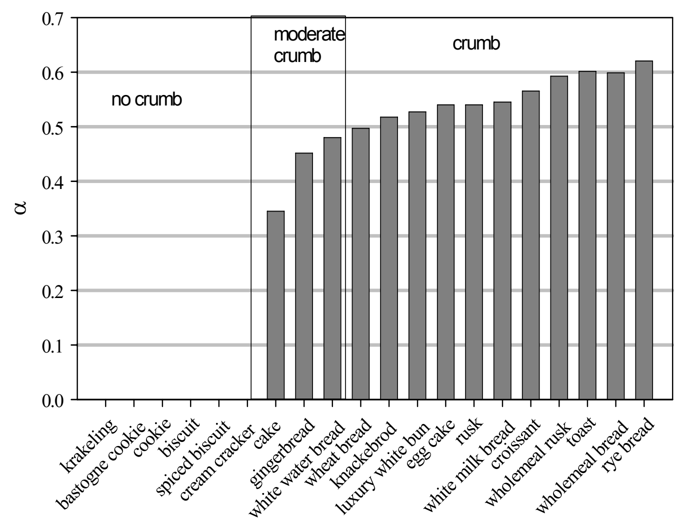


Figure 4. Total degree of gelatinization for bakery products and crumb classification

6.2. Consistency: softness and crispness

The consistency attributes softness and crispness of bakery products are related to the elasticity of the product during consumption. The degree of crispness is related with the difference between product temperature and glass transition temperature (T_g). The glass transition temperature is a function of water, sugar and starch content and is given in Eq. 23. Products are evaluated at room temperature; therefore the difference between room temperature and glass transition temperature is used to express crispness and softness.

$$\delta T = T_r - T_g. \tag{28}$$

Products with a negative value for δT are crispy products and crispness reaches a maximum value (crispness=1) when all water is evaporated which occurs for δT= -150°C. For the degree of crispness between δT =0 to δT=-150°C a linear expression is used:

$$crispness = \begin{cases} 0, & if \quad \delta T > 0 \\ -\delta T/150, & if \quad -150 < \delta T < 0 \\ 1, & if \quad \delta T < -150 \end{cases} \tag{29}$$

Softness is a combined function of the glass transition temperature and degree of gelatinization. A soft product is obtained for $\delta T>0$, but the gelatinization fraction has to be minimal 0.3 otherwise the product is experienced as staled. Maximal softness is obtained when all starch is gelatinized. Comparison of calculated values for Dutch bakery products yield that softness corresponds with the range δT=0-100°C. From this information the following expressing is defined:

$$softness(\delta T) = \begin{cases} 0, & if \quad \delta T < 0 \\ 0.01 \times \delta T, & if \quad 0 < \delta T < 100 \\ 1, & if \quad 100 < \delta T \end{cases}, \tag{30}$$

And for the degree of gelatinization

$$softness(\alpha) = \begin{cases} 0, & if \quad \alpha(t) < 0.3 \\ -\frac{3}{7} + \frac{10}{7}\alpha(t) & if \quad 0.3 < \alpha(t) < 1 \end{cases} \tag{31}$$

Total softness is calculated as

$$Softness = softness(\delta T) \times softness(\alpha) \tag{32}$$

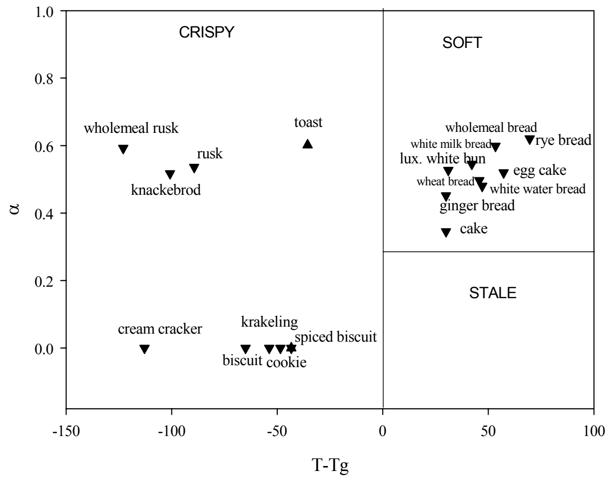


Figure 5. Crispness and softness of products in terms of the difference between room temperature, glass transition temperature and degree of gelatinization. T_g varies for the products and is calculated from the composition and by using Eq 23

Fig 5 shows the valuation of Dutch bakery products for their crispness and softness by using Eqs 18-23, 27-32 and initial composition for each product (Table 4). From the model follows that crackers, biscuits, *knåckebrod* and toasts fall in the category of crispy products, while bread types and cakes fall in the group of soft products. These results correspond to the consumers experiences. Due to retrogradation the degree of gelatinization of soft products decrease and for a<0.3 the soft products become staled. Crisp products do not retrogradate because they are in the glass state.

6.3 Brownness model

Brownness is important for appearance and is influenced by the Mailard reaction which is non enzymatic reaction producing melanoidins (m_e) as a color compound. Moreover, product color is also a function of the initial color of the dough, and the follow-up reactions caramelization and carbonization, which occur when the product temperature is above 150°C. Although oven temperatures above 150°C are being used the temperature of the surface seldom exceeds 150°C. Therefore caramelisation and carbonisation are not considered in this work.

Even though the correlation between melanoidins and color development was reported as linear relation (Martins and Boekel, 2003), in this work it is assumed that with increasing number of melanoidins, the color will reach saturation and goes to a maximum value (dark brown). This is achieved with the following expression:

$$brownness = 1 - (1 - brownness(0))\exp(-0.23 m_e) \quad (33)$$

where *brown (0)* is the initial brownness of the dough

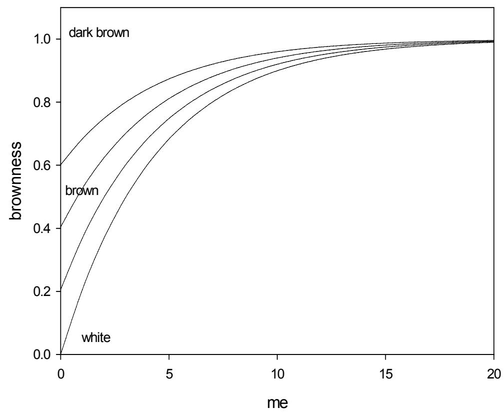


Figure 6. Correlation between melanoidins and brownness development

Figure 6 shows the relation between melanoidins and brownness formation. It shows that the color formation goes to a maximum level of brownness in the range of white (brownness=0) to dark brown (brownness=1). Figure 6 and Equation 33 also show that the brownness development can start from different initial color due to other color compounds and melanoidins in the dough.

7. Simulation Method

Bakery products are 3 dimensional products and the quality depends on the position in the product. Heat and mass transfer calculations are done with finite element calculations by multi-physic package of COMSOL 3.2 (www.comsol.com). For the simulation, the bakery products were considered as a cylinder with height (H) and radius (R) as shown in Fig 7. The shaded region is the sub domain where the simulation was performed and the two points were used to represent the center (point 1), and the surface (point 2). The symmetrical boundary condition (eq 16-17) is applied at the boundary line a, and the flux boundary condition (eq 14 -15) to boundary lines b,c and d. The heat and mass transfer model and the boundary conditions are given in Eqs. 1-17.

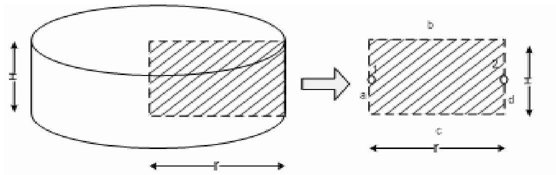


Figure 7. The simulation domain. a,b,c and d represent the boundary conditions. Point 1and 2 represent the center and surface characteristic of products.

The model allows the simulation of a variety of bakery products. In the next section three different bakery products (bread, biscuit and cake) illustrate the results for product transformation and product quality. The products and properties are specified in Table 5.

Table 5. Parameter specification of simulated bakery products

Properties	**Products**		
	Bread	**Biscuit**	**Cake**
Size (H, r) (m)	(0.03,0.05)	(0.0025,0.025)	(0.03,0.05)
Baking time (s)	1800	800	1800
T_{oven} (°C)	200°C	200°C	200°C
Initial condition			
W_0 (kg/kg)	0.45	0.19	0.30
Z (kg/kg)	0.37	0.49	0.16
S (kg/kg)	0.02	0.15	0.23
C(kg/kg)	0.15	0.09	0.10
Product properties			
ρ_s (kg/m^3)	705	540	880
c_p (J/kg.K)	1712.5	1712.5	1951
k (W/mK)	0.4	0.2	0.4
D_{vc} (m/s)	2.10^{-5}	2.10^{-5}	2.10^{-5}
D_w (m/s)	1.10^{-10}	1.10^{-10}	1.10^{-10}
h_c(1/s)	15	15	15
h_v(1/s)	0.2	0.2	0.2

8. Results and Discussions

8.1. Product temperature and water distribution

The predicted temperature and water content for bread, cake and biscuit during baking at an oven temperature of 200°C are given in Fig. 8. The lines represent the change of temperature and water content in the center and just below the surface. The temperature near the surface of the products increases more rapidly than in the center and come closer to the oven temperature. For all products, the temperature in the center remains during some time around the evaporation temperature (100°C). Due to the relatively high water content the period around 100°C is longer for bread and cake than for the other products. The center temperature for biscuits, with low water content, remains only a short time at 100°C and rises when the majority of water has been evaporated.

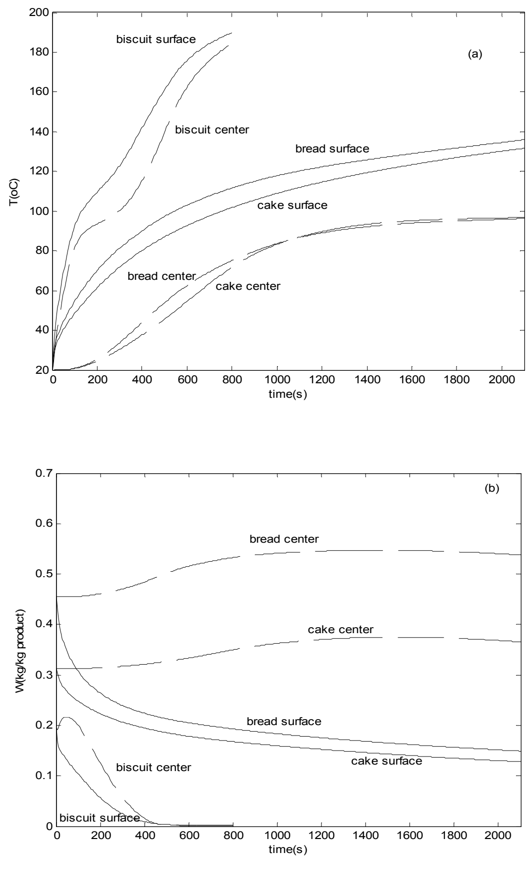


Figure 8. Temperature (a) and water (b) profiles for three products during baking.

For all products, the high evaporation rate in the surface region results in rapid decrease of the water content. In the first phase of baking, the water in the center of the products is almost unchanged as the heat does not yet penetrate into the center. Then the water content increases due to the condensation effect. For biscuits the center of the product starts to dry in a third phase and finally the water contents becomes zero. Bread and cake show the same phenomena but with a different pattern. The water content in the center increases but due to the larger product dimensions and the limited heat penetration, it takes a long time before the water content in the center starts to decrease. This result corresponds to the work of Thorvaldsson and Janestad (1999).

8.2. Crumb formation

Crumb formation is important since it develops the pore structure in the products. Crumb formation is a result of starch gelatinization which depends on the actual water content, the composition and product temperature. Fig 9 shows the degree of crumb formation that corresponds to degree of gelatinization formation of the three products. The result shows that degree of gelatinization at the surface is significantly faster than in the center which corresponds with the temperature profile. The simulations (combining Fig 8 and 9) show that gelatinization is completed at 78°C for bread and 81°C for cake; the degree of gelatinization is 0.50 and 0.31 respectively. Biscuit, which has low water content, does not gelatinize. The consequences of gelatinization on the crumb formation are also shown in Fig 9. In bread full crumb is formed while in cake the degree of crumb is partial because of the degree of gelatinization is below 0.5. The structure in cake is not fully developed and pores formation is partial. For biscuit the crumb is absent.

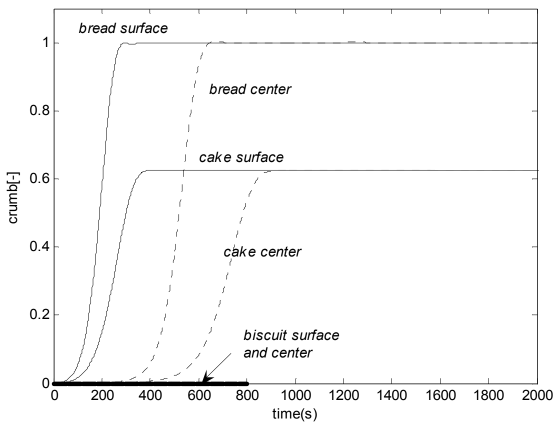


Figure 9. Crumb formation for three products during baking. The formation corresponds to twice value of gelatinization degree.

8.3. Softness and crispness

Softness and crispness are also derived from the degree of gelatinization. During product heating, starch gelatinizes and water evaporates into the oven. Gelatinization affects the mechanical strength of the products which also increases with decreasing amount of water in the product. As a result the products loose first their softness and then become crispy.

Figure 10 shows softness and crispness of the simulated bakery products. Softness follows the pattern of decreasing water content and becomes zero when the product temperature comes below the glass transition temperature (T_g). When T_g is achieved, the product changes from rubber to glassy state. The glass transition temperature for bread, which has a high water content, is T_g =-25°C and for cake T_g=-10°C, while biscuit has a high glass transition temperature T_g =80°C. These values explain the differences in the soft and crispness of the products at consumption temperature. Fig.10 also shows that softness in the center of cake and bread hardly changes, while significant changes in crispness occur in the biscuit center. This is directly related to current water content in the product which evaporates faster than for the two other products.

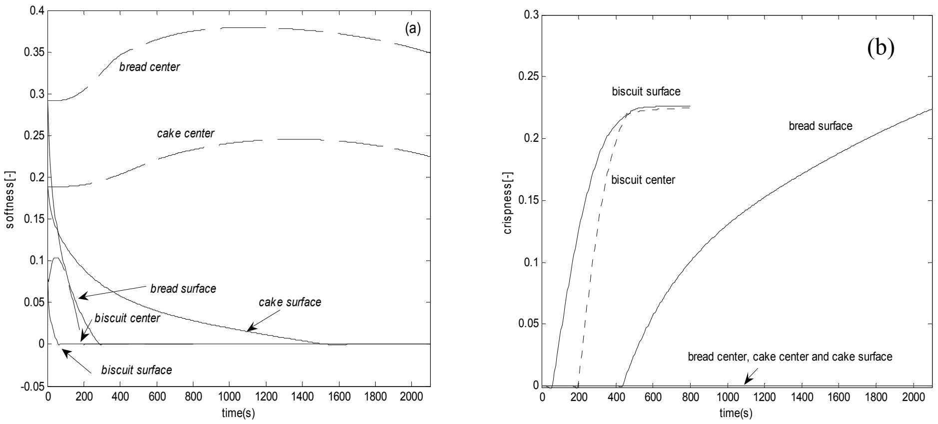


Figure 10. Softness (a) and crispness (b) development for three products during baking.

8.4. Color

The color, expressed in the level of brownness, is influenced by the composition of the dough, the water content and process conditions during baking process. The Maillard reaction is the main responsible for color development at temperatures below 150°C.

Figure 11 shows the development of brownness during baking for the three products due to the formation of melanoidins. The development of brownness on the surface is faster than in the center due to quick increase of surface temperature. The fast increase of temperature together with the fast decrease of the water content in the surface accelerates the Maillard reaction between sugar and amino acids which gives more melanoidins during baking.

Bread shows significant colour change at the surface and only a moderate change in the center. This is result of the high water content and low temperature in the center which gives a low amount of melanoidins.

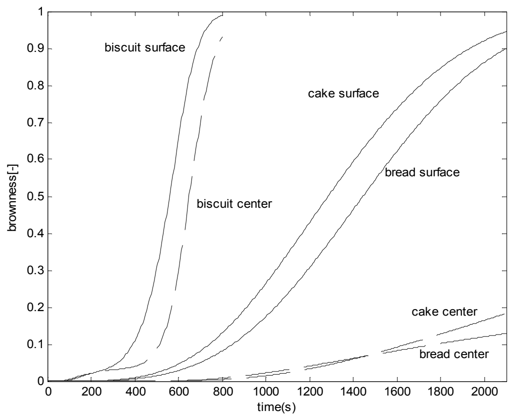


Figure 11. Development of brownness during baking.

The formation of melanoidins in biscuit is faster than in the bread. The low water content and small dimension have the effect that water is quickly evaporated and the product is dried out faster. The low water activity would result in a low reaction rate, but the increased temperature effect on colour formation surpasses the water activity contribution. Cake shows also a different pattern than bread; the final brownness is higher. This is due to the larger amount of sugar in cake which gives a higher amount of melanoidins.

8.5. Size (Height)

The height is a result of the pressure difference between the total pressure in the product and pressure in the oven. The pressure difference causes product deformation resulting in extension of height.

Fig 12 shows the extension for the three products. The height of the biscuit increases during the first 200s and starts to decrease when the product structure is open. The pressure difference between product and oven becomes less and at about 400 seconds the pressure difference is constant. The simulation shows that for biscuits the initial height is doubled (i.e. 100% extension). Bread height increases to a slightly higher value (120% extension), but there is not a prominent maximum in the curve. Cake shows lowest degree of extension (60%). This also related to degree of gelatinization which is not fully achieved during baking.

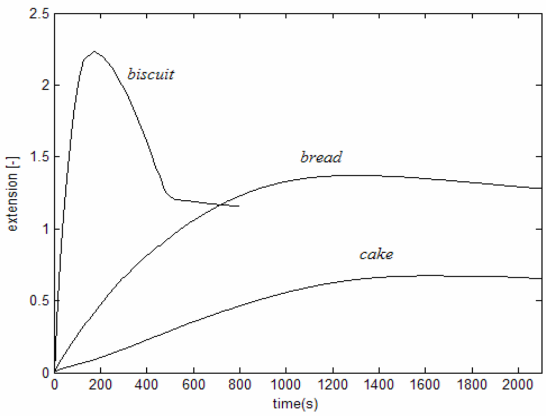


Figure 12. The extension of product height during baking.

8.6. Retrogradation during storage

As biscuits are in the glass state retrogradation does not occur for this product and therefore only retrogradation for bread and cake is presented in Fig 13. To demonstrate the effects of storage temperature, different settings of temperature are applied: 20^{o}C (room temperature) for 2 days followed by -20^{o}C (freezer temperature) for 4 days and 2 days at 5^{o}C (refrigerator temperature).

During storage at room temperature the degree of gelatinization lowers due to retrogradation and the product is experienced more staled. Retrogradation is enhanced by water uptake from the air around the product (see also contribution of water content in Eq 21 and Table 3). For cake there is hardly retrogradation because of the higher glass temperature (-18°C) and the lower water content. Therefore, the product can be stored under room temperature for 1 week with minimal staling. In frozen state the retrogradation of bread is minimized and therefore long term storage under this temperature is recommended to keep quality. However, when bread is stored under refrigerator conditions (5^{o}C), retrogradation will start again.

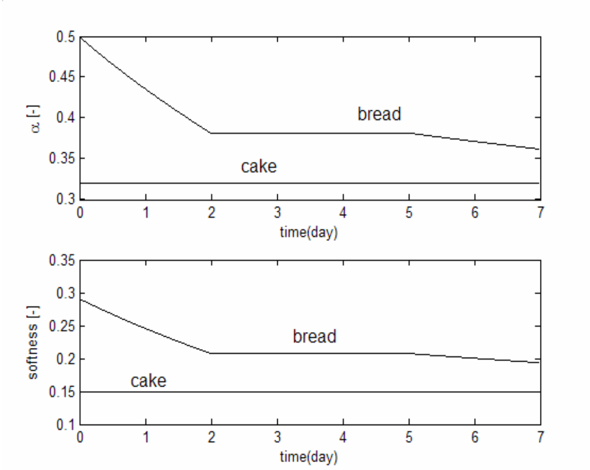


Figure 13. Changes in degree of gelatinization and softness during storage caused by retrogradation. Temperature is 20°C for 2 days, then -20°C for 3 days and finally 5°C for 2 days.

8.7. Directions for quality control

The overall influence of control parameters on the selected quality attributes were derived from simulations. The changes in final product quality for bread (composition given in Table 5) were calculated for 20% changes of oven temperature, initial water content, sugar, and starch components. The sensitivity indicators are given in Table 6. The sensitivity changes are categorized into 5 categories: o = changes below ±1%, +/-= moderate changes in the range 1-10% (increase/decrease), ++/--= significant changes in the range 10-20% (increase/decrease), and +++/---= major changes above 20 % (increase/decrease).

The product surface is directly exposed to the oven temperature. Therefore it is the main variable that affects the product quality attributes (water content, crispness, height and color) of the product at the surface. An increase of the initial water content results in a strong increase of softness in the product center and at the same time crispness of the surface decreases. Crumb formation is highly affected by a decrease of initial water content. Sugar and starch concentrations are mainly important for the crispness of the surface and softness in the center and no significant changes are found for other quality attributes.

Combination of two opposite sensitivities does not always compensate each other. For example, the effects of changes in crispness at the surface due to increase of oven temperature are surmounted by the effect of increased initial water content.

Table 6. The variation of bread quality attributes after baking for changed values of input variables with 20%. The changes of quality attributes are relative to a standard product (as given in previous sections).

Parameter*	W		crumb		crispness		softness		color		height
	s	c	s	c	s	c	s	c	s	c	
T_{ext} : $\Uparrow$	--	-	o	o	+++	o	o	--	++	+	+
T_{ext} : $\Downarrow$	+++	+	o	o	---	-	o	+	---	o	--
W_o:$\Uparrow$	++	+++	o	o	---	o	+	+++	-	o	o
Z$\Uparrow$;	o	o	o	o	-	o	-	+++	o	o	-
S$\Uparrow$;	o	o	o	o	-	o	o	--	o	o	-
$T_{ext,}$ $\Uparrow$ $W_{o,}$ $\Uparrow$	-	++	o	o	-	o	+	+++	+	+	++
$T_{ext,}$ $\Uparrow$ $W_{o,}$ $\Downarrow$	---	---	---	---	+++	o	o	---	++	+	-
$T_{ext,}$ $\Downarrow$ $W_{o,}$ $\Downarrow$	-	--	---	---	-	o	o	---	---	o	---
$T_{ext,}$ $\Downarrow$ $W_{o,}$ $\Uparrow$	+++	+++	o	o	---	o	o	+++	---	o	--

Note: s = surface, c=center, W_o=Initial water content, T_{ext}=oven temperature, Z=Starch, S= Sugar
$\Uparrow$ = increase of parameter value=20%, $\Downarrow$= decrease of parameter value=20%,
o = less than 1% change, + = increase 1-10%, **-** =decrease 1-10%, **++** = increase 10-20%,
-- =decrease 10-20%, +++ = increase >20%, --- =decrease >20%,
*: other parameters which are not mentioned use standard value.

9. Conclusion

Initial phases in food process design are enhanced by using mathematical models to explore the feasibility of alternatives, to compare alternatives and to reduce the time span for process development. The main objective of such feasibility phase is to rank different production methods with respect to the obtained product quality.

Baking is a process where several transformations occur for which a lot of information is available on specific aspects. To deal with the complexity of the product-process interaction, a systems approach is used, by splitting the process in three sequential parts:

- mass and heat transfer in porous media
- transformations of starch and the formation of color forming components
- quality properties (crumb, crust, color, softness and crispness)

Models of these parts were based on the dominant phenomena in the system. Although the accuracy of the model predictions might be limited, the proposed approach covers the interconnection between the separate parts, it learns to understand the phenomena that occur in the product and will also help to find which additional experiments are required to improve the prediction.

Because of the transport phenomena in bakery products, the qualities depend on the position in the products and also on the size and form of the product. Therefore it is necessary to use spatial models. The model predicts how the quality changes by the choice of the dough composition and energy as input variables.

The transformation of starch is derived from the behavior of polymers as a function of temperature and composition. The glass transition, melting and gelatinization temperature are important indicators. The degree of starch gelatinization is used as the main indicator for softness and crispness of the products. In storage the degree of gelatinization decreases by starch retrogradation, which results in staled products. The Maillard reaction is the main reaction for color formation.

Heuristic knowledge on quality attributes was captured by using rules with a minimum and maximum value (0-1 rules). This approach showed realistic predictions for Dutch bakery products and offer therefore good opportunities for use in the feasibility phase of process design.

As the model is not yet calibrated, the model will not give full accuracy. However, the model shows the tendency of the effects of input variables (composition and outside temperature) on the product quality, and is therefore suitable to explore production alternatives and to compare them by ranking in the initial phase of food process design. Moreover, the model supports to understand the interconnection between the phenomena.

Acknowledgement

This research has been financially supported by VLAG Graduate School, The Netherlands

Annotations

Symbols	Description	Unit
a_w	Water activity	[-]
C	Other water binding components	Kg kg^{-1}
c_p	Heat capacity	J kg^{-1} K^{-1}
D_{vc}	Gas diffusivity	m^2 s^{-1}
D_w	Liquid diffusivity	m^2 s^{-1}
e	Extension of height	[-]
f	Fusion factor	[-]

E	Elasticity modulus	Pa
E_a	Activation energy	J mol^{-1}
G_0	Reference retrogradation rate	s^{-1}
H	Height of product	m
I_v	Evaporation rate	kg $m^{-3}s^{-1}$
I_c	Production rate of CO_2	kg $m^{-3}s^{-1}$
h_c	Convective heat transfer coefficient	W $m^{-2}K^{-1}$
h_v	mass transfer coefficient	m s^{-1}
k	Thermal conductivity of product	$Wm^{-1}K^{-1}$
K_g	Constant	[-]
k_{me}	Reaction rate of Maillard reaction	s^{-1}
m_v	Mass flux of water vapor	kg $m^{-2}s^{-1}$
m_e	Melanoidins	[-]
m_c	Mass flux of CO_2 gas	kg $m^{-2}s^{-1}$
M_w	Molecular weight of water	kg mol^{-1}
P	Total pressure	Pa
$p_{v,sat}$	Saturated pressure of water vapor	Pa
R	Gas constant	J $mol^{-1}K^{-1}$
r	Product radius	m
R_{C0}	CO_2 generation rate	kg $kg^{-1}.s^{-1}$
S	Sugar content	kg kg^{-1}
T_∞	Hypothetical temperature	K
U^*	Activation energy for product during recristalization	J mol^{-1}
V_c	CO_2 gas concentration	kg kg^{-1}
V_v	Water vapor concentration	kg kg^{-1}
W	Water content	kg kg^{-1}
Z	Starch content	kg kg^{-1}
T_g	Glass transition temperature	K
T_m	Melting temperature	K
T_α	Gelatinization temperature	K
S/Z	Ratio sugar to starch	[-]

Greek letters

α	Total degree of starch gelatinization	[-]
α_{max}	Maximum degree of starch gelatinization	[-]
ε	Porosity	[-]
η	Dynamic viscosity	Pa.s
κ	Permeability	m^2

λ	Evaporation heat	$J.kg^{-1}$
ρ_s	Density of solid matrix	$kg.m^{-3}$
υ	Kinematic viscosity	$m^2.s^{-1}$
ϕ	Flux	$kg.m^{-2}s^{-1}$

References

Bates, L., Ames, J.M., Mac Dougall, D.B., and Taylor, P.C.(1998). Laboratory Reaction Cell to Model Maillard Colour Development in a Starch –Glucose-Lysine System. *Journal of Food Science*, 63(5), 991-996.

Bruin, S. (1999). Phase Equilibria for Food product and process design. *Fluid Phase Equilibria, 158-160, 657-671*

Chinachoti, P., and Vodovotz, Y. (2001). Bread Staling. *CRC Press. Boca Raton.*

Cuq, B., Abecassis,J. and Guilbert,S. (2003). State Diagrams to help describe wheat bread processing. *International Journal of Food Science and Technology*, 38, 759-766.

Diefes, H.A., Okos, M.R., and Morgan, M.T. (2000). Computer-aided process design using Food Operations Oriented Design System Block Library Morgan. *Journal of Food Engineering, 46(2), 99-108*

Douglas, J.M. (1988). Conceptual Design of Chemical Processes. *McGraw-Hill, Inc.*

Eliasson, A.C., in Cereals in bread making, Ed.A.C.Eliason. (1993). Marcel Dekker, Inc. New York p.96

Fan, J., Mitchell, J.R., and Blanshard, J.M.V. (1999). A model for the oven rise of dough during baking. *Journal of Food Engineering*, 41, 69-77.

Farhat, I.A., Blanshard, J.M.V., and Mitchell J.R. (1999). The Retrogradation of waxy maize starch extrudates: effects of storage temperature and water content. *Biopolymers*, 53, 411-422.

Farhat, I.A, Blanchard, J.M.V., Descamps, M., and Mitchell, J.R. (2000). Effects of sugars on retrogradation of waxy starch-sugar extrudates. *Cereal chemistry, 77, 202-208*

Fessas, D., and Schiraldi, A. (2000). Strach Gelatinization Kinetics in bread Dough, DSC Investigations on Simulated Baking Process. *Journal of Thermal Analysis and Calorimetry*, 61, 411-423.

Fryer. (1994). Mathematical-Models in Food-Processing. *Chem. Ind-London, 13, 515-518.*

Jadhav, N.Y., van der Stappen, M.L.M., Boom, R.M., Bierman, G. and Grievink J. (2002). Mass balance and capacity optimization in the conceptual design of processes for structured products. *European Symposium on Computer Aided Process Engineering-12, Elsevier Science.*

Karapantsios, T.D., Sakondiou, E.P. and Raphaelides, S.N. (2002). Water Dispersion Kinetics during starch gelatinization. *Carbohydrate Polymer 49*,479-490;

Levine, H. and Slade, L. (1990). Influences of the glassy and rubbery states on the thermal, mechanical, and structural properties of dough and baked products. In: Faridi H, Faubion JM (eds) Dough rheology and baked product texture. Van Nostrand Reinhold, New York, pp 157–330

Martins, S.I.F.S., and van Boekel, M. A. J. S.(2003). Melanoidins extinction coefficient in the glucose/glycine Maillard reaction. *Food Chemistry 83(1),135-142*

Meeuse, F.M., Grievienk, J., Verheijen, P.J.T., and vander Stappen M.L.M. (2001). Conceptual Design of Processes For Structured Products. *Conference Foundations of Computer Aided Process Design, Breckenridge*

Morales, F.J., and van Boekel, M.A.J.S. (1998). A study on advanced maillard reaction in heated casein/sugar solutions: Colour formation. *International Dairy Journal*, 8, 907-915.

Roos, Y.H. (1992). Phase transition and Transformations in Food Systems. in Heldman,D.R and D.B. Lund, hand Book of Food Engineering., Marcel Dekker,Inc New York.

Roos, Y.H. (1995). Phase transition in Foods. *Academic Press, London.*

Sablani, S.S., Marcotte, M., Baik, O.D., and Castaigne, F. (1998). Modeling of Simultaneous Heat and Water Transport in the Baking process. *Lebensm-Wiss. U Technology 31, 201-209*

Schiraldi,A., Piazza,L., Brenna,O., and Vittadini,E. (1996). Structure and Properties of Bread Dough and Crumb,Calorimetric, rheological and mechanical investigations on the effects produced by hydrcolloids, pentosans and soluble proteins. *Journal of Thermal Analysis*,47,1339-1360

Siirola, J.J. (1996). Strategic Process Synthesis: Advances in the Hierarchical Approach. *Computer Chem. Engineering, 20, 1637-1643*

Thorvaldson, K., and Jenested, H. (1999).A Model for simultaneous heat, water and vapour diffusion. *Journal of Food Engineering, 40, 167-172*

van Boekel, M.A.J.S. (2001). Kinetic Aspects of the Maillard Reaction: a critical review. *Nahrung/ Food*, 45(3), 150-159.

Wibowo, C., and Ng Ka M. (2001). Product Oriented Process Synthesis and development: Cream and Pastes. *Process System Engineering, 47(12), 2746-2767*

Zanoni, B., Schiraldi, A. and Simonetta, R. (1995). A naive model of starch gelatinization kinetics. *Journal of Food Engineering, 24(1), 25-33*

Zhang, J. and Datta , A.K.(2006). Mathematical modelling of bread baking process. *Journal of Food Engineering, 75(1), 78-89*

CHAPTER 4

Product Quality Driven Design of Bakery Operations using Dynamic Optimization

This Chapter has been accepted for publication as: Hadiyanto, D.C. Esveld, R.M. Boom, G. van Straten and A.J.B van Boxtel. (2007). Product Quality Driven Design of Bakery Operations using Dynamic Optimization. *Journal of Food Engineering*

Abstract

Quality driven design used specified product qualities as a starting point for process design. By backward reasoning the required process conditions and processing system were found. In this work dynamic optimization was used as a tool to generate processing solutions for baking processes by calculating optimal operation strategies which give a basis for process and unit operation design. Two different approaches for dynamic optimization have been applied: calculation of continuous trajectories based on the calculus of variations (1) and calculation of switching trajectories by using control vector parameterization (2). Optimization of bakery processes was performed for different product specifications and by using different heating sources: convective, microwave and radiation heating. Moreover, effects of variations in dough properties on the optimal processing system were also evaluated. The results showed that dynamic optimization procedures were versatile tools to achieve a better and a more flexible design by generating a number of solutions from the specified final product qualities. Furthermore, the results underpinned the well known empirical fact that different final product specifications require different baking strategies. It was also shown that the initial dough properties have significant effect on baking procedures, and that combining several heating inputs improves the flexibility of the process operation. In addition, optimization for continuous trajectories gave overall a better result than using the switching trajectories.

Key words: Baking, optimal operation, process design, optimization, quality, model.

1. Introduction

During their passage through a chain of processing equipment, raw food materials are transformed into the final products. Product quality develops due to the process conditions and treatments to which the raw materials are exposed. At the end of the chain the product quality should meet the product specifications.

The standard procedure for process design starts from the raw materials, for which a number of unit operations are put in the required sequence. The conditions are chosen in such way that the required product qualities are more or less obtained. This approach is mostly driven by experience and knowledge of the equipment.

In contrast to the standard design procedure, product quality driven process design starts from the specified product quality and searches in the backward direction using a systematic approach towards for a processing route and process conditions that satisfy the requirements. In this approach knowledge of the fundamental process underlying product (trans) formations is a main factor. To support the backward reasoning procedure, a solution generator is required, i.e. an algorithm that searches for the best process conditions throughout the equipment to obtain the product quality attributes.

The majority of process optimization applications in the food industry concern static optimizations, i.e. optimization towards the best choice of decision variables which are constant in time. These procedures satisfy well for systems without transient characteristics. However, the heat and mass transfer and the product transformations are transient phenomena. Here, dynamic optimization with an objective function that includes quality criteria has potential to find improved solutions. Several positive results of dynamic optimization in food engineering could be found in literature. For example thermal sterilization (Barreiro, Perez, and Guariguata, 1984; Banga, Perez-Martin, Gallardo, and Casares, 1991; Chalabi, van Willigenburg, and van Straten, 1999; García, Balsa-Canto, Alonso, and Banga, 2006), uniformity in food-heating (Saa, Alonso, and Banga, 1998; Stigter, Scheerlinck, Nicolaï, and van Impe, 2001), heat exchanger and membrane fouling control (van Boxtel, Otten, and van der Linden, 1992; van Boxtel and Otten, 1993), cooking of meat patties (Zorrila, Banga, and Sing, 2003) and drying processes (Boss, Filho, and Eduardo de Toledo, 2004; Barttfeld, Alleborn, and Durst, 2006). However, to our knowledge there was no work on the use of dynamic optimization to generate process design routes for bakery processes.

Baking is the main stage in bakery production and heating is applied to induce the transformations in the product. The type and settings of different heating sources (convective, microwave and radiation heating) can be altered to control the transformations in the product. Product qualities as crumb, crispness, softness, volume and color are the result of starch gelatinization, volume expansion, and browning reactions (Hadiyanto, Asselman, van Straten, Boom, Esveld, and van Boxtel, 2007). Most studies on the improvement of baking processes by manipulating these sources were based on experimental optimization, e.g. Therdthai, Zhou, and Adamczak (2002); Sumnu, Sahin, and Sevimli (2005); Keskin, Sumnu, and Sahin, (2004); Baucour, Cronin, and Stynes, (2003); Flander, Salmenkallio-Marttila, Suortti, and Auito, (2006) and Mevik, Færgestad, Ellekjær, and Næs, (2001). In contrast to these applications, our work concerns the design of an optimal baking strategy by employing a model-based dynamic optimization approach. The ultimate goal is to design the process (i.e. the heating systems) in such way that products with distinct quality are obtained.

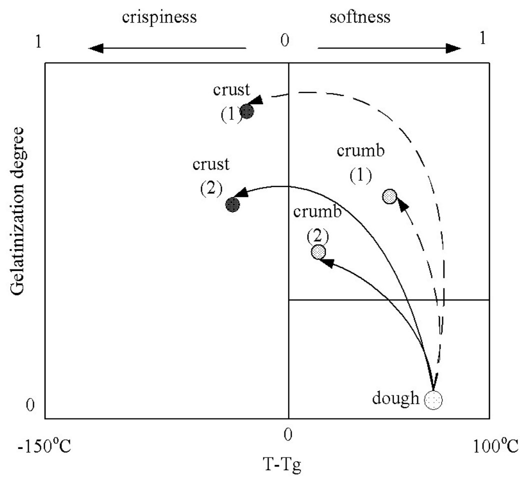


Figure 1. Two products with different crispness and softness at surface and center in a temperature-gelatinization diagram.

Figure 1 gives a schematic example of a state diagram which illustrates the state of the product in two dimensions: in this case the degree of gelatinization (α) and the difference between the product temperature and the products' glass transition temperature (T_r-T_g). The state diagram illustrates schematically how product quality can be manipulated in terms of the two parameters. Baking starts with dough and due to heating the final product quality, here chosen as softness in the crumb part (center) and crispness of the crust part (surface), are achieved for point 1. However, a product that should have different qualities (point 2) requires a different heating strategy or should start with different dough properties.

The product quality driven process design method using dynamic optimization can be applied to find the process conditions and equipment necessary to end with the product qualities of point 1 or with those of point 2. It thus yields the dough properties and operation strategies as a result.

This paper presents the design of baking processes by using dynamic optimization procedure. The dynamic optimization is used to generate design solutions. Two optimization methods are proposed in this work: gradient search optimization and control vector parameterization method. This paper also shows intension on how the final product specifications give different operation for the operations and how the initial properties of products can increase the flexibility of design.

2. Dynamic Optimization

Dynamic optimization yields the optimum input trajectory *u(t)* on the time interval from start to the end $[t_o\ t_f]$ by minimisation of the performance index (*J*) while respecting the lower and upper bounds $[u^L\ u^U]$ of the input variables and subject to a set (differential and algebraic) equations which describe the system dynamics and interconnections:

$$\min J = \phi(x(t_f)) + \int_{t_0}^{t_f} L(t, x, u, \theta)dt \tag{1}$$

$$\begin{aligned} s.t. \quad & \dot{x} = f(t, x, u, \theta),\ x(0) = x_0 \\ & u^L \le u \le u^U \end{aligned} \tag{2}$$

where x is a vector of state variables, θ the process parameter vector, J the performance index which is the sum of the objectives at final time ($\phi(x_{tf})$) and the integral of the running costs ($L(t, x, u, \theta)$).

There are several methods to solve the optimization problem. Indirect methods based on calculus of variations which solve the optimization problem as a two point boundary value problem are intensively discussed by Bryson and Ho (1975), Bryson (1999), and von Stryk and Bulirsch (1992). Other methods to solve the optimization problem are direct methods using control vector parameterization (Vassiliadis, Balsa-Canto, and Banga, 1993; Binder, Cruse, Villas, and Marquardt, 2000; Biegler, Cervantes, and Wächter, 2002; Balsa-Canto *et al.*, 2002a,b; Schlegel *et al.*,2005), dynamic programming (Bellman, 1957, Luus,1993), and stochastic or genetic algorithm based search methods (Roubos, van Straten, and van Boxtel,1999).

From a dynamic optimization point of view there are two extremes in searching for optimal baking strategies. One extreme is to find continuous trajectories for the input variables, the other extreme is to consider baking as a sequence of piece-wise constant inputs variables with unknown switching levels and switching moments (Figure 2). In this work the continuous trajectories are calculated by an indirect method based on the calculus of variation (Bryson, 1999) and the switching trajectories by control vector parameterization (CVP).

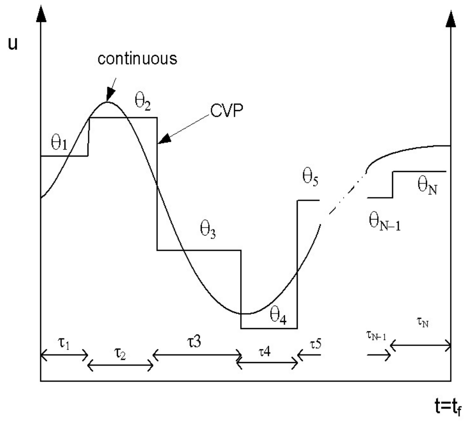


Figure 2. Schematic representation of input trajectories from continuous and control vector parameterization (CVP).

In the indirect method, the process behaviour is combined with the performance index by using a vector of time dependent Lagrange multipliers λ *(t)* (Bryson, 1999):

$$J = \phi(x(t_f)) + \int_{t_0}^{t_f} [L(t,x,u,\theta) + \lambda(t)^T (f(t,x,u,\theta) - \dot{x})]dt \tag{3}$$

The Lagrange multipliers are related to the actual process variables and consequently time dependent. To determine the input trajectories, the integral part of Eq.3 is considered (Bryson, 1999; von Stryk and Bulirsch, 1992) and it is expressed more concisely in terms of Hamiltonian function (*H*) defined by:

$$H = L(t,x,u,\theta) + \lambda(t)^T f(t,x,u,\theta) \tag{4}$$

According to the theory (Bryson, 1999), the performance index is minimized / maximized if the following necessary conditions are satisfied:

$$\frac{d\lambda(t)}{dt} = -\frac{dH}{dx} = -\frac{dL}{dx} - \lambda(t)^T \frac{df}{dx}, \text{ with } \lambda(t_f) = \frac{d\phi(tf)}{dx} \qquad (5)$$

$$\frac{dH}{du} = 0 = \frac{dL}{du} + \lambda(t)^T \frac{df}{du} \qquad (6)$$

Equations 2, 5 and 6 have to be satisfied for the optimum. As the boundary conditions of equations 2 and 5 are given at different moments (respectively $t=0$ and $t=t_f$) the problem is also named as a two point boundary value problem. Equation 6 represents the gradient of performance index (J) with respect to u while holding x_0 constant and satisfying Eq.2. Eq. 6 assists in the search towards the optimal input trajectories $u(t)$. Bryson and Ho (1975) and Bryson (1999) discuss several methods for solving the two-point boundary problem based on adjusting $u(t)$ to satisfy eq.6 by using gradient methods.

Control vector parameterization considers the optimal control problem as a nonlinear programming problem. The control trajectory is represented by a finite number of parameters by using suitable basis functions. Piecewise constant and piecewise linear are frequently used representations of the control vector.

Control vector parameterization has a limited potential for finding the true optimum due to the discretization of the control vector in time and there is no guarantee that these methods end in a global minimum. Nevertheless, the method has the advantage that the adjoint variables and Lagrange functions are not required (von Stryk and Bulirsch, 1992) and these methods are easy to apply.

Conventional baking processes are mostly performed in two processing periods: heating and cooling, each at a constant temperature. This process corresponds to a control vector parameterization problem with a switching function between two levels and choosing the switching time:

$$u = \begin{cases} \theta_1 & for \quad 0 \le t \le \tau_1 \\ \theta_2 & for \quad \tau_1 < t \le t_f \end{cases} \qquad (7)$$

$$\min J = \phi(x(t_f)) + \int_{t_0}^{t_f} L(t, x, \theta) dt \qquad (8)$$

$$\begin{aligned} s.t. \quad & \dot{x} = f(t, x, \theta) \\ & \theta^L \le \theta \le \theta^U \end{aligned} \qquad (9)$$

With $\theta = [\theta_1 \ \theta_2 \ \tau_1]$. The optimization for control vector parameterization is performed with the *pattern search* procedure from Matlabs' optimization toolbox.

3. Application to baking process

3.1. Product and Process Description

Bread is the best known bakery product and is appraised by the consumer on its characteristics. Bread types are differentiated by the initial composition and quality attributes: structure, volume, crispness, softness and color. Bread surface color together with its texture is the most important criteria for design (Purlis and Salvadori, 2006). Therefore, this work considered bread product with different color and texture attributes i.e crispness at the surface as key parameter for design. The other quality parameter is the interior water content which must be in the range of 0.35-0.4 kg/kg to ensure that the product has a smooth crumb texture (Cuq *et al.*, 2003). These attributes are mainly formed in the heating process where several product transformations occur simultaneously due to different heating modes.

During heating state transformations and product quality development are driven by heat and mass transfer. The product quality crispness, softness, brownness, size and crumb are the result of physical and chemical transformations starch gelatinization, volume expansion and the Maillard reaction (Hadiyanto *et al.*, 2007).

Convective, microwave and infra red radiation heating are potential heating modes for baking. Convective heating results in heat transfer from the surface towards the product center. In homogeneous products as bread microwave fields generate heat inside the product, while IR radiation only heats the product surface. Traditionally, baking of bread is performed in ovens at constant temperature in the range of 180-200^{o}C for about 30 minutes (Thorvaldsson and Janestad, 2001). Then the bread is cooled to the room temperature which is achieved between 0.5-1.5 hour after baking (depending on size and the environmental conditions).

3.2. Model development and assumptions

For optimization a baking model was required that describes the baking process and the processes taking place inside the product. In previous work a spatial model was presented that covers the main phenomena during baking (Hadiyanto *et al.*, 2007). The model was built around three main processes: heat and mass transfer of liquid water, of water vapor and of CO_2 (1), state transformations (2) and product quality formation (3), which are modelled as sequential processes (Figure 3). The full model which was presented in the previous work (Hadiyanto *et al.*, 2007) are discussed briefly and presented in Table 1a. Additional equations and boundary conditions are given in Table 1b and Table 1c.

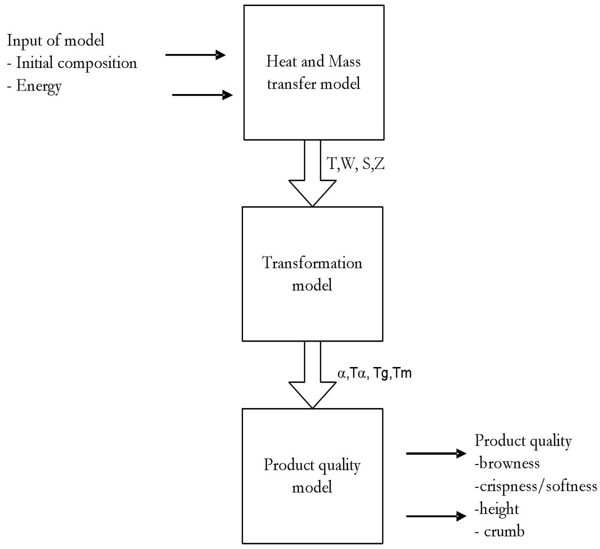


Figure 3. The model structure of baking system (Hadiyanto *et al.*, 2007)

For simulation discretization of one dimension model in 10 segments was found to be satisfactory. This discretization resulted in a system with 108 ordinary differential equations (ODEs) which were solved with integration procedures for stiff sets of ODE (Matlabs' ode15s or ode23s).

3.2.1. Heat and mass transfer

The heat and mass balances for liquid water, water vapour and CO2 gas (Eq. 10-13) follow from the conservation laws for mass and include water evaporation, heat conduction and heat fluxes due to internal convection during baking. The other heating source is microwave which generates heat inside the product. The local changes of liquid water in the product are result of the rates of diffusion fluxes and evaporation (I_v). For additional equations see Table 1a ,1b and 1c. The thermal properties of bread product are described in Table 1d.

Table 1a. The main baking models

Laws of conservation		
Energy	$\rho c_p \frac{\partial T(r,t)}{\partial t} + \frac{\rho \lambda}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = k \frac{\partial^2 T(r,t)}{\partial r^2} - \lambda I_v(r,t) - \frac{\partial (m_v H_v)}{\partial r} - \frac{\partial (m_c H_c)}{\partial r} + Q_{mw}(r,t)$	(10)
Liquid water	$\rho \frac{\partial W(r,t)}{\partial t} + \frac{\rho W(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_w \frac{\partial W}{\partial r}) - I_v$	(11)
Water vapour	$\rho \frac{\partial V(r,t)}{\partial t} + \frac{\rho V(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial V}{\partial r} - m_v) + I_v$	(12)
CO_2	$\rho \frac{\partial V_c(r,t)}{\partial t} + \frac{\rho V_c(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial Vc}{\partial r} - m_c) + I_c$	(13)
State transformations		
Product extension	$\eta \frac{de(r,t)}{dt} + Ee(r,t) = P - P_{atm}$	(14)
Degree of gelatinization	$\frac{d\alpha(r,t)}{dt} = k_{gel}(\alpha_{\max} - \alpha(r,t)) - k_{retro}\alpha(r,t)$	(15)
Melanoidine formation	$\frac{dm_e(r,t)}{dt} = k_{me}(r,t)$ (Maillard reaction)	(16)
Quality attributes		
crumb	$\begin{cases} 0 \quad if \quad \alpha(r,t) = 0 \\ 2\alpha(r,t) \quad if \quad \alpha(r,t) \le 0.5 \\ 1 \quad if \quad \alpha(r,t) > 0.5 \end{cases}$	(17)
crispness	$-\frac{0.0067.(T - T_g(r,t))}{1+\exp(3.(T - T_g(r,t)))}$	(18)
softness	$-k_{soft} \frac{0.01.\exp(3(T - T_g(r,t)))}{1+\exp(3.(T - T_g(r,t)))}$	(19)
brownness	$1 - (1 - m_e(0))e^{-0.23(m_e(r,t))}$	(20)

Table 1b. Additional equations for the baking model

In equation	Descriptions
10-13	$m_v = -\frac{\kappa}{\nu}\frac{V(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
10-13	$m_c = -\frac{\kappa}{\nu}\frac{V_c(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
14	$P = pv + pc$
10	$Q_{mw}(r,t) = \frac{2\alpha_{mw}RP_{0,r}}{r}\exp\left(-2\alpha_{mw}(R-r)\right)$, $P_0,r = \frac{P_{mw}}{2\pi R(L+R)}$
10-13,16	$a_w = \frac{1.05W(r,t)}{0.09+W(r,t)}$
15	$k_{gel} = 2.8.10^{19}\exp(\frac{-139000}{R_g T(r,t)})$
15	$k_{retro} = G_0.\exp\left[\frac{-U^*}{R_g(T(r,t)-T_\infty)}\right]\exp\left[\frac{-K_g}{T(r,t).\Delta T.f_r}\right]$ *if* $T<298^o K$
15,17,19	$\alpha_{\max} = \begin{cases} 0 & \text{if } W<0.5(S+C) \\ \frac{(W-0.5S-0.5C)}{S} & \text{if } 0.5(S+C)<W<0.5(3S+C) \\ 1 & \text{if } 0.5(3S+C)<W \end{cases}$
16	$k_{mr}(r,t) = 4.9\times10^{-3}\times\frac{\exp(9a_w)}{2\times10^3+\exp(11.3a_w)}\exp\left[\frac{-E_a}{R_g}\left(\frac{1}{T(r,t)}-\frac{1}{363}\right)\right]$
19	$k_{soft} = (\frac{-3}{7}+\frac{10}{7}\alpha_{\max}).\frac{\exp(500.(\alpha_{\max}-0.3))}{1+\exp(500.(\alpha_{\max}-0.3))}$
Boundary condition for heat and mass transfer :	
Surface	$k\left.\frac{\partial T}{\partial r}\right\|_{r=R} = h_c(T_{oven}-T(R,t)) - \lambda\rho D_w\left.\frac{\partial W}{\partial r}\right\|_{r=R} + F\varepsilon_r(T_r^4 - T(R,t)^4)$
	$D_{vc}\left.\frac{\partial V}{\partial r}\right\|_{r=R} = h_v(V_{ext}-V(R,t))$
center	$k\left.\frac{\partial T}{\partial r}\right\|_{r=0} = D_{vc}\left.\frac{\partial V}{\partial r}\right\|_{r=0} = 0$

Table 1c. Equation for glass transition and melting temperature

$$T_{g/m} = p_1 + p_2(S/Z) + p_3.W + p_4(S/Z)W + p_5(S/Z)^2 + p_6(W)^2 + p_7(S/Z)^2W^2$$

Parameters	p_1	p_2	p_3	p_4	p_5	p_6	p_7
T_g	457.10	-396.32	-853.21	716.76	430.27	778.44	-1424.71
T_m	472.69	-180.90	-519.97	419.63	124.46	471.87	-749.88

Table 1d. The thermal properties of bread product used in this study

Parameter	Value	Unit
Attenuation factor (α_{mw})	0.2	[1/cm]
Emmisivity (ε_r)	0.9	[-]
Thermal conductivity (k)	0.4	W/mK
Heat capacity (c_p)	2000	J/kg K

3.2.2. State transformations

Product extension (e) gives the change of size (height) compared to the initial height of the product (equation 14). The change of height follows model for visco-elastic systems.

Protein thermosetting reactions and starch state transformation from crystalline state into the gel state and *vice versa* are the main transformations for product texture. Protein thermosetting reactions only solidify the network. Therefore, starch gelatinization and retrogradation are the main transformations relevant for texture properties. The net rate of change of the degree of gelatinization is equal to the rate of gelatinization (Zanoni, Schiraldi, and Simonetta, 1995) minus the rate of retrogradation (equation 15). Here α_{max} is the maximum attainable degree of gelatinization which is a function of the initial composition of the product (content of water, starch and other water binding components in dough) (Hadiyanto *et al.*, 2007).

Gelatinization occurs at higher temperatures and is faster then retrogradation. Therefore gelatinization generally takes place during baking and retrogradation during storage (staling of product). Additional equations are given in Table 1b and 1c.

Browning of bakery products is mainly caused by Maillard reactions which form melanoidins as colouring compounds (eq 16). These reactions are zero order (van Boekel, 2001) and the reaction rate depends on temperature and water content in the product (see also Table 1b)

3.2.3. Product quality model

Crumb (i.e. the open network structure in the center of bread) is linked to the degree of starch gelatinization (Hadiyanto *et al.*, 2007). For a range of Dutch bakery products the relation between crumb and degree of gelatinization given by equation 17 is found.

Crispness and softness of bakery products are linked to the difference between the current product temperature (T_p) and the glass transition temperature of the product (T_g). A product is crisp when T_r-T_g<0 (equation 18). The glass transition temperature is a function of the product composition at the end of baking (see Table 1b). Softness is a combined function of T_r-T_g and the degree of gelatinisation. Products are soft for T_r-T_g >0 but requires a minimum value for the degree of gelatinization above 0.3 (equation 19).The relation between brownness and the amount of melanoidins (*me*) is given by equation 20.

3.3 Defining the optimization problem

3.3.1. Performance index

In a quality driven design procedure, the goal of the design procedure is based on the final product properties after baking. Thus emphasis is on the terminal states in Eq 1 and the running costs are set to zero.

The applied objective function is the sum of the squared deviation of the final quality from their specified value, each multiplied with a weight factor:

$$J = \sum_{i=1}^{N} w_i (x_i(t_f) - x_{s,i})^2 \tag{21}$$

Where w_i is a weight factor for each quality, $x_i(t_f)$ a final quality and $x_{s,i}$ the specified value for the final quality. Different setting values of product attributes are chosen for the surface and product center. Table 2 presents four different specifications products (P-1, P-2, P-3 and P-4) chosen such that there is clear differentiation between the brownness and crispness of the crust while the interior attributes (water content) are equal for all products.

Table 2. The specified values for the final quality and applied weight factors.

Optimized quality	weight factor [unit]	Setting value of product			
		P-1	**P-2**	**P-3**	**P-4**
brownness surface	1 [-]	0.8	0.8	0.65	0.65
crispness surface	10 [-]	0.65	0.8	0.8	0.65
water content center [kg/kg]	10 [(kg/kg)$^{-2}$]	0.38	0.38	0.38	0.38
temperature (surface)	0.0001 [(°C)^2]	25°C	25°C	25°C	25°C

3.3.2. Initial conditions and lower- upper bounds

The initial dough composition was chosen as 0.53 kg/kg for the water content, 0.37 kg/kg for the starch content, 0.02 kg/kg for the sugar content, 0.02 kg/kg for protein content and the rest are additional minor components. The total mass of dough was 0.12 kg with initial height of 0.08 m, radius 0.04 m and the dough was placed in the oven at a room temperature of 25°C.

The applied heating sources for baking were convective heating from the oven temperature (T_{oven}), microwave heating given by the used microwave power (P_{mw}) and radiation heating by the temperature of the radiation source (T_r). Upper and lower bounds (Table 3) are set on these control inputs.

Table 3 Upper and lower bounds on input variables

Input (u)	Continuous		Switching function		
	U^L	U^U	θ_1	θ_2	τ_1
Oven temperature (T_{ext})-°C	20	250	20-250	20-250	0-2.5 hrs
Microwave (P_{mw})-W	0	200	0-200	0-250	0-2.5 hrs
Radiation(T_r)- °C	20	250	20-250	20-250	0-2.5 hrs

4. Results and Discussion

4.1. Convective heating strategies for different products

The main interest of the optimization was to find input (processing) trajectories for different product specifications (P-1, P-2, P-3 and P-4). At this stage optimization is performed with one heating mode (convective heating). Two approaches were compared: a continuous trajectory from the calculus of variations and an optimal switching trajectory obtained from the control vector parameterization method (section 2). The iterations for the first optimization approach were started with a constant temperature trajectory of 120°C. A process time of 2.5 hour is chosen. For the second approach, the control input was transformed into three decision variables: two control parameters θ_1 and θ_2 for the temperature levels and τ_1 for the switching time. Initial condition for the iterations was 120°C for θ_1 , θ_2 and 1.5 hour for τ_1.

Figure 4 gives the obtained input trajectories and corresponding state diagrams for the four product specifications. The trajectories from both approaches show significant differences in processing strategies for the different products. This illustrates that these products require individual treatments, and that these treatments can be found effectively from the dynamic optimization procedures. The state diagrams (Fig 4b and 4d) illustrate differences in the course of the state variables water content and temperature in different parts of the product (surface and center) during different baking strategies.

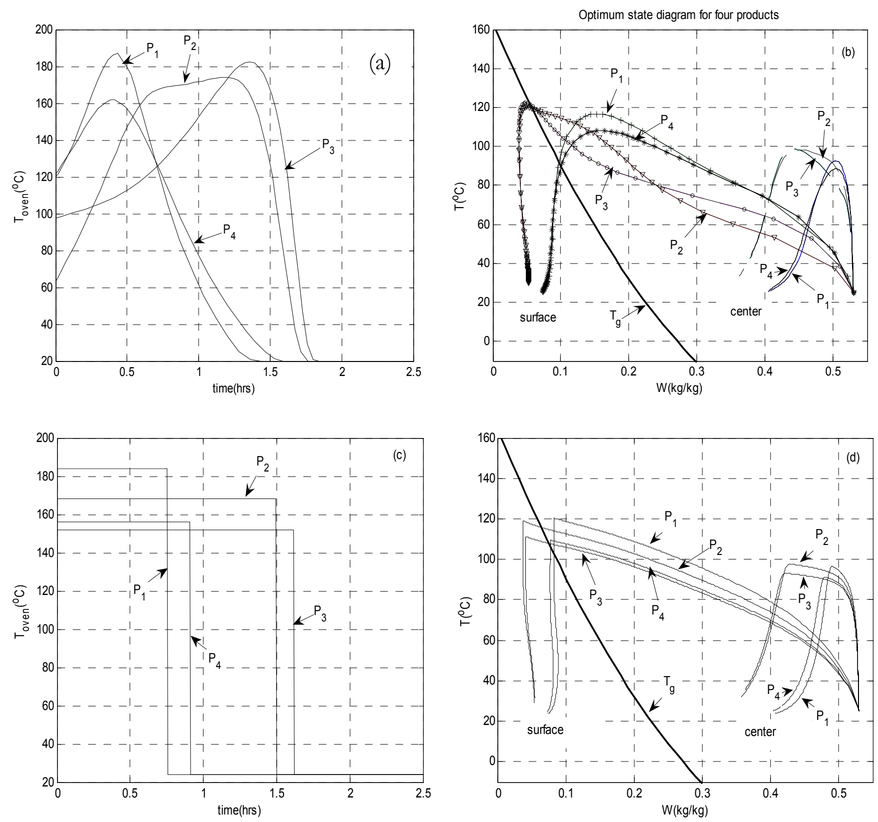


Figure 4. Optimal input trajectories for convective heating of three products and corresponding state diagrams for surface and center. Results from continuous (Fig 4a and 4b) and switching function optimization (Figure 4c and 4d). In both methods, Product P1 and P4 require shorter baking time than P2 and P3 as effect of lower crispness value. To achieve higher brownness value, the products need higher temperature as shown by P1 and P2. The state diagrams show the different routes to form the different products.

In both approaches, product P-1 and P-4 require a shorter heating time than the product P-2 and P-3. However, product P-1 needs a higher oven temperature than product P-4 as a consequence of the higher required level for brownness. The longer baking periods for products P-2 and P-3 make that the maximum product temperature is achieved at lower water content which can be compared with the low crispness products P-1 and P-4. The state diagram also shows the different routes to form different products (Figure 4b). The longer baking period results in more evaporation for the surface only, later followed by the product center region.

For the switching trajectories Figure 4c shows that product P-1 is obtained by heating for 40 minutes at 185°C, which is sufficient to form the surface attributes as shown in table 4. Analogous to the results for the continuous gradient optimization, a longer heating period at lower temperatures is also found for product P-2 and P-3. This procedure yields qualitatively similar results for product P-4 as for the continuous trajectories: a shorter baking period at lower oven temperature. Figure 4d shows the state diagram of temperature - water content for the optimal switching trajectory. The lower brownness values for products P-1 and P-4 are obtained at lower product temperature (110°C) while the higher brownness levels are obtained at higher peak temperatures. The crisp products P-2 and P-4 achieve their maximum temperatures at lower water content values.

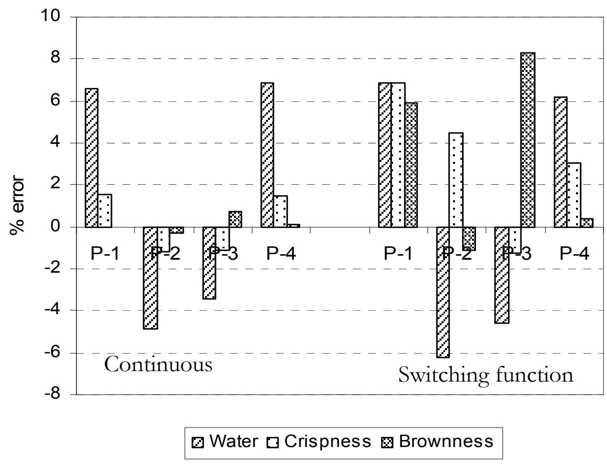


Figure 5 The relative error of each product for optimization using continuous and switching trajectories. The relative error is calculated as $\frac{(x(t_f)-x_s))}{x_s}100\%$

Table 4. Result of baking optimization with convective heating for four different products

Quality	**Continuous**				**Switching Function**			
	P-1	**P-2**	**P-3**	**P-4**	**P-1**	**P-2**	**P-3**	**P-4**
T [^{o}C] -s	25.4	29.8	31.4	25.9	23.8	28.9	31.3	24.7
W [kg/kg]- c	0.4051	0.3615	0.367	0.406	0.4062	0.3564	0.3625	0.4034
crispness [-]	0.6599	0.7907	0.7913	0.6595	0.6576	0.8356	0.7897	0.6696
brownness [-]	0.7998	0.7977	0.6549	0.6507	0.8475	0.7910	0.7039	0.6527
J [-]	0.007327	0.0066533	0.006574	0.007452	0.009885	0.009214	0.00951	0.009355

Comparison of both approaches yields the conclusion that using continuous trajectories result in an adequate process operation and design: the final values for brownness and crispness are close to their specifications (Table 4). The deviation from the specification for the switching (CVP) trajectories is clearly larger (Figure 5). Both approaches do not attain the specified water content in the center of the product. Changing the weight coefficient for the water content in the center of product results in values that are closer to the specifications, however, then the specifications on brownness and crispness are not met. Based on our experiences, the weight values in Table 2 are most satisfactory.

4.2. Multi heating strategies

Convective heating contributed mainly to the development of product attributes at the surface. The product attribute that still farthest away from the required value, was the crumb (water content) in the product center. This was especially true for product P-1 (see table 4 and Fig 5). Evidently, the single heating mode (convection heating) did not suffice to obtain the complete set of required product quality attributes. Thus, we need to change the process configuration. Therefore, convective heating is combined with microwave and radiation heating as option of heating sources.

Figure 6 presents the results for product P-1 obtained with a combination of microwave, radiation and convection heating, both using continuous trajectories (Fig 6a) and switching trajectories (Fig 6b). The contribution of convective heating to the formation of the product properties at the surface is now reduced. Convective heating starts now from a lower temperature. This implies that no preheating of the equipment is required. The radiation temperature starts at 65^{o}C, goes up to 135^{o}C after 20 minutes of baking and decreases subsequently.

The microwave system generates heat inside the product and is able to reduce the water content in the center to close to the specified value. The microwave power starts at 190 Watt, and then decreases to 150 Watt after 40 minutes of baking. At this moment, the contribution of the microwave to reduce the water content in the center is sufficient and the microwave is switched off in the following 5 minutes.

Figure 6b depicts the results for the switching strategy for the combined heating inputs. Convective heating is lowered from 185^{o}C in the previous calculations to 155^{o}C. 135 Watt microwave heating is applied for 45 minutes and a radiation temperature of 100^{o}C is used for nearly one hour.

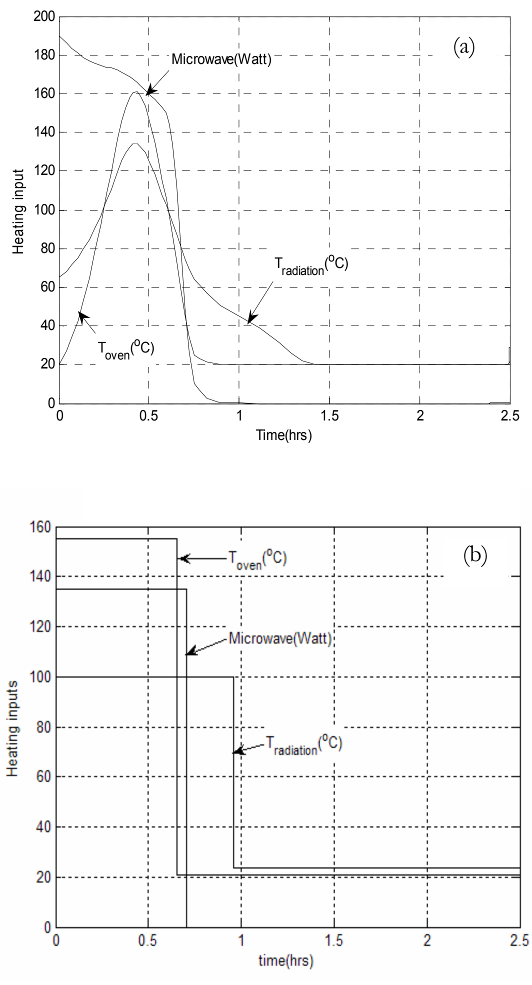


Figure 6 Optimization of baking process with combination of three heating sources: convection, microwave and radiation.

Compared to convective heating only (section 4.1) the combined application of the heating sources improves the overall baking process performance. The deviation from specifications is significantly reduced; the ultimate value of the objective function for both methods is about 25% of that for convective heating only (Table 5). Again, the operations with continuous trajectories perform better than the switching operations, but the difference is smaller.

Table 5. Results for multi-input heating and comparison with convective heating only. The results concern two approaches of dynamic optimization for product P-1.

Quality	Convection		Oven-microwave-radiation	
	Continuous	Switching Function	Continuous	Switching Function
T(°C)-s	25.4	23.8	23.5	26.5
W (kg/kg)	0.4051	0.4062	0.3897	0.3909
Crispness[-]	0.6599	0.6576	0.6581	0.6591
Brownness [-]	0.7998	0.8475	0.7959	0.7885
J [-]	0.007327	0.009885	0.0016574	0.002341

Figure 7 presents the state diagram of the four different heating strategies for product P-1. The figure shows that the product histories obtained with for convective heating only are different from those obtained with combined heating sources.

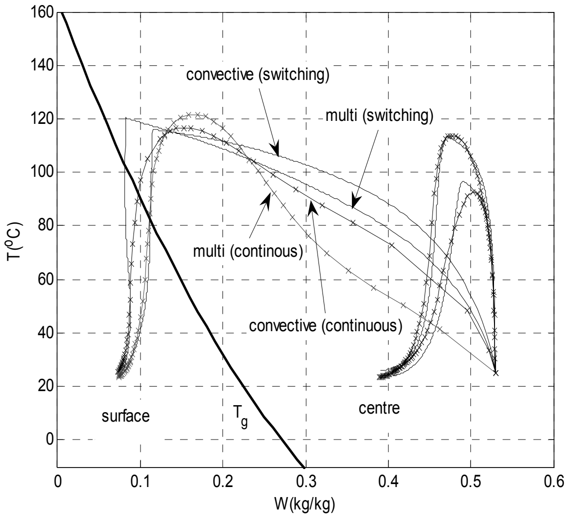


Figure 7 State diagram for the three heating sources: convective, microwave and radiation heating

Due to the microwave heating, the combined heating strategies yield a significant higher product temperature in the center, which intensifies water transport. Radiation shortens the time needed to attain the maximum temperatures of the crust and it is attained at higher water contents. The crust temperature is kept low in the initial process while at the end of process radiation still plays a role in increasing the crust temperature and to perform the brownness formation (see also Fig. 6a).

Figure 8 shows the relative deviation of both methods in terms of optimal final product quality. The continuous method generally gives better performance than the switching method, and application of multi-heating sources could significantly reduced the relative deviations.

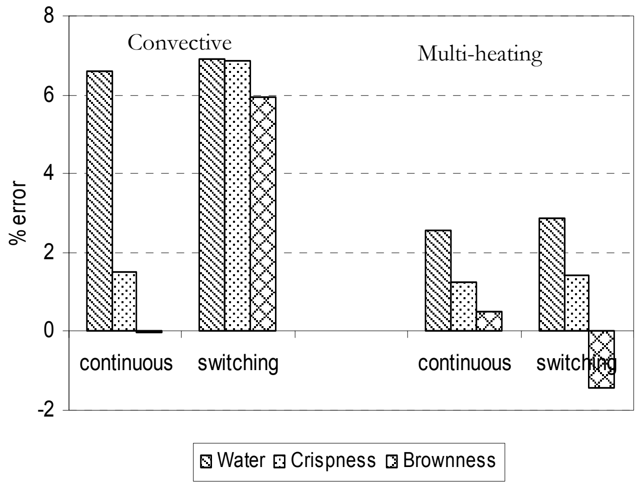


Figure 8. The relative error of optimum quality compared to the setting value for convective and multi-heating inputs. The relative error is calculated as $\frac{(x(tf)-x_s))}{x_s}100\%$

4.3. Variations of dough properties

The final product qualities depend not only on the applied process conditions but also on the dough properties. The dough temperature and water content are of specific interest, however other effects of the composition (starch, fat and sugars) can be investigated in a similar way. Product P-1 was considered as an example; for matter of clarity only convective heating was applied.

4.3.1. Effect of dough temperature

The dough temperature was chosen in the range of 10-55°C. The maximum total baking time was set at 2.5 hours and the initial water content was (as in previous calculations) set to 0.53 kg/kg. Optimization iterations were started with a constant oven temperature trajectory of 120°C over the total baking time.

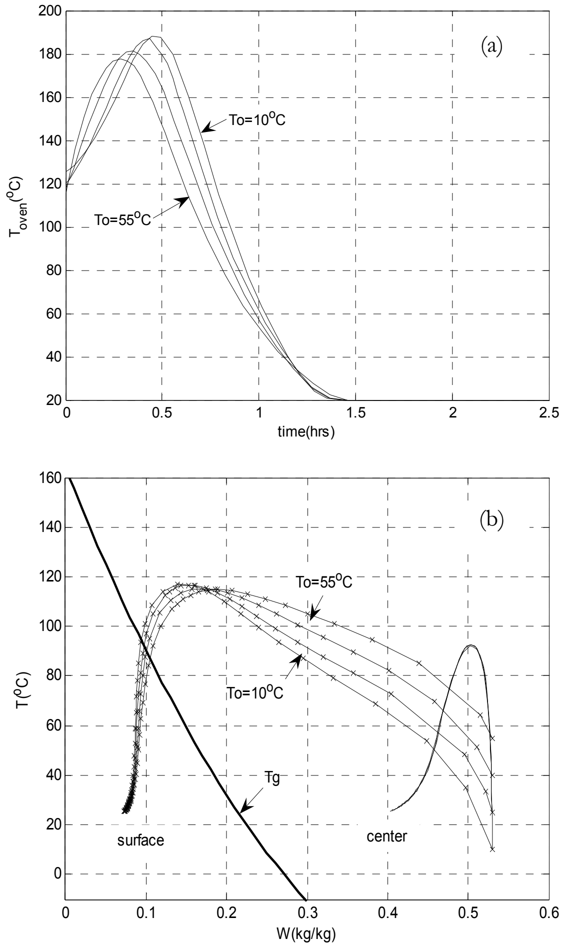


Figure 9. The effect of dough temperature (10-55°C) on the trajectories for convective heating input (a) and the state diagram of water content versus product temperature (b) for product P-1.

Figure 9a presents the optimal heating trajectories for the different initial dough temperatures. Low dough temperatures require higher oven temperatures to compensate. The required time for baking is in all cases nearly the same (1.5 hour).

The state diagram in Figure 9b shows that the starting points of the lines differ with respect to the initial temperatures. The state history for the crust differs in the initial stage of baking, but towards the end the lines are close to each other. The initial dough temperature has no effect on the changes of state in the center. The lines for the center in Figure 9b fall together. Baking with a dough temperature above room temperature gives better baking performance (Table 6). This is mainly result of the lower deviation of the final water content in the center compared to its specified value.

Table 6. Obtained product quality with dynamic optimization for variations in dough temperature for product P-1.

Quality	Dough temperature			
	10°C	25°C	40°C	55°C
T(°C)	25.5	25.4	25.3	25.3
W (kg/kg)	0.4060	0.4051	0.4036	0.4012
Crispness[-]	0.6608	0.6599	0.6598	0.6587
Brownness [-]	0.8006	0.7998	0.8018	0.8010
J[-].	0.0079648	0.007327	0.006556	0.005826

4.3.2. Effect of dough water content

The water content has an important role in product texture development, since it affects the degree of gelatinization that is achieved during baking (see Eq 15) and as a consequence it strongly influences the softness and crispness properties of the product. Rapid evaporation may lead to insufficient gelatinization. Therefore, dough types with different water content will require different baking strategies. Optimization calculations were performed for dough types with water content in the range 0.47-0.55 kg/kg. The initial temperature was set to at 25°C, and the available baking time was 2.5 hour.

Figure 10a shows that the oven temperature trajectories depend strongly on the dough water content. A low initial water content in the dough requires a short heating period at a high temperature, while a high water content in the dough requires a 3 times longer heating period with a 50°C lower maximum value. These values are linked directly to the amount of water that has to be evaporated. Dough with a high water content could be processed during a shorter time at high temperatures, but in that case the crust properties would be compromised.

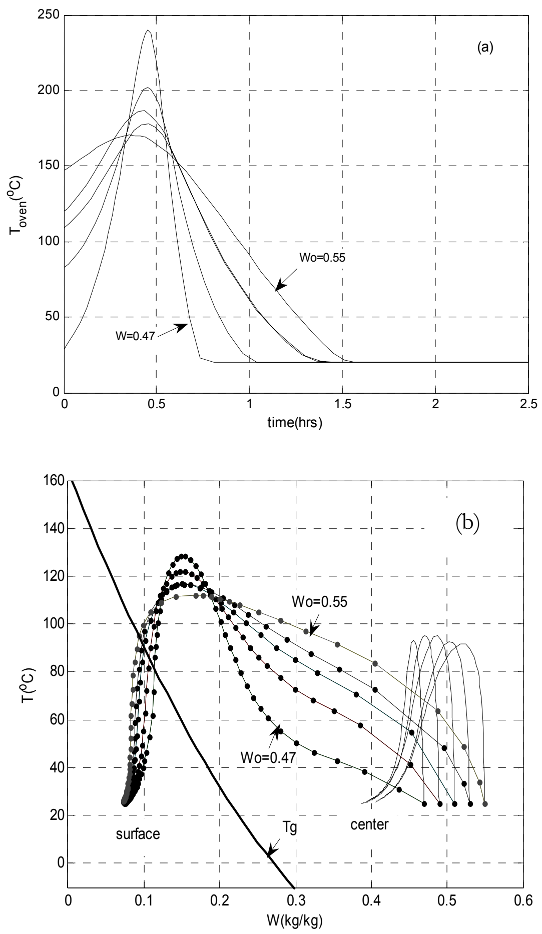


Figure 10 The effect of dough water content (0.47-0.55 kg/kg) on the trajectories for convective heating (a) and the state diagram of water content versus temperature (b) for product P-1.

Figure 10b presents the state diagram for the variations of dough water content. Important differences are observed for the crust. Dough with low water content has stronger evaporation at low temperatures, and a high maximum temperature. This strategy is necessary to obtain sufficient crispness at the surface while at the same time ensuring that the center does not loose too much water. For this dough composition, the deviation of final brownness and crispness of the surface from the specified values is the largest, but the water content in the center is closer to the target than for the other baking procedures.

The state diagram shows that the maximum temperatures for the center differ only a few degrees. For dough with a water content above 0.54 kg/kg, the required product specification in the center is difficult to achieve. Thus additional microwave heating is recommended for these dough types.

Table 7. Obtained product quality with dynamic optimization for a variation of dough water content for product P-1.

Quality	Dough water content (kg/kg)				
	0.47	0.49	0.51	0.53	0.55
T(°C)	25.01	25.3	26.0	25.4	26.15
W (kg/kg)	0.3865	0.3924	0.3985	0.4051	0.4124
Crispness[-]	0.6566	0.6561	0.6581	0.6599	0.6616
Brownness [-]	0.7955	0.7972	0.7998	0.7998	0.8027
J[-]	0.000883	0.0019	0.00420	0.007327	0.0121

4.4. Optimal initial dough parameters

As discussed before, the dough temperature and water content clearly affect the operation strategy of baking processes. The combined effects of variation of these parameters on the value of the objective function are given for convective baking and multi-heating of product P-1 in Fig 11a and Fig 11b.

For convective heating only (Fig 11a), P-1 can attain the required brownness, crispness and internal water content for dough with a water content between 0.47 - 0.48 kg/kg, while the best dough temperature is above room temperature. However, the dough temperature seems not critical.

Figure 11b shows that for the multi-heating system the attained values of the objective function (contour lines) are lower than in figure 11a, which means that the baking process is better. Figure 11b also shows that with multi-heating input, the optimal region is extended, which means that it is less sensitive to the dough water content and temperature. So, there is more freedom to correct variations in initial water content and temperature during the baking process, or in other words the process operation is more flexible.

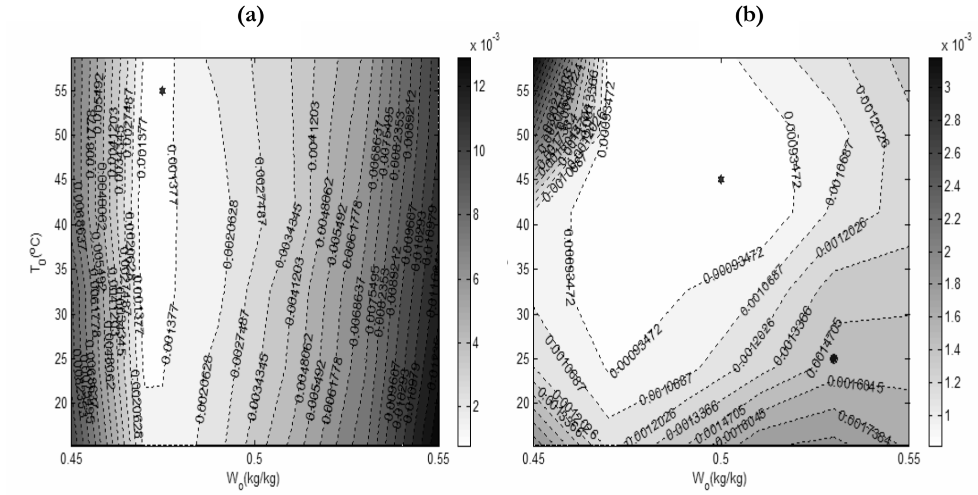


Figure 11. Contour lines for the attained objective function values for combined dough water content (W_o) and dough temperature (T_o) for product P-1 using convective (Fig. 11a) and multi-heating inputs (Fig 11b).

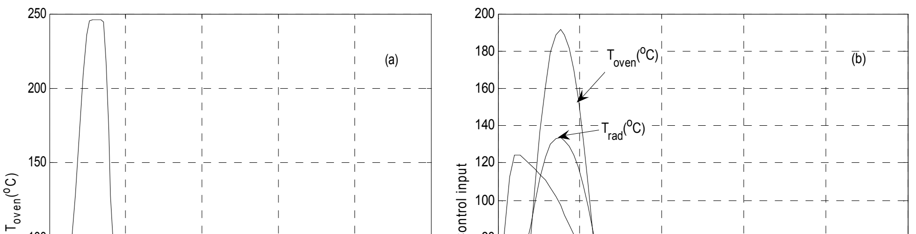


Figure 12. Optimal input trajectories at point [0.475 50°C] for convective (Fig 12a) and [0.51 45°C] for multi-heating inputs (Fig 12b), respectively.

Figure 12 gives the input trajectories for corresponding standard and optimum parameters. A shorter period of heating and higher oven temperature was found for an optimum dough (water content and initial temperature) (Fig 12a). For multi-heating (Fig 12b), the optimal water content was lower than used standard (see Fig 6a), and requires less microwave power.

The main reason for the differences arises from the amount of water that has to be evaporated from the product. The standard convective heating procedure that results in good brownness and crispness, is not long/high enough to evaporate all the water from the product. A lower initial dough moisture content helps therefore. Another alternative is the use of microwave heating which enhances the evaporation.

5. Conclusions

In quality driven process design, product specifications are the starting point for the process design procedure. One needs to find a sequence of product treatment procedures that satisfies the final product specifications. In this work dynamic optimization is applied to find this sequence for some baking products during their passage through baking equipment. The estimated trajectories have still to be transformed into zones for baking equipment with continuous product transport; however this is a standard equipment design problem. The following conclusions are drawn:

- Operation strategies for baking can be calculated by dynamic optimization based on the calculus of variations which results in continuous trajectories, or by control vector parameterization, which results in a switching strategy. Baking using continuous trajectories gives overall a better performance compared to using switching functions.
- Different product quality specifications require different heating strategies. Convective heating can be used to obtain the right product properties at the product surface, but it cannot be easily used to obtain the right product properties in the center.
- Simultaneous heating with different heating sources improves the baking result significantly. Microwave and radiation heating assist convective heating to achieve the specified product qualities, while processing time is reduced. The microwave helps to attain the required water content in the center, while radiation helps the convective heating to obtain the surface qualities.
- The initial properties of the dough have a strong effect on the optimum operation strategies. First, the baking strategies differ for different dough properties. Secondly, by changing the dough properties the objectives can be realized more closely. Therefore,

process and raw materials (trajectory and dough) optimization must be regarded as an integrated problem.

- The approach followed here is illustrated for baked products, however it can be easily extended to other types of product, by development of suitable product models and deciding on an objective function..

Acknowledgement

The authors gratefully acknowledge the financial support from the Graduate School VLAG, the Netherlands. The authors also would like to thank Dr. ir. L.G. van Willigenburg for providing gradient search method algorithm.

Annotations

Symbol	Description	Unit
a_w	Moisture activity	[-]
C	Non-starch moisture binding components	kg kg^{-1}
c_p	Heat capacity	J kg^{-1} K
D_v	Gas diffusivity	m^2 s^{-1}
D_w	Liquid diffusivity	m^2 s^{-1}
e	Relative extension of height	[-]
f_r	Fusion factor	[-]
F	Stefan-Boltzman (5.67E-8)	W m^{-2}K^{-1}
E_a	Activation energy	J mol^{-1}
E	Elasticity	Pa
G	Retrogradation rate constant	s^{-1}
G_0	Reference value for retrogradation rate	s^{-1}
H_c	Enthalpy of moisture vapour	J kg^{-1}
H_v	Enthalpy of CO_2 gas	J kg^{-1}
h_c	Convective heat transfer coefficient	W m^{-2}K^{-1}
h_v	Mass transfer coefficient	m s^{-1}
J	Performance index	[-]
k	Thermal conductivity of product	W m^{-1}K^{-1}
K_g	Retrogradation Constant	[-]
L	Length of product	[m]
k_{me}	Reaction rate constant for Maillard reaction	s^{-1}
k_{soft}	Constant for gelatinization	[-]
k_{gel}	Rate constant for gelatinization	[-]
k_{retro}	Rate constant for retrogradation	[-]
m_v	Mass flux of moisture vapour	kg m^{-2}s^{-1}
me	melanoidines	[-]
m_c	Mass flux of CO_2 gas	kg m^{-2}s^{-1}

M_w	Molecular weight of moisture	kg $kmol^{-1}$
P	Total pressure	Pa
$P_{0,r}$	Incident power of microwave	Watt m^{-3}
P_{mw}	Microwave power	Watt
$p_{v,sat}$	Saturated pressure of moisture vapour	Pa
pv	Partial pressure of water vapour	Pa
pc	Partial pressure of CO_2	Pa
Q_{mw}	Microwave power	[W m^3]
R_g	Gas constant	J $mol^{-1}K^{-1}$
R	Height of product	[m]
R_{CO2}	CO_2 production rate	Kg m^{-2} s^{-1}
S	Sugar content	kg kg^{-1}
t	Time	s
t_f	Final time of process	s
T_∞	Hypothetical temperature	K
To	Initial dough temperature	K
U^*	Activation energy for recrystallization	J mol^{-1}
V_c	CO_2 gas concentration	kg kg^{-1}
V_v	Moisture vapour	kg kg^{-1}
W	Moisture content	kg kg^{-1}
W_o	Initial moisture content	kg kg^{-1}
w	Weight factor	
x	State variable	
Z	Starch content	kg kg^{-1}
T_g	Glass transition temperature	K
T_m	Melting temperature	K
T_r	Radiation temperature	K
u	Input variable	
S/Z	Ratio sugar and starch	[-]

Greek letters

α	Total degree of starch gelatinization	[-]
α_{max}	Maximum attainable degree of gelatinization	[-]
$\alpha_{,mw}$	Attenuation factor	[m^{-1}]
λ	Evaporation heat	J kg^{-1}
ε	Porosity	[-]
ε_r	emissivity	[-]
υ	Kinematics viscosity	m^2 s^{-1}
ρ	Density of product	kg m^{-3}
η	Dynamic viscosity	Pa s
κ	Permeability	kg m^{-3} Pa^{-1} s^{-1}

References

Balsa-Canto, E., Banga, J.R., and Alonso, A.A.(2002a). A Novel, efficient and reliable method for thermal process design and optimization. Part II: applications. *Journal of Food Engineering,* 52, 235-247.

Balsa-Canto, E., Banga, J.R., and Alonso, A.A.(2002b). A Novel, efficient and reliable method for thermal process design and optimization. Part 1: theory. *Journal of Food Engineering,* 52,227-234.

Banga, J.R, Perez-Martin, R.I., Gallardo, J.M., and Casares, J.J.(1991). Optimization of the thermal processing of conduction-heated canned foods: Study of several objective functions,.*Journal of Food Engineering, 14, 25-51*

Barreiro, J.A., Perez, C.R., and Guariguata, C.(1984). Optimization of energy consumption during the heat processing of canned foods, *Journal Food Engineering,* 3, 27–37

Barttfeld, M., Alleborn,N., and Durst, F.(2006). Dynamic optimization of multiple-zone air impingement drying processes. *Computers and Chemical Engineering, 30(3), 467-489*

Baucour, P., Cronin, K., and Stynes, M. (2003). Process optimization strategies to diminish variability in the quality of discrete packaged foods during thermal processing. *Journal of Food Engineering, 60(2), 147-155*

Bellman, R.(1957). *Dynamic programming*, Princeton University Press, Princeton, NJ.

Boss, E.A., Filho, R.M., and Eduardo de Toledo, C.V.(2004). Freeze drying process: real time model and optimization. Chemical *Engineering and Processing, 43(12)*

Biegler, L.T., Cervantes, A.M., and Wächter, A.(2002). Advances in simultaneous strategies for dynamic process optimization. *Chemical Engineering Science, 24, 39*-51

Binder, T., Cruse, A., Villas, C., and Marquardt, W. (2000). Dynamic optimization using a wavelet based adaptive control vector parameterization strategy. *Computers and Chemical Engineering,* 24, 1201–1207

Boekel, M.A.J.S. van .(2001). Kinetic aspects of the Maillard reaction: A critical review. *Nahrung/ Food,* 45 (3), 150–159

Boxtel, A.J.B. van, Otten, Z.E.H., and van der Linden, H.J.L.J.(1992). Dynamic Optimization of a one-stage reverse osmosis installation with respect to membrane fouling. *Journal of Membrane Science* , 65, 277–293

Boxtel, A.J.B. van, and Otten, Z.E.H. (1993). New strategies for economic optimal membrane fouling control based on dynamic optimization. *Desalination*, 90, 363–377

Bryson,A.E.(1999). Dynamic optimization, Editorial Addison Wesley Longman, Inc, Menlo Park, CA.

Bryson, A.E., and Ho,Y.C.(1975). Applied optimal control, New York; hemisphere Pub. Corp.

Chalabi, Z.S., Willigenburg, L.van., and Straten, G.van. (1999). Robust optimal receding horizon control of the thermal sterilization of canned foods. *Journal of Food Engineering*, 40(3), 207–218

Cuq, B., Abecassis, J. and Guilbert,S. (2003). State diagrams to help describe wheat bread processing. *International Journal of Food Science and Technology*, 38(7), 759-766.

Flander,L., Salmenkallio-Marttila, M., Suortti,T., and Auito, K.(2006). Optimization of ingredients and baking process for improved wholemeal oat bread quality. *LWT – Food Science and Technology, article in press*

García,M.S.G, Balsa-Canto,E., Alonso,A.A, and Banga,J.R. (2006). Computing optimal operating policies for the food industry. *Journal of Food Engineering,* 74(1),13-23

Hadiyanto, Asselman, A., van Straten, G., Boom, R.M., Esveld, D.C., and van Boxtel, A.J.B. (2007). Quality Prediction of bakery products in the initial phase of process design. *Innovative Food Science and Emerging Technologies*, 8(2), 285-298

Keskin,S.O., Sumnu,G., and Sahin,S.(2004). Bread baking in halogen lamp–microwave combination oven. *Food Research International,* 37(5), 489-495

Luus ,R.(1993). Application of dynamic programming to differential-algebraic process systems**.** *Computers and Chemical Engineering,* 17(4), 373-377

Mevik,B.H.**,** Færgestad, E.M., Ellekjær,M.R., and Næs,T. (2001). Using raw material measurements in robust process optimization**.** *Chemometrics and Intelligent Laboratory Systems,* 55(1-2), 133-145.

Purlis, E. and V. O. Salvadori. (2007). Bread browning kinetics during baking. *Journal of Food Engineering*, 80(4), 1107-1115.

Roubos, J.A., van Straten,G., and van Boxtel,A.J.B.(1999). An evolutionary strategy for fed-batch bioreactor optimization; concepts and performance. *Journal of Biotechnology*, 67, 173–187.

Saa,J., Alonso,A.A., and Banga, J.R.(1998.) Optimal control of Microwave Heating Using Mathematical Models of Medium Complexity, AcoFoP IV, Goteborg, Sweden.

Schlegel, M., Stockmann,K., Binder,T., and Marquardt, W.(2005). Dynamic optimization using adaptive control vector parameterization. *Computer Chemical Engineering,* 29 (8), 1731–1751

Stigter, J.D., Scheerlinck, N., Nicolaï, and Van Impe, J.F. (2001). Optimal Heating Strategies for a Convection oven. *Journal of Food Engineering,* 48, 335-344

Stryk,O von., and Bulirsch, R.(1992). Direct and Indirect Methods for Trajectory Optimization. *Annals of Operations Research,* 37, 357-373

Sumnu, G., Sahin, S., and Sevimli, M.(2005). Microwave, infrared and infrared-microwave combination baking of cakes **.** *Journal of Food Engineering,* 71(2), 150-155

Therdthai, N., Zhou, W., and Adamczak.(2002). Optimisation of the temperature profile in bread baking **.***Journal of Food Engineering*, 55(1), 41-48

Thorvaldsson,K., and Janestad, H.(1999). A model for simultaneous heat, water, and vapor diffusion. *Journal of Food Engineering,* 40, 167–172

Vassiliadis,V.S., Balsa-Canto, E. and Banga, J.R. (1999). Second order sensitivities of general dynamic systems with application to optimal control problems. *Chemical Engineering Science,* 54, 3851–3860

Zanoni, B., Schiraldi, A., and Simonetta, R.(1995). A naive model of starch gelatinization kinetics. *Journal of Food Engineering,* 24 (1), 25–33

Zorrila, S.E., Banga, J.R., and Sing, R.P. (2003). Dynamic optimization of double-sided cooking of meat patties. *Journal of Food Engineering,* 58(2), 173-182

CHAPTER 5

Control Vector Parameterization with Sensitivity Based Refinement Applied to Baking Optimization

This Chapter has been published as: Hadiyanto, D.C. Esveld, R.M. Boom, G. van Straten and A.J.B van Boxtel. (2007). Control Vector Parameterization with Sensitivity Based Refinement Aplied to Baking Optimization. *Special Symposium Innovations in Food Technology, Denmark*. The manuscript has been invited for submission in Journal Food and Bioproducts Processing

Abstract

In bakery production product quality attributes as crispness, brownness, crumb and water content are developed by the transformations that occur during baking and which are initiated by heating. A quality driven procedure requires process optimization to improve bakery production and to find operational procedures for new products. Control vector parameterization (CVP) is an effective method for the optimization procedure. However, for accurate optimization with a large number of parameters (representing the control vector), CVP optimization takes a long time for computation. In this work, an improved method for direct dynamic optimization using CVP is presented. The method uses a sensitivity based step size refinement for the selection of control input parameters. The optimization starts with a coarse discretization level for the control input in time. In successive iterations the step size was refined for the parameters for which the performance index has a sensitivity value above a threshold value. With this selection, optimization is continued for a selected group of input parameters while the other non sensitive parameters (below threshold) are kept constant. Increasing the threshold value lowers the computation time, however the obtained performance index becomes less. A threshold value in the range of 10-20% of the mean sensitivity satisfies well. The method gives a better solution for a lower computation effort than single run optimization with a large number of parameters or refinement procedures without selection.

Keywords: Baking, optimal operation strategy, baking model, product quality, optimization.

1. Introduction

Quality driven process design can help to meet the challenges of the food industry to produce high quality products. Moreover, the approach also can create flexibility to produce a wide range of products. In quality driven process design, one starts with a process model, which describes the conversion process from ingredients and process conditions, to the product. Next, the product specifications are translated to an objective function. An optimization procedure is applied to find the required product treatment as a function of time and time dependent process conditions. Finally, the treatments are translated into processing equipment (Hadiyanto *et al.,* 2007b; Garcia *et al.*, 2006).

To solve the optimization problem for the processing time indirect and direct methods for dynamic optimization are available. Indirect methods are based on the calculus of variations and use adjoint variables. It follows from the calculus of variations that optimal conditions have been obtained when the derivative of the Hamiltonian with respect to the inputs equals to zero for any point at the input trajectories (Bryson and Ho, 1975). Therefore indirect methods require the computation of the gradient and a search for the control variables trajectories for which the gradient is zero. Betts and Huffman (1998) mentioned two main drawbacks for this approach. First, the necessary conditions for optimization have to be defined and for complicated nonlinear dynamic system this can be quite daunting task. Second, the region of convergence may be surprisingly small, especially when the adjoint variables values do not have a clear physical meaning.

For direct methods the dynamic optimization problem is transformed into a nonlinear programming problem. The main advantage is that there is no requirement to satisfy the necessary conditions for the Hamiltonian function or to use adjoint variables. The control variables are adjusted and optimize the objective function directly. A well known direct method parameterizes the input trajectory over the time interval; this approach is named control vector parameterization (CVP) (Betts and Huffman, 1998).

Both methods (indirect and direct) have been applied for baking processes (Hadiyanto *et al.*, 2007b). Optimization resulted in optimum heating trajectories which can be translated into design for unit operations. The direct method is based on a low discretization level of the control input for heating and cooling. As a consequence, the results obtained with the direct method were of less quality compared to that of the indirect method. Proper choice of the discretization level is a point of concern. Low numbers may not yield optimal results, while a high number mostly may end in local minima and an input trajectory with strong switching values (see Roubos *et. al*, 1999).

The computational time required for direct methods increases significantly with the number of parameters. In recent years a number of methods to reduce computational time of large-scale optimization problems were proposed; for example *refinement of control input* (Binder *et al.*, 2000; Schlegel *et al.*, 2005) or *successive re-optimization* (Garcia *et al.*, 2006). These refinement methods start the optimization with a rough grid (a few parameters) and subsequently the grid is refined to increase the resolution of the control inputs (Binder *et al.*, 2000 and Schlegel *et al.*, 2005). After some refinement iterations a smooth grid is obtained for an acceptable computation time. In the approach of Garcia *et al.* (2006) the refinement is applied to all positions in the time grid by halving the step size from previous refinement iteration until the stopping criteria are fulfilled. However, it must be noted that not all parameters have significant effect on the improvement of the objective function. Therefore, one can reduce the necessary computation time by applying the step size refinement only at points in the time grid with enough sensitivity. This paper illustrates the use of the sensitivity based refinement method for the design of optimal baking operations.

2. Dynamic Optimization

2.1 Problem formulation

Dynamic optimization, also known as open loop optimal control, computes a set of control variables as a function of time that minimizes or maximizes an performance index. The performance index (*J*) composed from the terminal (*Φ)* and running cost (*L*) is optimized within the constraints of the process ($\dot{x} = f(t,x,u)$), and the defined lower and upper bounds of input variables (*u*):

$$
\begin{aligned}
&\min_{u,p,tf} J = \phi(x(t_f)) + \int L(x,t,u)\, dt \\
&st: \quad \dot{x} = f(t,x,u) \quad [t_o, t_f] \quad x(0) = x_0 \\
&\qquad u^L \le u \le u^U \qquad [t_o, t_f]
\end{aligned}
\tag{1}
$$

2.2. Control Vector parameterization

For direct dynamic optimization the optimal control problem is transformed into a Non Linear Programming (NLP) problem. Control vector parameterization implies that the control input is discretized and approximated by a basis function with a limited number of parameters. The state variables in the process model remain in the form of continuous differential equations (Goh and Teo, 1988) (Figure 1). These differential equations are solved by forward integration and for the endpoint ($t=t_f$) the performance index is evaluated and optimized over a number of iterations.

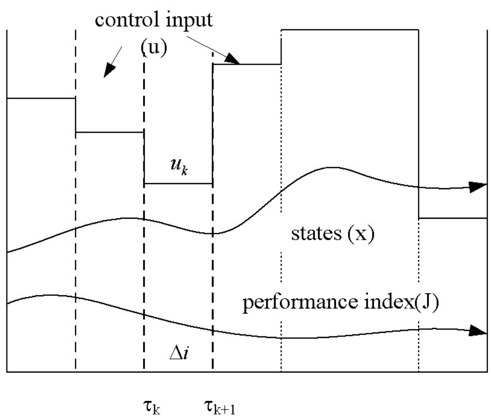


Figure 1. Example of a piece wise constant discretized control input and continuous trajectories of the states and the development of the performance index.

Mostly a low order B-spline function (for example piece-wise constant or piece-wise linear functions) is used to represent the control inputs. Polynomial functions such as Chebychev polynomials can also be used.

For piece-wise constant functions the control input is formulated as:

$$u(t) = u_k, \quad t \in [\tau_k \quad \tau_{k+1}] \\ for\ k = 0,1,..N-2 \tag{2}$$

2.3. Refinement Procedure

A fine grid for the discretization of the control vector in time improves the quality of the control strategy, but it has significant effect on the computational effort. Therefore, to limit the computational effort, we propose to start with optimisation by starting with a low number of parameters (coarse grid). When this optimization has reached a plateau, a step size refinement is applied for a next iteration to achieve better performance. Such refinement procedure has been considered important in the improvement of direct optimization methods. Binder (2000) and Schlegel *et al.*, (2005) used a local resolution based analysis to point out which control parameter needs to be refined further while Balsa-Canto *et al.* (2001) and Garcia *et al.* (2006) applied grid refinement throughout the trajectory.

However, for process optimization, we found that there are several intervals where adjustment of the control parameter has no significant effect on the improvement of the performance index. These intervals can be excluded from further optimization. The selection uses a threshold value for the sensitivity *(*ε_s*)* which separates the control parameters into two groups: u^{opt} , with sensitivity above the threshold value and which will be considered for refinement and further optimization, and u^{const} , with a sensitivity below the threshold value and which are excluded from further optimization. Figure 2 illustrates the selection of control input based on its sensitivity.

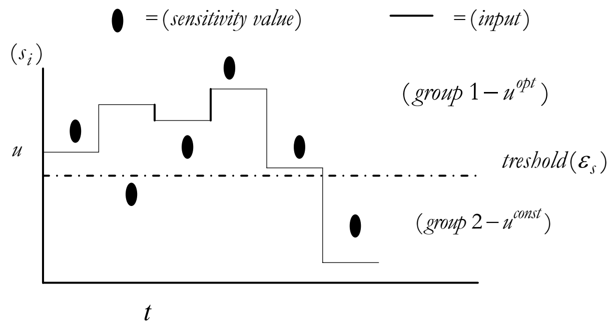


Figure 2. Selection of parameters for refinement based on the sensitivity

The sensitivity (s_i) of each parameter input is given by:

$$s_k = \frac{\partial J}{\partial u_k} \tag{3}$$

$$\varepsilon_s = r_\varepsilon . \bar{s}_k \tag{4}$$

and the selection by

$$\begin{aligned} u_k^\ell (s_k >= \varepsilon_s) \in u_k^{\ell,opt} \\ u_k^\ell (s_k < \varepsilon_s) \in u_k^{\ell,const} \end{aligned} \tag{5}$$

with s_k the sensitivity of parameter with index k, and ε_s the threshold value which fraction (r_ε) of the average sensitivity $(\bar{s}_k)$. In this work the sensitivities are numerically calculated by small perturbations for each individual parameter with δu =10^{-6}.

The threshold value is chosen such that the less sensitive parameters are separated from the parameters to be optimized. Here, the threshold value is linked to the mean sensitivity by multiplication with a proportionality factor (r_ε). The proportionality factor value is an indicator for the range below mean sensitivity; $r_\varepsilon = 0$ means that all input parameters are above the threshold value and therefore they are always refined and further optimized. Using the value $r_\varepsilon = 0$ corresponds to the work of Balsa-Canto (2001) and Garcia *et al.* (2006). By increasing the r_ε value, more parameters will be transferred to the second group that is not optimized further.

The optimization procedure is given by the following pseudo-algorithm. In the first step, the initial number of control parameter input (N_u) and their values (u^0) are defined together with the threshold parameter (r_ε), stopping criteria of optimization, and the maximum number of refinement (l_{max}). For the first iteration ($l=1$), all control parameters are above the threshold value and therefore they are all parameters to be optimized $(u_k^{0,opt})$. The optimizations were performed for this set of parameters and at the end the obtained parameters were evaluated for their sensitivity in regard to performance index (see equations 3 and 4). After grouping by using the threshold value and sensitivity values, a new set of input parameters is obtained by doubling the number of parameters from previous iteration $N_u^{\ell+1} = 2N_u^{\ell}$. The new set of parameters optimized and will be subject for a following refinement. The procedure is repeated until l_{max} is reached.

Pseudo Algorithm

Choose number of input parameters, initial control profiles and final time: N_u^{ℓ} , u^0 , t_f

Specify tolerances, and maximum number of refinement: *TolMesh,TolFun, TolX,* r_ε, l_{max}

For $\ell=1,..\ \ell_{\max}$

$u_k^0 = \left[u_k^{0,opt} \right]$ and $u_k^{0,const} = [\ ]$ (*for initial iteration*)

Do optimization problem with initial guess u_k^0 ,

⟶ store the optimal solution $u_k^{*,\ell}, J^{*,\ell}$

if $\ell < \ell_{\max}$ t hen

Calculate s_i *and* ε_s

(i) $u_k^{*,\ell}\left(s_k^{\ell} > \varepsilon_s\right) \rightarrow u_k^{\ell,opt}$

(ii) $u^{*,\ell}{}_k\left(s_k^{\ell} < \varepsilon_s\right) \rightarrow u_k^{\ell,const}$

⟶refine : $u_k^{\ell+1,opt} = \text{interp}(u_k^{\ell,opt}, \tau_k^{l+1})$,

$$u_k^{\ell+1} = u_k^{\ell+1,opt} \quad , \quad u_k^{l+1,const} = u_k^{l,const}$$

Else

Exit

end if

end for

→ optimal solution: $J_k^*, u_k^{*,\ell}$

For optimization, a direct search by using *Patternsearch* from Matlabs' optimization toolbox is applied. The method is normally used for highly nonlinear functions and if other direct gradient-based methods are not reliable anymore. *Patternsearch* operates from a set of points that form a pattern and it does not require derivatives to determine the descent direction. The pattern is reflected, expanded or shrunk, depending on whether any point within the pattern has a lower objective function value than the current point. The stopping criteria for the procedure are related to those characteristics. If the progress in optimization, expressed in terms of changes in the objective function (*TolFun*), and in changes of the mesh (*TolMesh*), and the changes in the parameters (*TolX*) is below the values as given in Table 1, the optimization ends.

Table 1 Setting of stopping criteria of *patternsearch*

Options	**value**
TolMesh	10^{-4}
TolX	10^{-5}
TolFun	10^{-5}
SearchMethod	*Positive basis Np1*
Mesh Contraction	*2*
Mesh refinement	*0.3*

2.4. Evaluation of the procedure on a reference process

For evaluation of the procedure a reference case on the optimal production of protein in a fed-batch reactor is used. This case was originally formulated by Park and Ramirez (1988). The objective of this case is to maximize the secreted heterologous protein by a yeast strain in a fed-batch culture. The model and its description are given in the work of Park and Ramirez (1988) and Balsa-Canto *et al.* (2001).

Luus (1995) applied dynamic programming while Banga *et al.* (1998) used control vector parameterization without refinement to solve this optimization problem. The attained performance index values were J=32.686 and J=32.562, respectively. To test the effect of refinement to this particular case, we first did a single run optimization (i.e. without refinement) with 40 parameters. The result of this optimization (Figure 3) shows strong variations in values of the succeeding parameters which is the result of local optima of the solution. The calculation time was 35 minutes and the obtained performance index J=32.7297.

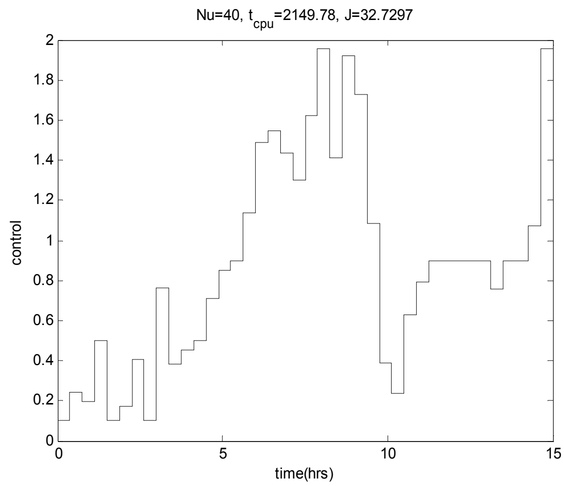
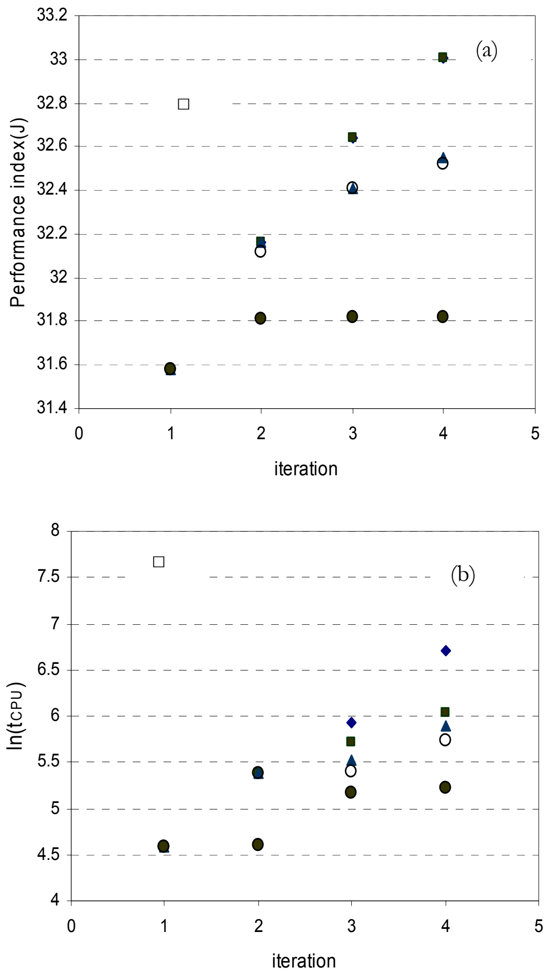


Figure 3 Single run optimization for optimal production of protein with a control vector parameterization by 40 parameters.

In the refinement method the choice for the threshold value is important. Its value has effect on the obtained result and the parameters used during the refinement iterations. The threshold is a fraction (r_ε) of the mean current sensitivity. Figure 4 gives the obtained value of the performance index and the final number of optimization parameters for threshold factors (r_ε) varying from 0 to 1. Increasing threshold factors reduce the number of parameters for optimization (u^{opt}) and consequently lower computation time, but at the same time the final obtained performance index is reduced, meaning that the optimum solution is not attained. The threshold of r_ε =0, which mean all parameters are optimized, could give better performance index, however the computation time is high. Therefore, the choice for the threshold factor is recommended in the range r_ε =0.1-0.2.



♦ r_ε=0 ■ r_ε=0.15 ▲ r_ε= 0.4 O r_ε=0.6 ● r_ε=1 □ single run

Figure 4. The effects of threshold factor *(r_ε)* variation to the final obtained value of the performance index (a) and the required computation time (logarithmic scale) (b)

Figure 5 shows the development of the input trajectories and the sensitivity values for *(r_ε)*=0 and 0.15 respectively. The first refinement iteration started with 5 parameters and after optimization the sensitivity of each parameter is still above the threshold value. Thus, all input parameters are refined and the number of parameters for the second refinement is doubled to 10.

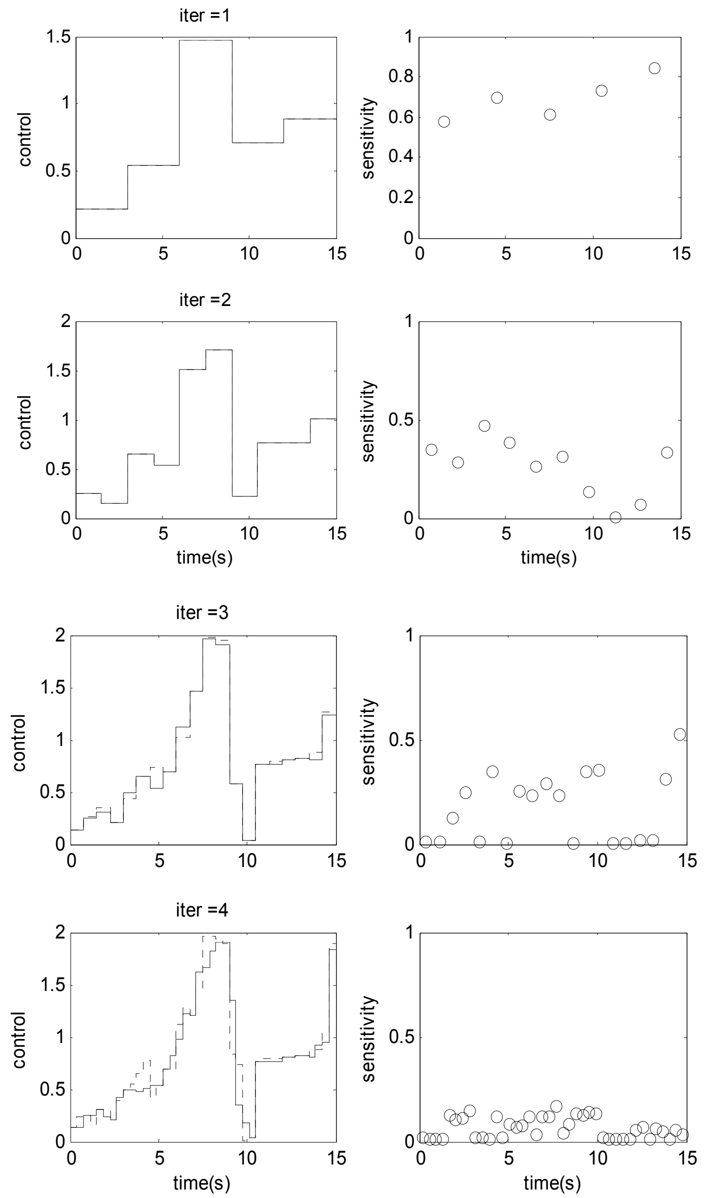


Figure 5 Trajectories for optimal production of protein by using step size refinement with (r_ε=0, dashed line) and (r_ε=0.15, solid line) from the mean sensitivity value.

After optimization in the second refinement iteration, the sensitivity values are evaluated and now there is only one parameter with sensitivity below the threshold value. Therefore, in the third refinement step, the control input to be optimized (u^{opt}) has 18 parameters and one parameter is not optimized further. During the fourth iteration there are only 22 parameters to be optimized which make the computation time is less than full optimization and the result after this step is given in the last graph of Figure 5.

Table 2. Computation time and performance index for optimal protein production optimization

Iteration	Refinement on all CVP-points (r_ε=0)			Refinement with threshold value (r_ε=0.15)			Single run	
	u^{opt}	J	t_{cpu} (s)	u^{opt}	J	t_{cpu} (s)	u^{opt}	J
1	5	31.5805	98	5	31.5805	98	40	32.7297
2	10	32.1610	218	10	32.1612	218		
3	20	32.6412	376	18	32.6392	303		
4	40	33.0028	813	22	33.0032	451		
Total t_{cpu}			*1506*			*1071*		*2149*

u^{opt} : number of parameters for optimization in this step, J: performance index value, t_{cpu}= computation time(s). Computation time on Intel Pentium M processor 1.40 GHz ,Matlab 7.0.

The results in Table 2 show that the required computational time for the refinement based on threshold sensitivity method (r_ε=0.15) is favourable compared to the refinement with no threshold value (r_ε=0) as was used by Balsa-Canto *et al.*, (2001) and Garcia *et al.*, (2006). However, both refinements in Table 2 perform better than the single run optimization (40 parameters, 2149 seconds) in terms of the performance index and computation time. Furthermore, comparing to previous studies (Balsa-Canto *et al.*, 2001; Banga *et al.*, 1998; Luus, 1995) an interesting improvement for the performance index is realized.

3. Application to baking process

In section 2.4 the method has been tested to a standard problem from literature in which the objective function was maximized, and now the method will be applied to bakery production (baking process) optimization. The general purpose of baking optimization is to minimize the deviation of final qualities from the aimed values.

3.1 Formulation of baking optimization problem

The objective of baking optimization is to find optimal heating strategies that result in the specified final product qualities. Baking can be performed by applying different heating inputs as: convective, radiation and microwave heating. Each heating input has a different role in the improvement of baking performance. Convective heating is the most applied type; heat is transferred to the product surface and then penetrates into product by convection and conduction. Microwave heating generates heat inside the product. Radiation (usually infrared) directly heats the upper layer of the product, by exciting rotational/vibration modes in the present molecules. Hadiyanto *et al.*, (2007b) showed that depending on the required final product quality, different optimal heating strategies can be found by optimization.

For optimization the required final qualities have to be translated into a performance index. The following formulation is used to express the performance index.

$$\min \ J = \sum_{i=1}^{N} w_i . (x_i(t_f) - x_{s,i})^2 \qquad (6)$$

where $x_{s,i}$ represent the setting values of the states (qualities) at the end of baking time, and w_i are weighting factors for each product quality. The results in this work are based on the setting values and weight factors as given in Table 3. Please note that while in the validation example of section 2.4 the objective function was maximized, we will here minimize the objective function. This does not give any differences in results or method.

Table 3. Applied setting values for the final product qualities and weight factors

Optimized quality (*x*)	**weight factor (w_i)**	**setting value (x_s)**
brownness surface	1 [-]	0.8
crispness surface	10 [-]	0.65
water content center [kg/kg]	10 [(kg/kg)$^{-2}$]	0.38
temperature [°C]	0.0001 [(°C)^2]	25

3.2 Baking model development

The baking model concerns a series of three sequential processes:

1. Heat and mass transfer of liquid water, water vapour and CO_2,
2. Product transformations
3. Product quality development

The full model was presented in previous work (Hadiyanto *et al.*, 2007a); here the main equations are briefly discussed and presented in Appendix 5.1 (Table 1a, 1b and 1c). Discretization of 1-D in 10 segments was found to be satisfactory. This resulted in a system with 108 ordinary differential equations (ODEs) which were solved with integration procedures for stiff sets of ODEs (Matlabs' ode15s or ode23s).

3.2.1. Heat and mass transfer

The heat and mass balances for liquid water, water vapour and CO_2 gas (eqs. A1-A4) follow from the laws for mass and energy conservation and include water evaporation/condensation. The heat transport is described by convection augmented with a (microwave) source term. The mass transport is described by diffusion equations. The local change of liquid water in the product is the result of the diffusion and the evaporation rate (I_v). For additional equations see Appendix 5.1 (Tables 1a, 1b and 1c) of this chapter. The model parameters were described in Chapter 3 and 4 in this thesis.

3.2.2. State transformations

The product extension (e) gives the change of size (height) compared to the initial height of the product (equation A5). The extension of height is based on Kelvins-Voight' model for visco-elastic material. Protein thermosetting reactions and starch state transformation from crystalline state into the gel state and reverse are the main transformations for product texture. Protein thermosetting reactions only solidify the network. Therefore, starch gelatinization and retrogradation are the main transformations relevant for textural properties. The changes of the degree of gelatinization are equal to the gelatinization rate (Zanoni *et al.*, 1995) minus the retrogradation rate (equation A6). Here is α_{max} the maximum attainable degree of gelatinization which is a function of the initial composition of the product, i.e. content of water (W), starch (S) and other water binding components (C) in dough (Hadiyanto *et al.*, 2007a). Gelatinization occurs at higher temperatures and is faster than retrogradation. Therefore gelatinization takes place during baking and retrogradation during storage (staling of product). Browning of bakery products is mainly caused by the Maillard reaction which forms melanoidins as coloring compounds (eq A7). These reactions are zero order (van Boekel, 2001) and the reaction rate depends on temperature and water content in the product .

3.2.3. Product quality model

Crumb (i.e. the open network structure in the center of bread) is linked to the degree of starch gelatinization (Hadiyanto *et al.*, 2007a). For a range of Dutch bakery products the relation between crumb and degree of gelatinization given by equation A8 is found. Crispness and softness of bakery products are linked to the difference between the current product temperature (T_r) and the glass transition temperature of the product (T_g). A product is crisp when T_r-T_g<0 (equation A9). The glass transition temperature is a function of the product composition. Softness is a combined function of T_r-T_g and the degree of gelatinisation. Products are soft for T_r-T_g >0 but softness requires a minimum value of the degree of gelatinization above 0.3 (equation A10). The relation between brownness and the amount of melanoidins (*me*) is given by equation A11.

4. Results and Discussion

4.1. Case 1: Baking using convective heating

We first discuss baking with convective heating only. The set points for the quality attributes are given in Table 3. A single run optimization ($l = 1$) with 45 parameters and 120°C as initial value for all parameters resulted in a computation time of around 5 hours. The obtained performance index is J = 0.0071432. The optimization result (Figure 6) shows several irregular peaks of the control input which are not expected for a continuous process. This phenomenon is common for CVP with a large number of parameters and illustrates that the final result is in a local minimum.

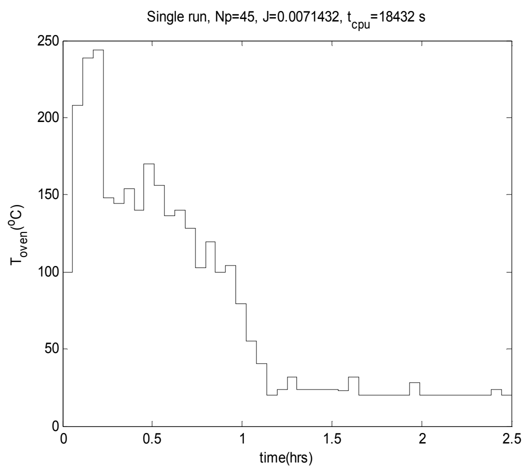


Figure 6 Single run optimization for convective baking with an input represented by 45 parameters

The procedure with refinement is started with 6 parameters and 120°C as initial values for the parameters. Two cases are considered, with $r_\varepsilon = 0$ and 0.2, respectively. Figure 7 gives the development of the input trajectories for convective heating and the sensitivity values used for refinement for the case $r_\varepsilon = 0.2$. For both cases the trajectories fall almost together and have a much more regular form than for the single run optimization. The convergence to optimal solution is illustrated by the decrease of the sensitivity values at each refinement.

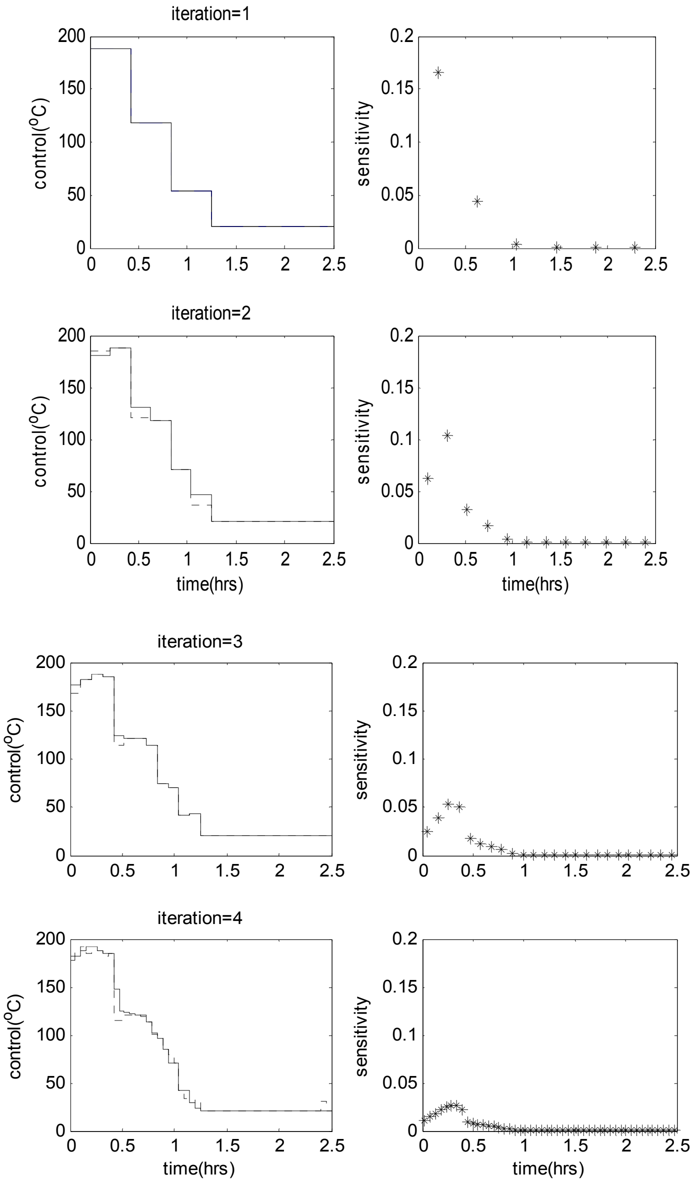


Figure 7 Convective heating baking operation. Succeeding iterations for the optimization procedure with refinement for iteration 1 to 4. (–) with threshold value r_e = 0.2, (--) without threshold value (r_e = 0).

For a factor r_ε=*0.2*, similar trajectories are obtained as for r_ε=*0* while the computation is almost halved (Table 4). The computation time is also about 4 times faster than that for a single run optimization. Moreover, compared to single run optimization the refinement procedure with a threshold factor r_ε=*0.2* gives a clear improvement of the performance index.

Table 4. Computational time and performance index for three different methods

Iteration	Refinement on all CVP-points (r_ε=*0*)			Refinement with threshold value (r_ε=*0.2*)			Single run	
	u^{opt}	J	t_{cpu} (s)	u^{opt}	J	t_{cpu} (s)	u^{opt}	J
1	6	0.00718145	382	6	0.00718145	382	45	0.0071432
2	12	0.00697551	869	6	0.00697542	537		
3	24	0.00692146	1718	12	0.00692135	1078		
4	48	0.00686000	4941	24	0.00684551	2245		
Total t_{cpu}			*7911*			*4243*		*18432*

u^{opt} : number of parameters for optimization in this step, J: performance index value, t_{cpu}= computation time(s). Computation time on Intel Pentium M processor 1.40 GHz using Matlab 7.0.

4.2. Case 2: Baking with multi-heating inputs

Multi-heating baking is another application with setting values as given in Table 3. The applied heating sources are convective heating, characterized by the oven temperature (T_{oven}), radiation, characterized by the temperature of the radiating element (T_{rad}) and microwave power (P_{mw}). The use of the three heating sources makes the baking system more flexible and can result in a better achievement of the product quality goals (Hadiyanto *et al.*, 2007b).

First, the multi-heating system is optimized by a single run optimization and applying 45 parameters for each input, which results in a total of 135 of parameters for optimization (u^{opt}). Trajectories are presented in Figure 8. The single run optimization results in a performance index of J = 0.003725 and required about 11 hours of computation time. The trajectories are more irregular than for the single input optimization and are not very intuitive for a continuous process.

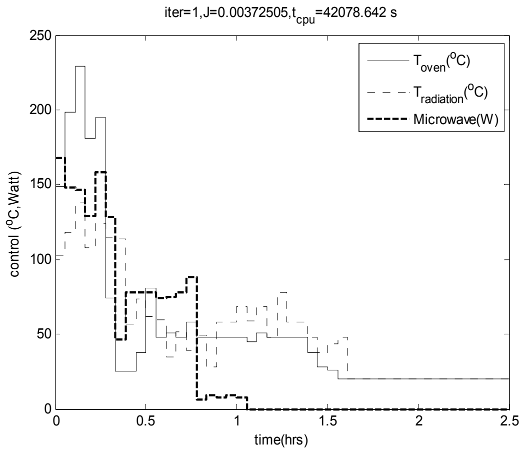


Figure 8. Single run optimization for multi-heating baking. Each input is represented by 45 parameters.

In the case with only convective heating, we concluded that the refinement procedure with r_e = 0.2 performed best. Thus we only apply this procedure here. The results for the step size refinement are given in Figure 9 and Table 5.

Figure 9 shows the development of the trajectories and the sensitivity values for four succeeding refinement steps. At the start, each input is represented by 6 parameters which results in a total of 18 parameters. This set of parameters can be optimized quickly. In the next refinement iteration only 6 input parameters with sensitivity above the threshold value are optimized (18 for total). This strongly reduces the computation time compared to a procedure in which all parameters are refined (36 parameters).

Table 5 shows that finally 50% of the control parameters are selected for u^{opt}. Control parameters in the first 1.25 hour are the most sensitive (u^{opt}), while the rest are not sensitive and are not varied. Compared to the single run optimization, the refinement method gives a much better performance index (80% improved) and requires much less computation time (a factor 6 less). Moreover the trajectories have a more regular form that complies to the continuous nature of the process.

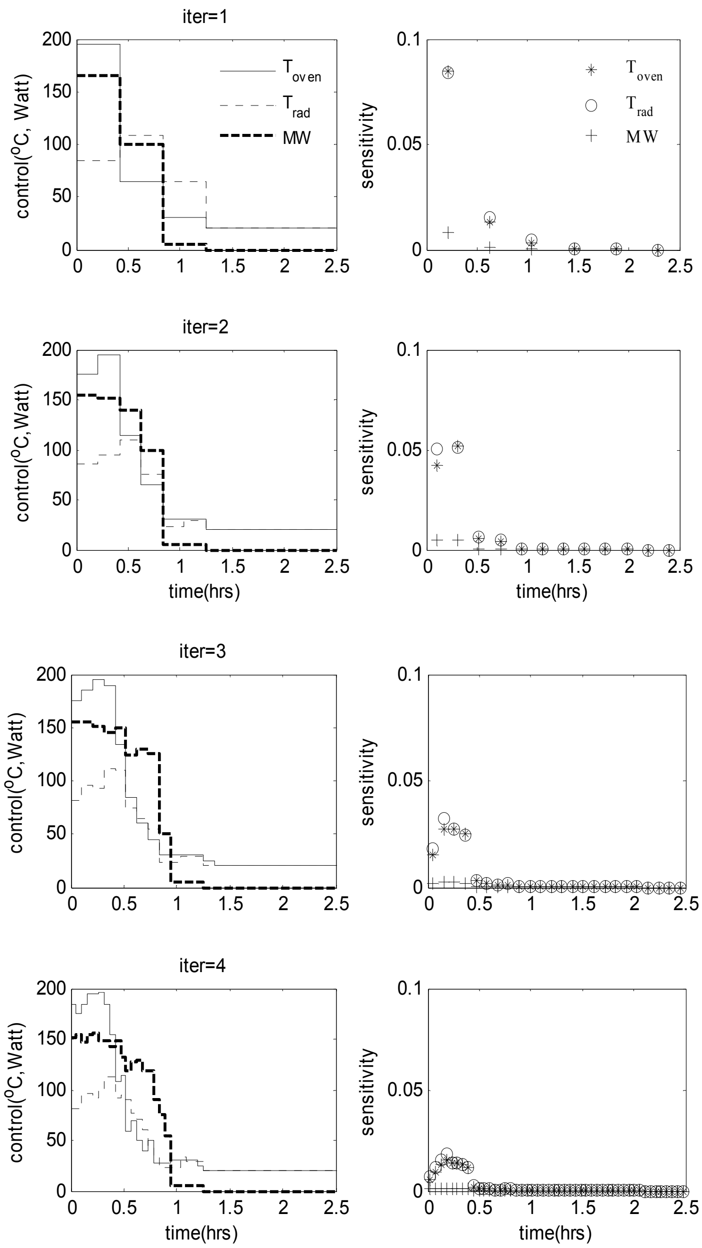


Figure 9. Succeeding iterations optimization procedure for multi-heating baking operation with refinement for iteration 1 to 4 and threshold factor r_ε=0.2.

Table 5. Results of optimization with refinement for multi-heating baking process. The optimization is performed with threshold factor r_ε=0.2 and compared to single run optimization.

Iter(l)	Refinement with r_ε=0.2			Single run	
	u^{opt}	J	t_{CPU} (s)	u^{opt}	J
1	18	0.00370194	785	45	0.0071432
2	18	0.00205799	1264		
3	36	0.00156933	2057		
4	76	0.00144551	3245		
Total t_{cpu}			*7352*		*42078*

5. Conclusion

The improvement of control vector parameterization in optimization by using sensitivity functions has been presented. Starting with a low number of parameters, the refinement method showed a significant reduction of computation time while the achieved performance index was still equal as compared to full control vector parameterization. The refinement method used a threshold sensitivity to group input parameters. The reduction of the number of input parameters to be optimized (above threshold value) resulted in lower computational effort, and in this work it was found that the recommended threshold value is in the range of 10-20% of the mean sensitivity.

Keeping computational time within limits becomes critical for larger complex systems. A significant reduction of the computation time was achieved with convective and multi-heating baking, including a heating and cooling period. The control parameters in the cooling period have minimal effect on the performance index and therefore these parameters were hardly considered in the optimisation procedure. The optimization focused itself on the heating period, by which the performance index is the most affected. Refinement gives a good estimate of the optimal process.

The proposed control vector parameterization method has two-fold benefit. First, it is useful for optimization of the design and operation of large process systems, but also identifies critical control points in the production process, yielding more insight in what factors determine the quality of the product. For example, the layout and operation of complete or parts of complex food production systems, or even supply chains with long periods of cooling where product quality is not very sensitive to the settings, as long as they stay in a certain (low) region. Secondly, the method identifies the parameters that are most important to the product quality. This critical control point analysis will facilitate further study and improvement of the production system.

Acknowledgement

This work is financed by the Graduate School VLAG, the Netherlands. The authors acknowledge Dr. Hans Stigter (Wageningen University) for his highly valuable suggestions and discussions for this work.

Annotations

Symbol	Description	Unit
a_w	Water activity	[-]
C	Non-starch water binding components	kg.kg^{-1}
D_v	Gas diffusivity	m^2.s^{-1}
D_w	Liquid diffusivity	m^2.s^{-1}
e	Relative extension of height	[-]
f	Fusion factor	[-]
E_a	Activation energy	J.mol^{-1}
G	Retrogradation rate constant	s^{-1}
G_0	Reference value for retrogradation rate	s^{-1}
H_c	Enthalpy of water vapour	J.kg^{-1}
H_v	Enthalpy of CO_2 gas	J.kg^{-1}
h_c	Convective heat transfer coefficient	Wm^{-2}K^{-1}
h_v	Mass transfer coefficient	m.s^{-1}
J	Performance index	[-]
k	Thermal conductivity of product	Wm^{-1}K^{-1}
K_g	Constant	[-]
k_{me}	Reaction rate constant for Maillard reaction	s^{-1}
k_{soft}	Constant for gelatinization	[-]
k_{gel}	Rate constant for gelatinization	[-]
k_{retro}	Rate constant for retrogradation	[-]
m_v	Mass flux of water vapour	kg.m^{-2}s^{-1}
me	melanoidines	[-]
m_c	Mass flux of CO_2 gas	kg.m^{-2}s^{-1}

M_w	Molecular weight of water	$kg.kmol^{-1}$
Nu	Total number of input parameter	[-]
P	Total pressure	Pa
$P_{0,r}$	Incident power of microwave	$Watt.m^{-3}$
P_{mw}	Microwave power	Watt
$p_{v,sat}$	Saturated pressure of water vapour	Pa
Q_{mw}	Microwave power	[W m^3]
R_g	Gas constant	J $mol^{-1}K^{-1}$
R	Height of product	[m]
R_{CO2}	CO_2 production rate	kg m^{-2} s^{-1}
S	Sugar content	kg kg^{-1}
t	Time	s
T_∞	Hypothetical temperature	K
To	Initial dough temperature	K
$U*$	Activation energy for recrystallization	$J.mol^{-1}$
V_c	CO_2 gas concentration	kg kg^{-1}
V_v	Water vapour	kg kg^{-1}
W	Water content	kg kg^{-1}
W_o	Initial water content	kg kg^{-1}
Z	Starch content	kg kg^{-1}
T_g	Glass transition temperature	K
T_m	Melting temperature	K
Tr	Radiation temeparture	K
S/Z	Ratio sugar and starch	[-]
s	Sensitivity	
u^{opt}	Input parameter subjected for optimized group	
u^{const}	Input parameter subjected for constant group	
r_ε	Factor of sensitivity threshold	[-]
l_{max}	Maximum refinement iteration	[-]
t_f	Final time of processes	[s]

Greek letters

α	Total degree of starch gelatinization	[-]
α_{max}	Maximum attainable degree of gelatinization	[-]
$\alpha_{,mw}$	Attenuation factor	[m^{-1}]
λ	Evaporation heat	J kg^{-1}
ε	Porosity	[-]
ε_s	Treshold value for sensitivity	[-]

ε_r	emissivity	[-]
υ	Kinematics viscosity	$m^2\ s^{-1}$
ρ	Density of product	$kg\ m^{-3}$
η	Dynamic viscosity	Pa s
κ	Permeability	$kg\ m^{-3}\ Pa^{-1}\ s^{-1}$
τ	Time knot	[s]

References

Balsa-Canto, E., Banga, J.R., Alonso, A.A., and Vassiliadis,V.S. (2001).Dynamic Optimization of Chemical and Biochemical Processes Using restricted second order information. *Computer and Chemical Engineering, 25*, 539-546.

Balsa-Canto, E., Banga, J. R., Alonso, A.A., and V. S. Vassiliadis.(2002). Restricted Second Order Information for the Solution of Optimal Control Problems using Control Vector Parameterization. *J. Process Control*, 12 (2), 243–255.

Banga, J.R., Irizarry, R. and Seider, W.D., (1998). Stochastic optimization for optimal and model-predictive control. *Computers and Chemical Engineering,* 2, p. 603.

Banga, J.R., Balsa-Canto, E., Moles, C.G., and Alonso, A.A. (2003). Improving food processing using modern optimization methods. *Trends in Food Science and Technology, 14(4), 131-144*

Betts, J., T., and Huffman W. P. (1998). Mesh refinement in direct transcription methods for optimal control. *Optimal Control Applications and Methods,19(1), 1-21*

Binder, T., Cruse, A., Cruz Villar, C.A and Marquardt, W. (2000). Dynamic optimization using a wavelet based adaptive control vector parameterization strategy. *Computers and Chemical Engineering, 2*4(2-7), 1201.

Boekel, M.A.J.S. van .(2001). Kinetic aspects of the Maillard reaction: A critical review. *Nahrung/ Food,* 45 (3), 150–159

Bryson, A.E. (1999). Dynamic optimization, Editorial Addison Wesley Longman, Inc, Menlo Park, CA.

Bryson, A.E., and Ho, Y.C.(1975). Applied Optimal Control Optimization, Estimation and Control. Hemisphere Publication Company, New York

Garcia, M.S.G, Balsa-Canto,E., Alonso, A.A. and Banga,J.R. (2006). Computing optimal operating policies for the food industry. J*ournal of Food Engineering. 74(1),*13-23

Goh,C.J. and Teo,K.L.(1988).Control parameterization: A unified approach to optimal control problems with general constraints. *Automatica*.24(1), 3-18

Hadiyanto, Asselman, A, van Straten, G., Boom, R.M., Esveld, D.C and van Boxtel, A.J.B.(2007a). Quality prediction of bakery products in the initial phase of process design. *Innovative Food Science and Emerging Technologies*, 8(2),285-298

Hadiyanto, Esveld, D.C., Boom, R.M. , van Straten, G. and van Boxtel, A.J.B. (2007b). Product Quality driven design of baking operation using dynamic optimization, *submitted*

Luus, R.(1995).Sensitivity of control policy on yield of a fed-batch reactor. *IASTED International Conference on Modelling and Simulation.* Pittsburgh, PA..

Park, S. and Ramirez, W.F. (1988). Optimal production of secreted protein in fed-batch reactors. *AIChE Journal.* 34(8),. 1550–1558.

Roubos, J.A., Straten, G van and van Boxtel, A.J.B. (1999). An evolutionary strategy for fed-batch bioreactor optimization: Concepts and performance. *Journal of Biotechnology,* 67, 173–187

Schlegel, M., Stockman, K. , Binder, T., and Marquardt, W. (2005). Dynamic optimization using adaptive control vector parameterization. *Computers and Chemical Engineering,* 29(8), 1731.

Zanoni, B., Schiraldi, A., and Simonetta, R.(1995). A naive model of starch gelatinization kinetics. *Journal of Food Engineering,* 24 (1), 25–33

Zhang, J and Datta, A.K. (2005). Mathematical modelling of bread baking process. *Journal of Food Engineering,* 75, 78-89

Appendix 5.1

Table 1a. The main baking models

Laws of conservation		
Energy	$\rho c_p \frac{\partial T(r,t)}{\partial t} + \frac{\rho\lambda}{1+e(r,t)}\frac{\partial e(r,t)}{\partial t} = k\frac{\partial^2 T(r,t)}{\partial r^2} - \lambda I_v(r,t) - \frac{\partial(m_v H_v)}{\partial r} - \frac{\partial(m_c H_c)}{\partial r} + Q_{mw}(r,t)$	A1
Liquid water	$\rho \frac{\partial W(r,t)}{\partial t} + \frac{\rho W(r,t)}{1+e(r,t)}\frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_w \frac{\partial W}{\partial r}) - I_v$	A2
Water vapour	$\rho \frac{\partial V(r,t)}{\partial t} + \frac{\rho V(r,t)}{1+e(r,t)}\frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial V}{\partial r} - m_v) + I_v$	A3
CO_2	$\rho \frac{\partial V_c(r,t)}{\partial t} + \frac{\rho V_c(r,t)}{1+e(r,t)}\frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial Vc}{\partial r} - m_c) + I_c$	A4
State transformations		
Product extension	$\eta \frac{de(r,t)}{dt} + Ee(r,t) = P - P_{atm}$	A5
Degree of gelatinization	$\frac{d\alpha(r,t)}{dt} = k_{gel}(\alpha_{\max} - \alpha(r,t)) - k_{retro}\alpha(r,t)$	A6
Melanoidine formation	$\frac{dm_e(r,t)}{dt} = k_{me}(r,t)$ (Maillard reaction)	A7
Quality attributes		
crumb	$\begin{cases} 0 & if \quad \alpha(r,t) = 0 \\ 2\alpha(r,t) & if \quad \alpha(r,t) \le 0.5 \\ 1 & if \quad \alpha(r,t) > 0.5 \end{cases}$	A8
crispness	$-\frac{0.0067.(T - T_g(r,t))}{1+\exp(3.(T - T_g(r,t)))}$	A9
softness	$-k_{soft}\frac{0.01.\exp(3(T - T_g(r,t)))}{1+\exp(3.(T - T_g(r,t)))}$	A10
brownness	$1 - (1 - m_e(0))e^{-0.23(m_e(r,t))}$	A11

Table 1b. Additional equations for the baking model

In equation	Descriptions
A1-A4	$m_v = -\frac{\kappa}{\nu}\frac{V(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
A1-A4	$m_c = -\frac{\kappa}{\nu}\frac{V_c(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
A5	$P = pv + pc$
A1	$Q_{mw}(r,t) = \frac{2\alpha_{mw}RP_{0,r}}{r}\exp\left(-2\alpha_{mw}(\mathrm{R}-r)\right)$, $P_0,r = \frac{P_{mw}}{2\pi \mathrm{R}(L+\mathrm{R})}$
A1-A4,A7	$a_w = \frac{1.05W(r,t)}{0.09+W(r,t)}$
A6	$k_{gel} = 2.8.10^{19}\exp(\frac{-139000}{R_g T(r,t)})$
A7	$k_{retro} = G_0.\exp\left[\frac{-U^*}{R_g(T(r,t)-T_\infty)}\right]\exp\left[\frac{-K_g}{T(r,t).\Delta T.f_r}\right]$ $if \quad T<298^o K$
A7,A9,A10	$\alpha_{\max} = \begin{cases} 0 & if \quad W<0.5(S+C) \\ \frac{(W-0.5S-0.5C)}{S} & if\ 0.5(S+C)<W<0.5(3S+C) \\ 1 \quad if \quad 0.5(3S+C)<W \end{cases}$
A7	$k_{me}(r,t) = 4.9\times10^{-3}\times\frac{\exp(9a_w)}{2\times10^3+\exp(11.3a_w)}\exp\left[\frac{-E_a}{R_g}\left(\frac{1}{T(r,t)}-\frac{1}{363}\right)\right]$
A10	$k_{soft} = (\frac{-3}{7}+\frac{10}{7}\alpha_{\max}).\frac{\exp(500.(\alpha_{\max}-0.3))}{1+\exp(500.(\alpha_{\max}-0.3))}$

Boundary condition for heat and mass transfer :

Surface

$$k\left.\frac{\partial T}{\partial r}\right|_{r=\mathrm{R}} = h_c(T_{oven}-T(\mathrm{R},t)) - \lambda\rho D_w\left.\frac{\partial W}{\partial r}\right|_{r=\mathrm{R}} + F\varepsilon_r(T_r^{\,4}-T(\mathrm{R},t)^4)$$

$$D_{vc}\left.\frac{\partial V}{\partial r}\right|_{r=\mathrm{R}} = h_v(V_{ext}-V(\mathrm{R},t))$$

center

$$k\left.\frac{\partial T}{\partial r}\right|_{r=0} = D_{vc}\left.\frac{\partial V}{\partial r}\right|_{r=0} = 0$$

Table 1c. Equation for glass transition and melting temperature

$$T_{g/m} = p_1 + p_2(S/Z) + p_3.W + p_4(S/Z)W + p_5(S/Z)^2 + p_6(W)^2 + p_7(S/Z)^2W^2$$

Parameters	p_1	p_2	p_3	p_4	p_5	p_6	p_7
T_g	457.10	-396.32	-853.21	716.76	430.27	778.44	-1424.71
T_m	472.69	-180.90	-519.97	419.63	124.46	471.87	-749.88

CHAPTER 6

Multi-objective Optimization to Improve the Product Range of Baking Systems

This Chapter has been submitted for publication as: Hadiyanto, R.M.Boom, G. van Straten, A.J.B van Boxtel, and D.C. Esveld. (2007). Multi-objective Optimization to Improve the Product Range of Baking Systems. *Journal of Food Process Engineering*

Abstract

The operational range of a food production system can be used to obtain a variation in certain product characteristics. The range of products characteristics that can be simultaneously realised by an optimal choice of the process conditions is inherently limited. Knowledge of this feasible product range and the limitations therein would be of great help to the process/product innovator. In this paper the method of Pareto analysis in combination with dynamic optimisation is introduced to map the feasibility range for multi-objective optimization problems. The Pareto front obtained for a set of conflicting objectives divides the product specification space in a feasible and a non-feasible area. For process design such an analysis is a versatile tool to evaluate different options and to search for extension of the operational range. In this paper, Pareto analysis is applied for bakery production. Bakery products might have conflicting specifications for the final quality (crispness, brownness and moisture content). The analysis showed how the feasible area is changed as the initial dough water content is modified. Furthermore it is proven that by modification of the process (i.e., application of multi-heating systems - combined convective, microwave and radiation heating) the feasible area is extended significantly. Taking these options into account, the operational range of bakery systems is improved significantly.

Keywords: Baking, Multi-objective optimization, bakery, feasible solutions

1. Introduction

Food process design aims to find operation and processing strategies to obtain targeted product qualities. Food production systems should be able to produce products with varying specifications, and thus flexibility is an important aspect in food process design. Optimization is a versatile method for the design of flexible systems and it was shown that such methods are efficient to realize different product specifications by adaptation of the processing methods (Hadiyanto *et al.,* 2007b). Given the required product specifications and process characteristics, we see that usually a trade-off exists among the design specifications and for many applications such an inherent conflict in the design objectives exist. If the objectives are conflicting, then the design problem switches to finding the remaining possible design solutions rather than finding the globally optimal solution. This type of problem is known as multi-objective optimization which is still a challenging task in the area of food process design.

The solutions of multi-objective problems are conceptually different from single-objective optimization. In multi-objective optimization, there may not be a solution which satisfies all objectives. Instead, there are multiple sub-optimal solutions depending on how the multiple objectives are combined in a single criterion (Sarkar *et al.*, 2006; Zhang *et al.*, 2002). By changing the balance given to the different conflicting objectives, a family of so called Pareto-optimal solutions can be found. The Pareto set of solution forms a front that divides the solution space in a feasible and an unfeasible solutions subspace (Gurnani *et al.*, 2005). On the Pareto front each individual objective function component can only be improved by worsening at least one of the other individual objectives. Therefore the Pareto front is very useful, because it narrows the choices and helps to guide a decision maker in the selection of a desired process operation from the set of Pareto-optimal points (Zhang *et al.*, 2002).

Multi-objective optimization has been an object of interest to engineers for a long time, but only a few studies on multi-objective optimization have been reported in the mainstream of food engineering literature. Furthermore, most food processes deal with dynamic system and therefore the application of dynamic multi-objective optimization has more potential. The possibility of two or more conflicting objectives can be illustrated for bakery applications where a strategy to achieve one of the product qualities may worsen other qualities. For example, increasing surface brownness conflicts with the aim of having lower crispness. Therefore, it is an essential aspect in quality driven process design to find a set of possible solutions by means of multi-objective optimization. Single-objective function optimization to reach specified brownness, crispness and moisture content of bakery products was previously reported (Hadiyanto *et al.*, 2007a) and it was shown that the final product quality determines the optimal heating strategy during baking. In that application, the applied combination heating strategy of convective, microwave and radiation could enhance the flexibility of the process resulting in a larger diversification of possible products. This work focuses on the multi-objective optimization applications in the design of bakery production systems with conflicting product specifications.

2. Multi-objective Optimization

Multi-objective optimization problem is given as the simultaneous minimization of multiple objective functions *(J)* for separate specified criteria or quality attributes (q_i^*) , here defined by Eqs 1-2

$$J = \begin{bmatrix} J_1 & J_2 & \cdots & J_n \end{bmatrix}^T \tag{1}$$

$$J_i(u) = \left(Q(x_i(t_f)) - q_i^{\ *} \right)^2 \tag{2}$$

where u is a vector of design and input variables that determine the evolution of the state variables $x(t)$, Q is a vector of quality attributes that is evaluated at the end of the process (t_f) and q^* is the set point or target value of quality. The purpose is to find the optimal vector u^* that minimizes J in some sense. The standard approach of solving a multi-objective optimization problem is to create a single objective function as the weighted sum of the individual objectives (Zadeh, 1963):

$$\min \quad J = \sum_{i=1}^{n} w_i J_i \tag{3}$$

The weight factors (w) are typically chosen such that $\sum_{i=1}^{n} w_i = 1$. This method is straightforward and therefore frequently used to solve multi-objective optimization problems. The approach is not unbiased since it is relies on a prior decision about the distribution of the weight factors.

To solve the optimization problem in equation 3, the standard dynamic optimization method can be used, but solving such problem for a given weight vector yields only a single solution. The sensitivity of the solution for the choice of the weight vector can be evaluated by solving the optimization problem multiple times with different weight combinations. Figure 1a shows an example of the Pareto set for two objective functions. The point with the conflicting and thus unattainable objective functions J_1* and J_2* is called the utopia point J^*. Separate optimization of the two individual objectives J_1 and J_2 results in the two extremes A and B on the Pareto front, i.e. the line A-B, one objective can only be improved at the expense of the other. For any choice in w in eq 3 the dynamic optimization method finds the best suitable processing route resulting in the best possible product considering the utopia point as objective. The dynamic optimization method can hence be used to obtain the Pareto front, by varying the weight w over its full range.

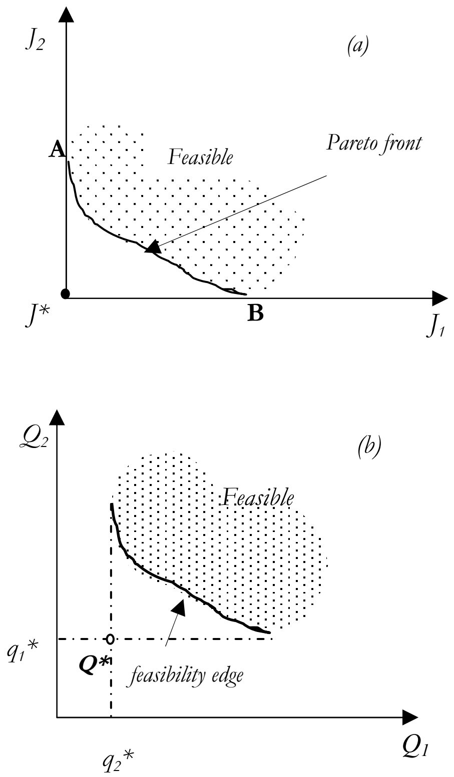


Figure 1. Example of Pareto front for two objective functions (Figure 1a) and the corresponding image of the Pareto front (feasibility edge) in quality space (Figure 1b). The Pareto front divides the space into feasible and non-feasible area for design.

Additional insight is obtained by scanning which quality target points lead to conflicting objectives, and which can be matched exactly. In the latter case, $J_1^*=J_2^*=\ldots=0$, and there is no Pareto front. These points can be called feasible points, as these qualities can be reached by choosing the decision variables trajectories u found by dynamic optimization, such that $J = 0$. The set of points that are feasible form a feasibility region in quality space, as depicted qualitatively in Figure 1b. If an utopia point is chosen outside the feasible region, it can be deduced from Figure 1a that the dynamic optimization will end up at the Pareto front for that utopia point. At the Pareto front the solution is just feasible, and hence in quality space will be at the edge of the feasible region. This edge can be viewed as an image of the Pareto front in quality space.

The Pareto analysis can hence be used as method to scan the boundary of the feasibility area. The use of other strategically chosen utopia points will reveal other Pareto lines, and consequently other boundary lines in quality space, which cover another part of the feasibility region. Together they can be used for the complete mapping of the feasibility area. A designer can use knowledge of the feasibility region to see the possibilities given by inherent flexibility of the process coupled to the inherent limitation of the product transformations. If the product specifications fall in the feasible region, then the products can be easily produced, while if the product specifications fall outside the feasible region, they cannot be realized at all. Then the best possible solutions lie on the edge of the feasible region *i.e* on the associated Pareto front and the designer has to make a choice based on his preferences or resort to changes in the production process or in the formulation. In the next application on bakery products it is further shown how this technique can be used to explore the effect of different choices in design parameters on the shift and enlargement of the feasibility space.

3. Methods

3.1. Model

Hadiyanto *et al.* (2007a) presented a model for bakery production. The model includes mass and heat transfer, starch state transformations and product quality formation. This model is briefly described in the following sections and the model equations are given in Appendix 6.1 of this chapter. The model parameters and thermal properties were described in Chapter 3 and 4.

3.1.1. Heat and mass transfer

The heat and mass balances for liquid water, water vapour and CO_2 gas (eqs. A1-A4) follow from the laws for mass and energy conservation and include water evaporation/condensation. The heat transport is described by convection augmented with a (microwave) source term. The mass transport is described by diffusion equations. The local change of liquid water in the product is the result of the diffusion and the evaporation rate (I_v). For the complete equations see Appendix 6.1 Tables 1a, 1b and 1c.

3.1.2. State transformations

The product extension (e) gives the (linear) change of size (height) compared to the initial height of the product (equation A5). The extension of height is based on a model for visco-elastic materials (Hadiyanto *et al.*, 2007a). Protein thermosetting reactions and starch state transformation from crystalline state into the gel state and the reverse are the main transformations for product texture. Protein thermosetting reactions only solidify the network. Therefore, starch gelatinization and retrogradation are the main transformations relevant for textural properties. The changes of the degree of gelatinization are equal to the gelatinization rate (Zanoni *et al.*, 1995) minus the retrogradation rate (equation A6). Here is α_{max} the maximum attainable degree of gelatinization which is a function of the initial composition of the product, i.e. content of water (W), starch (S) and other water binding components (C) in dough (Hadiyanto *et al.*, 2007a). Gelatinization occurs at higher temperatures and is much faster than retrogradation. Therefore gelatinization takes place during baking and retrogradation during storage (staling of product). Additional equations are given in appendix 6.1 Tables 1b and 1c. Browning of bakery products is mainly caused by the Maillard reaction which forms melanoidins as colouring compounds (eq A7). These reactions are zero order (van Boekel, 2001) and the reaction rate depends on temperature and water content in the product (see also Table 1b)

3.1.3. Product quality model

Crumb (i.e. the open network structure in the center of bread) is linked to the degree of starch gelatinization (Hadiyanto *et al.*, 2007a). For a range of Dutch bakery products the relation between crumb and degree of gelatinization given by equation A8 is considered. Crispness and softness of bakery products are linked to the difference between the current product temperature (T_r) and the glass transition temperature of the product (T_g). A product is crisp when T_r-T_g<0 (equation A9). The glass transition temperature is a function of the product composition (see Table 1c). Softness is a combined function of T_r-T_g and the degree of gelatinization. Products are soft for T_r-T_g >0 but softness requires a minimum value of the degree of gelatinization above 0.3 (equation A10). The relation between brownness and the amount of melanoidins (*me*) is given by equation A11.

3. 2. The multi-objective optimization problem

Surface crispness, brownness and the product water content in the product are the major quality attributes of bakery products, and these are considered as critical parameters for the bakery operation design (Hadiyanto *et al.*, 2007b).

The standard strategy for baking is convective heating, but combination with microwave and radiation heating gives extra flexibility. This is especially useful for larger products for which the internal heat transfer is becoming an inherent limiting factor. Hadiyanto *et al.* (2007b) showed that with combined heating sources the specified product qualities can be achieved more accurately, while the baking process is more flexible.

For multi-objective optimization the following quality objectives (Q_i) are considered:
1) Surface crispness (scaled to the range 0-1)
2) Surface brownness (scaled to the range 0-1)
3) Center moisture content. (Weight fraction)

Two different cases were studied;

a. Case I with two objectives: Optimization for surface attributes.

For this case, the design of the process operation concerns only the product surface attributes crispness and brownness in the objective function.

b. Case II with three objectives: Optimization for surface and center attributes

The second case concerns both surface and center attributes. The moisture content is important for the internal product quality. Cuq *et al.* (2003) reported that for good crumb properties of bread, the moisture content after baking should be in the range of 0.35-0.40 kg/kg. Therefore, in the three objective problems the product moisture content is included to represent an internal product quality attribute.

3.3. The feasibility domain

The study of the feasible operational domain is performed along four lines.:

1. Scanning method. The conflicting combinations of product specifications are determined by scanning over the domain of potential target values. This is done as follows. A grid of the specified quality parameters covering the full domain is chosen, and for each point in the grid a single-objective function, which combines the individual objectives with equal weights is optimized by using dynamic optimization. If it is possible to find a solution that meets the criteria (i.e. J is approximately= 0), then this is a feasible specification. The grid points where this is not the case reveals conflicting (unfeasible) quality specifications.
2. Pareto front method. Knowing roughly the feasible range allows to choose suitable utopia points for the Pareto front method. A point with conflicting objectives is chosen. Solving the multi-objective optimization problem by varying the weights from 0 to 1, making sure that $\sum_{i=1}^{n} w_i = 1$ generates the Pareto front and its image in quality space defines part of the boundary of the feasible area. When the context is clear we will for brevity simply use 'Pareto front' to indicate the image of the Pareto front in quality space. The weighted sum multi-objective optimization approach based on eq. 3 with varying weight values (Zadeh,1963) combined with a gradient search method for dynamic optimization (Bryson, 1999; Hadiyanto *et al.*, 2007b) is used to generate the Pareto front. The Pareto front divides the space of product quality specifications in feasible and non-feasible combinations.

3. Inspection of the operational strategies on the Pareto front. To this end the image of the Pareto front in quality space is divided in three regions and for a selection of a product specification from each of the regions the characteristic operation strategy/design is calculated by using a gradient search for dynamic optimization. The purpose is to see the degree of variation over the operational range along the edge of the feasibility region.
4. Sensitivity of the feasible area for design parameters. In this case the dough initial water content is taken as a design variable, to see how the feasible range changes.

4. Results and Discussions

4.1. Case I: Multi-objective optimization for surface properties

4.1.1. Scan for potential conflicting product specifications

Figure 2 presents the final solutions which are obtained by many single-objective optimizations towards a grid of utopia points which are equally distributed in the quality space of the surface attributes of brownness and crispness. Only convective heating is used for baking.

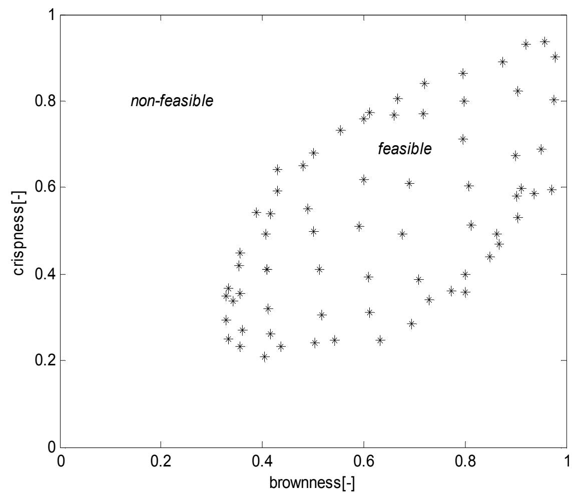


Figure 2. Solutions of single-objective optimization towards a grid of surface quality utopia points using dynamic operations of convective heating

The final quality plot gives a good indication which combinations of surface quality specifications are feasible or unfeasible. The feasible area is shown by the region of scattered points, and it shows that the convective heating is most suitable for products specifications in the middle area of the quality specification domain. The unfeasible area is formed by the regions of low crispness–high brownness and high crispness–low brownness. Thus, these combinations of product attributes are the focus of the following discussion.

4.1.2. Determination of the Pareto front

The inspection of the image of Pareto front in the quality domain will give the decision maker information about which combinations of quality specifications can be achieved. Moreover, it gives information how the specifications could be changed to produce a product with the required quality.

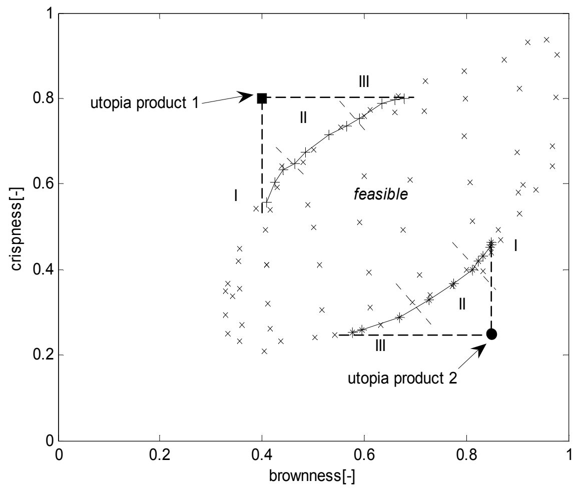


Figure 3 Pareto optimal set for two cases of conflicting product specifications, Product 1 with crispness=0.8 and brownness=0.4, and product 2 with crispness=0.25 and brownness=0.85. The dashed lines correspond to limit of Pareto point for each individual utopia point.

Figure 3 shows the Pareto images for two unfeasible products : Product 1 with high crispness and low brownness (chosen utopia point: brownness=0.4 and crispness =0.8), and product 2 with lower crispness and high brownness (chosen utopia point: brownness=0.85 and crispness =0.25). These Pareto fronts indicate which combinations of qualities can be obtained while maintaining optimality. All points on the Pareto front, which are weighted differently, show a trade off between objectives and they are possible solutions for corresponding utopia points. Figure 3 also shows that both Pareto fronts fall in the boundary of the feasible area and this gives indication that the Pareto front can indeed be used to determine the feasibility area without scanning all possibilities under the grid searching method. This is important, since for systems with many quality parameters, scanning the complete quality space become unpractical.

4.1.3 Inspection of the operational conditions on the edge of the feasibility region

Each point on the Pareto front is linked with a different convective heating strategy. To illustrate this effect, the Pareto front is split in three regions. In region I a small increase of brownness results in a significant increase of product crispness, while, in region III small changes in crispness of the product result in large changes in brownness. Region I is appropriate for consumers which accept a different crispness than the specified one, while region III delivers good products for consumers that prefer the good crispness instead of colour. Region II is the transition region between region I and III and hence represents a compromise between the two.

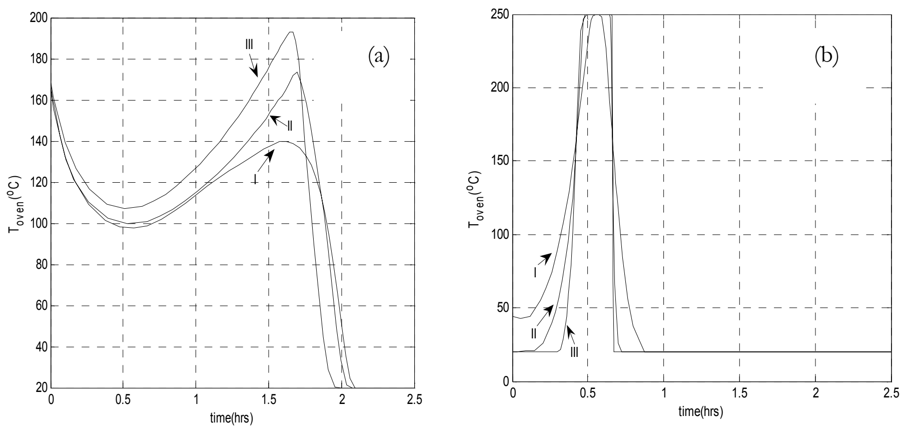


Figure 4 The corresponding heating strategies expressed by the oven temperature as a function of time for the three regions of product 1 (Fig 4a) and product 2(Fig 4b).

The solution family for the different regions in the Pareto front is given in Figure 4a and 4b. The two solution families show different characteristics of heating. Overall, product 1 (Figure 4a) requires longer heating period than product 2 (Figure 4b), while the temperature is lower. For product 1, the solutions in region III (which puts more emphasis to crispness) need higher temperatures to evaporate all the moisture in the surface while region I requires lower temperature to produce lower crispness. The solutions in region II are a balance between the two, and indeed its heating profile is in between that of regions I and III.

The optimization for product 2 with low crispness and high brownness shows different profiles for the solutions (Figure 4b). To achieve a high level of brownness the product temperature at the surface must be high for a short period to activate the Maillard reaction. Such a heating strategy makes also that a small amount of moisture is evaporated at the surface and as a result crispness can be maintained at a low value. This example illustrates nicely how the method reveals the large flexibility in operational strategies of the baking process.

4.1.4. Effect of design condition: initial dough water content

The initial dough water content has a significant effect on the final crust quality and it is an important aspect for design to determine the operating strategy (Hadiyanto *et al.* 2007b). In figure 5 the effect of variations of initial dough water content in the range 0.48-0.53 kg/kg for both the utopia points are given. The results show that by lowering initial water content of dough, the feasible area is shifted towards product 1, which means that higher crispness with low brownness can be achieved by reducing the initial water content. On the other hand, the lowering of the initial dough water content is detrimental for utopia product 2 with opposite quality attributes. Hence the whole feasible region is shifted by lowering the initial dough water content. This example shows that by means of the Pareto analysis it is possible to predict how the feasibility area will change as a result of a change in initial product composition.

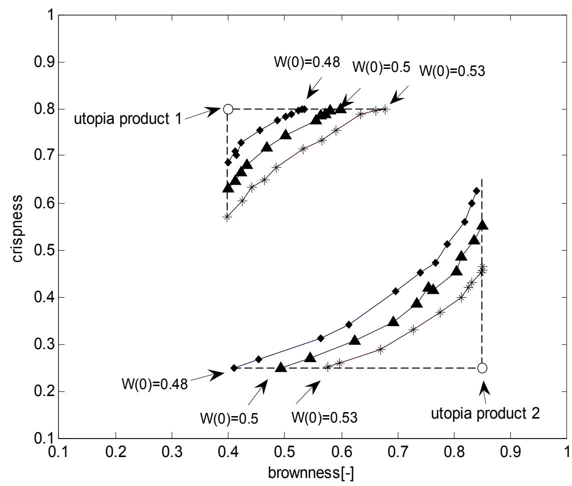


Figure 5 Effect of initial moisture content to Pareto front and feasibility area for convective heating baking of products. The dashed lines correspond to limit of Pareto point for each individual utopia point.

4.2 Case 2: Multi-objective optimization for surface and center attributes (brownness-crispness-water content)

The multi-objective optimization for the surface quality in previous section showed that optimization of conflicting quality attributes is a trade-off between the (partial) objective functions. Now, we look at this method when a third objective (water content) function is included. The considered case is to produce a final product with a low level of brownness (=0.4), high level of crispness (=0.8) and a final moisture content in center of the product (0.38 kg/kg). In a previous study (Hadiyanto *et al.*, 2007b) it was shown that by the use of only convective heating this combination of quality criteria could not be fully satisfied. Therefore now this situation is studied in more detail using the Pareto front analysis, and, in addition, a combination of convective, microwave and radiation heating was also studied. The purpose of this case is to show how we can use Pareto front analysis to deal with complex multi objectives and how the feasible area can be enlarged by process modification (i.e., applying multi-heating strategies).

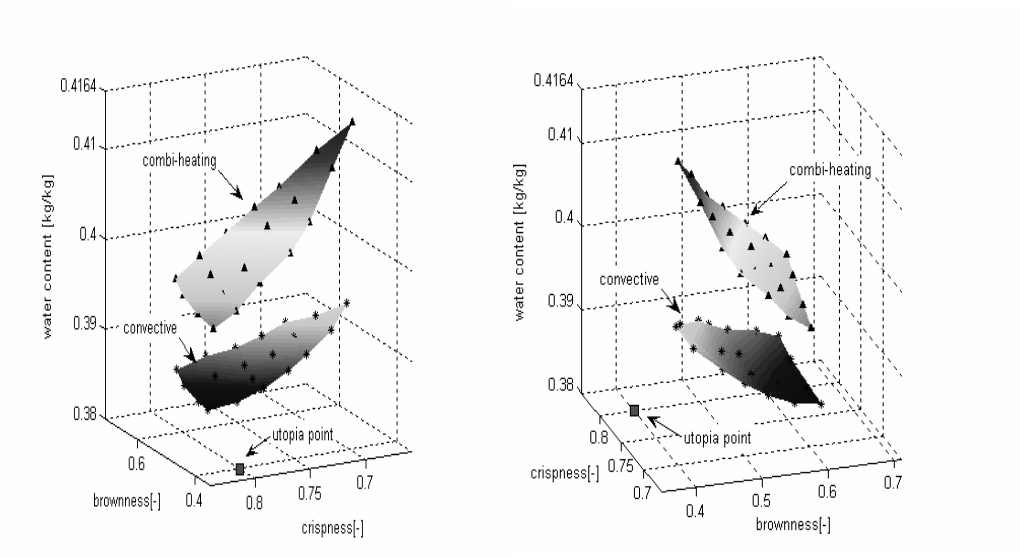


Figure 6 Visualizing Pareto solutions for three objectives in two different view angles. The utopia point is specified as brownness=0.4, crispness=0.8 and moisture content=0.38 kg/kg. The two Pareto surfaces represent dynamic convective heating and a combination of dynamic heating inputs.

The optimal solutions for this case are given in a three-dimensional plot as a surface (see Figure 6). The image of the Pareto front is not longer a line, but a surface represented by triangular areas constructed by several points (see Figure 6). Each individual Pareto point on the surface represents a different dynamic heating strategy. These Pareto fronts illustrate the trade-off among the three objectives. A brownness value of 0.4 is only possible with a low crispness while the moisture content is then above the specification. Vice versa, high crispness values are only possible by increasing the temperature of the surface, but then brownness goes up and the moisture decreases.

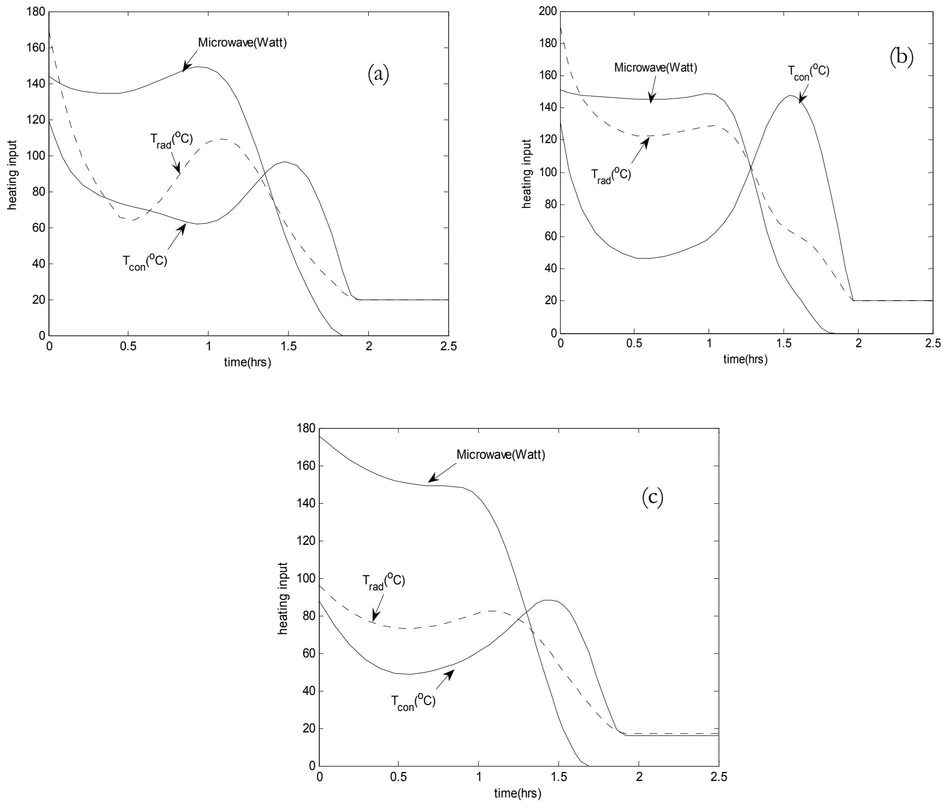


Figure 7. Heating strategies for different weight factors, (a) high weight for brownness, (b) high weight for crispness and (c) high weight for moisture content

The Pareto surface divides the quality space in feasible and unfeasible combinations of quality specification. For solutions on the surface one quality can not be improved by giving away for another quality. The results for convective heating show that all solutions on the Pareto surface are still far from the utopia point. The main reason is that this type of heating has a limited effect on the moisture removal from the center. The dynamic multi-heating strategy i.e. simultaneous convective, microwave and radiation heating significantly extends the feasibility surface towards the utopia point. This improvement is demonstrated in Figure 6 where the Pareto surface of the multi-heating system is closer to the utopia point. The outcome shows that multi-heating baking increases the flexibility of baking processes by extending the feasibility area.

The corresponding heating strategies for the three extreme points of the Pareto surface for combination heating are given in Figure 7a-c.

Figure 7a shows the heating strategy for products with emphasis on brownness. To develop the required brownness, the convective and radiation temperatures decrease in the first hour of baking, and then increase to form the brown colour by Maillard reaction. A different heating trajectory is required when the design gives higher importance to crispness (Figure 7b). The oven temperature increases remarkably in the last stage of baking to form crispness at the surface. This is necessary to evaporate the remaining water from the surface to achieve the required crispness. By giving higher importance to the internal moisture content, the heating strategy is changed consequently. From Figure 7c, it is clear that the microwave power increases to bring the water content in the center to the required value; while radiation and convective heating are kept lower.

5. Conclusion

In product and process development, designers are often confronted with conflicting objectives. Optimization of such problems results in a set of sub-optimal solutions instead of a single optimum solution. This set of solutions, represented by the Pareto front, separates the solution space in a feasible region and a non-feasible region. The feasibility area can be approximated by single-objective optimization towards a grid of utopia points and the border of the feasibility space can be scanned with the Pareto method. Inside the feasible region several combinations of objectives are possible, while at the Pareto front a better realization of one objective result in a negative effect on the other objectives. For a designer it is important to have a practical tool to map the feasible and non-feasible area, to balance the benefits and give-away for the objectives when operating at the Pareto front and finally to know how the feasible area can be extended.

By means of two cases in bakery it is illustrated how the Pareto front can be used by the designer to find possibilities to extend the feasible region and to improve the flexibility of the system. This can be achieved by changing the product formulation, and by changing the process system. The first is illustrated by the shift in the feasibility space by increasing the initial water content in the dough. The second is illustrated by the use of combination heating, which enlarged the possible product range by increasing the flexibility. Again the Pareto analysis is a versatile tool for the designer to find solutions that enlarge feasibility or flexibility of processes.

Multi-objective optimization is developed for systems where many objectives play a role. Multi-objective optimization up to three variables can be represented in a graphical way. However, for four or more objective functions the multidimensional Pareto results are difficult to interpret. Therefore, analysis for more complex systems constitutes a challenge for future research.

Acknowledgement

The authors gratefully acknowledge the financial support from the Graduate School VLAG, the Netherlands.

Annotations

Symbol	Description	Unit
a_w	Moisture activity	[-]
C	Non-starch moisture binding components	kg kg^{-1}
D_v	Gas diffusivity	m^2 s^{-1}
D_w	Liquid diffusivity	m^2 s^{-1}
e	Relative extension of height	[-]
f_r	Fusion factor	[-]
F	Stefan-Boltzman constant	J s^{-1} m^{-2}K^{-4}
E_a	Activation energy	J mol^{-1}
G	Retrogradation rate constant	s^{-1}
G_0	Reference value for retrogradation rate	s^{-1}
H_c	Enthalpy of moisture vapour	J kg^{-1}
H_v	Enthalpy of CO_2 gas	J kg^{-1}
h_c	Convective heat transfer coefficient	W m^{-2}K^{-1}
h_v	Mass transfer coefficient	M s^{-1}
J	Performance index	[-]
J^*	Utopia point in objective space	[-]
k	Thermal conductivity of product	W m^{-1}K^{-1}
K_g	Retrogradation Constant	[-]
k_{mc}	Reaction rate constant for Maillard reaction	s^{-1}

k_{soft}	Constant for gelatinization	[-]
k_{gel}	Rate constant for gelatinization	[-]
k_{retro}	Rate constant for retrogradation	[-]
m_v	Mass flux of moisture vapour	kg $m^{-2}s^{-1}$
me	melanoidines	[-]
m_c	Mass flux of CO_2 gas	kg $m^{-2}s^{-1}$
M_w	Molecular weight of moisture	kg $kmol^{-1}$
P	Total pressure	Pa
$P_{0,r}$	Incident power of microwave	Watt m^{-3}
P_{mw}	Microwave power	Watt
$p_{v,sat}$	Saturated pressure of moisture vapour	Pa
Q	Quality variable	[-]
Q^*	Utopia Point in quality domain	[-]
Q_{mw}	Microwave power	[W.m^3]
q^*	Setting value for final quality	[-]
R_g	Gas constant	J $mol^{-1}K^{-1}$
R	Height of product	[m]
R_{CO}	CO_2 production rate	kg m^{-2} s^{-1}
S	Sugar content	kg kg^{-1}
t	Time	s
t_f	Final time of process	s
T_∞	Hypothetical temperature	K
To	Initial dough temperature	K
U^*	Activation energy for recrystallization	J mol^{-1}
V_c	CO_2 gas concentration	kg kg^{-1}
V_v	Moisture vapour	kg kg^{-1}
W	Moisture content	kg kg^{-1}
W_o	Initial moisture content	kg kg^{-1}
x	State variable	
Z	Starch content	kg kg^{-1}
T_g	Glass transition temperature	K
T_m	Melting temperature	K
u	Input variable	
S/Z	Ratio sugar and starch	[-]

Greek letters

α	Total degree of starch gelatinization	[-]
α_{max}	Maximum attainable degree of gelatinization	[-]
$\alpha_{,mw}$	Attenuation factor	[m^{-1}]
λ	Evaporation heat	J.kg^{-1}
ε	Porosity	[-]
ε_r	emissivity	[-]
υ	Kinematic viscosity	m^2 s^{-1}
ρ	Density of product	kg m^{-3}

References

Boekel, M.A.J.S. van .(2001). Kinetic aspects of the Maillard reaction: A critical review. *Nahrung/ Food,* 45 (3), 150–159

Bryson, A.E. (1999). Dynamic Optimization. Addison-Wesley, Menlo Park.

Cuq, B., Abecassis,J. and Guilbert,S. (2003).State diagrams to help describe wheat bread processing. *International Journal of Food Science and Technology*,38**,** 759–766

Gunarni, A., Ferguson, S., Donndelinger, J., and Lewis, K. (2005). Feasibility Assessment in Preliminary Design Using Pareto Sets. *Proceeding of IDETC/CIE 2005*, California.

Hadiyanto, Asselman, A., Straten, G. v., Boom, R. M., Esveld, D. C. and van Boxtel, A. J. B.(2007a). Quality prediction of bakery products in the initial phase of process design. *Innovative Food Science and Emerging Technologies*, 8(2), 285-298.

Hadiyanto, Esveld, D. C., Boom, R. M., Straten G. van. and van Boxtel, A. J. B. (2007b). Product Quality Driven Design of Bakery Operations using Dynamic Optimization, *submitted*

Sarkar, D., Rohani,S., and Jutan, A. (2006). Multi-objective Optimization of Seeded batch crystallization process. *Chemical engineering Science,* 61,5282-5295

Sendin, O. H., Vera, J. Torres, N. V and Banga, J. R. (2001).Model based optimization of biochemical systems using multiple objectives: a comparison of several solution strategies. *Mathematical and Computer Modeling of Dynamical Systems,*12(5),469-487

Zadeh, L. (1963). Optimality and non-scalar-valued performance criteria. *IEEE Trans Automat Control*, 8,59–60

Zanoni, B., Schiraldi, A., and Simonetta, R.(1995). A naive model of starch gelatinization kinetics. *Journal of Food Engineering,* 24 (1), 25–33

Zhang, J and Datta, A.K. (2005). Mathematical modelling of bread baking process. *Journal of Food Engineering,* 75, 78-89

Zhang, Z., Hidajat,K. and Ray,A.K. (2002). Multi-objective Optimization of SMB and Varicol Process for Chiral Separation. *AIChE Journal*, 48(12), 2800-2816

Zorrilla, S. E., Banga, J. R. and Singh, R. P. (2003).Dynamic optimization of double-sided cooking of meat patties. *Journal of Food Engineering*, 58, 173-182.

Appendix 6.1.

Table Ia. The main baking models

Laws of conservation		
Energy	$\rho c_p \frac{\partial T(r,t)}{\partial t} + \frac{\rho\lambda}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = k \frac{\partial^2 T(r,t)}{\partial r^2} - \lambda I_v(r,t) - \frac{\partial(m_v H_v)}{\partial r} - \frac{\partial(m_c H_c)}{\partial r} + Q_{mw}(r,t)$	(A1)
Liquid water	$\rho \frac{\partial W(r,t)}{\partial t} + \frac{\rho W(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_w \frac{\partial W}{\partial r}) - I_v$	(A2)
Water vapour	$\rho \frac{\partial V(r,t)}{\partial t} + \frac{\rho V(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial V}{\partial r} - m_v) + I_v$	(A3)
CO_2	$\rho \frac{\partial V_c(r,t)}{\partial t} + \frac{\rho V_c(r,t)}{1+e(r,t)} \frac{\partial e(r,t)}{\partial t} = \frac{\partial}{\partial r}(D_{vc} \frac{\partial Vc}{\partial r} - m_c) + I_c$	(A4)
State transformations		
Product extension	$\eta \frac{de(r,t)}{dt} + Ee(r,t) = P - P_{atm}$	(A5)
Degree of gelatinization	$\frac{d\alpha(r,t)}{dt} = k_{gel}(\alpha_{\max} - \alpha(r,t)) - k_{retro}\alpha(r,t)$	(A6)
Melanoidine formation	$\frac{dm_e(r,t)}{dt} = k_{me}(r,t)$ (Maillard reaction)	(A7)
Quality attributes		
crumb	$\begin{cases} 0 \quad if \quad \alpha(r,t)=0 \\ 2\alpha(r,t) \quad if \quad \alpha(r,t) \le 0.5 \\ 1 \quad if \quad \alpha(r,t) > 0.5 \end{cases}$	(A8)
crispness	$-\frac{0.0067.(T - T_g(r,t))}{1+\exp(3.(T - T_g(r,t)))}$	(A9)
softness	$-k_{soft} \frac{0.01.\exp(3(T - T_g(r,t)))}{1+\exp(3.(T - T_g(r,t)))}$	(A10)
brownness	$1 - (1 - m_e(0))e^{-0.23(m_e(r,t))}$	(A11)

Table 1b. Additional equations for the baking model

In equation	Descriptions
A1-A4	$m_v = -\frac{\kappa}{\nu}\frac{V(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
A1-A4	$m_c = -\frac{\kappa}{\nu}\frac{V_c(r,t)}{V(r,t)+V_c(r,t)}\frac{\partial P}{\partial r}$
A5	$P = pv + pc$
A1	$Q_{mw}(r,t) = \frac{2\alpha_{mw} R P_{0,r}}{r}\exp\left(-2\alpha_{mw}(R-r)\right)$, $P_0, r = \frac{P_{mw}}{2\pi R(L+R)}$
A1-A4,A7	$a_w = \frac{1.05W(r,t)}{0.09+W(r,t)}$
A6	$k_{gel} = 2.8.10^{19}\exp(\frac{-139000}{R_g T(r,t)})$
A7	$k_{retro} = G_0.\exp\left[\frac{-U^*}{R_g(T(r,t)-T_\infty)}\right]\exp\left[\frac{-K_g}{T(r,t).\Delta T.f_r}\right]$ if $T < 298^o K$
A7,A9,A10	$\alpha_{\max} = \begin{cases} 0 & \text{if } W < 0.5(S+C) \\ \frac{(W-0.5S-0.5C)}{S} & \text{if } 0.5(S+C) < W < 0.5(3S+C) \\ 1 & \text{if } 0.5(3S+C) < W \end{cases}$
A7	$k_{me}(r,t) = 4.9\times10^{-3}\times\frac{\exp(9a_w)}{2\times10^3+\exp(11.3a_w)}\exp\left[\frac{-E_a}{R_g}\left(\frac{1}{T(r,t)}-\frac{1}{363}\right)\right]$
A10	$k_{soft} = (\frac{-3}{7}+\frac{10}{7}\alpha_{\max}).\frac{\exp(500.(\alpha_{\max}-0.3))}{1+\exp(500.(\alpha_{\max}-0.3))}$
Boundary condition for heat and mass transfer :	
Surface	$k\frac{\partial T}{\partial r}\Big\vert_{r=R} = h_c(T_{oven}-T(R,t)) - \lambda\rho D_w\frac{\partial W}{\partial r}\Big\vert_{r=R} + F\varepsilon_r(T_r^4 - T(R,t)^4)$
	$D_{vc}\frac{\partial V}{\partial r}\Big\vert_{r=R} = h_v(V_{ext}-V(R,t))$
center	$k\frac{\partial T}{\partial r}\Big\vert_{r=0} = D_{vc}\frac{\partial V}{\partial r}\Big\vert_{r=0} = 0$

Table 1c. Equation for glass transition and melting temperature

$$T_{g/m} = p_1 + p_2(S/Z) + p_3.W + p_4(S/Z)W + p_5(S/Z)^2 + p_6(W)^2 + p_7(S/Z)^2W^2$$

Parameters	p_1	p_2	p_3	p_4	p_5	p_6	p_7
T_g	457.10	-396.32	-853.21	716.76	430.27	778.44	-1424.71
T_m	472.69	-180.90	-519.97	419.63	124.46	471.87	-749.88

CHAPTER 7

Model Calibration and Parameter Identification for Bread Baking

Hadiyanto, R.M. Boom, G. van Straten, D.C. Esveld and A.J.B. van Boxtel

Abstract

Bread product quality is highly depending on the baking process. A model for the development of product quality, which was obtained by using quantitative and qualitative relationships, was calibrated by experiments at a fixed baking temperature of 200°C alone and in combination with 100W microwave power. The model parameters were estimated in a stepwise procedure. First, heat and mass transfer related parameters, then the parameters related to product transformations and finally some product quality parameters were determined. There was a fair agreement between the calibrated model results and the experimental data. The results learn that the applied simple qualitative relationships for quality perform above expectation. Furthermore, it is confirmed that the microwave input is most meaningful for the internal product properties and not for the surface properties as crispness and color. The model with adjusted parameters was applied in a quality driven food process design procedure to derive a dynamic operation pattern, which was subsequently tested experimentally to calibrate the model. Despite the limited calibration with fixed operatioan settings, the model predicted the behaviour under dynamic convective operation well and fairy well under combined convective and microwave operation. It is expected that the coreespondence between model and baking system could be improved further by performing calibration experiments at more temperature and microwave power levels.

Keywords: Baking , bread quality, process design, experimental validation

1. Introduction

The availability of accurate models to predict product quality is an essential requirement in quality driven food process design. Hadiyanto *et al.* (2007a) use a model to predict the development of product quality during bakery operations and they use the model also to generate design alternatives by calculating dynamic optimal operations (Hadiyanto *et al.*, 2007b). This model needs to be experimentally validated

Baking is a main operation in bakery production which is performed by convective heating systems or by combined heating systems using convective, microwave and radiation heating. Convective heating exposes the surface to a high temperature and the heat subsequently penetrates the product towards the center. This results water evaporation and a corresponding increment of the internal pressure which creates a driving force for vapor transport to the environment of the product. In contrast to convective heating, microwave radiation will generate the heat directly inside the product, which results in different moisture and temperature profiles for products in comparison to convective heating. Radiation heating only affects the product surface temperature and heat penetration to the product from this source is limited. Combined heating systems with convective, microwave and radiation heating increase the flexibility of baking operation whereas the operation time is reduced and a wider range of product quality can be realized (Ni and Datta, 2002; Keskin *et al.*, 2005; Hadiyanto *et al.*, 2007b; Sumnu *et al.*,2006).

Important quality attributes of bakery products are color, texture, crumb and size. These attributes are the consequence of browning reactions, starch gelatinization and retrogradation and gas expansion. The associated transformations are ruled by the heat and mass transfer within the products which are a result of the imposed process conditions. The model proposed by Hadiyanto *et al.* (2007a) is a sequential model that includes the chain of phenomena starting from heat and mass transfer followed by the state transformations and finally the product quality formation. The heat and mass transfer part of the model was based on well recognized relationships for transport phenomena (Zhang and Datta, 2006). The state transformations and quality formation, however, were derived from qualitative expert knowledge. Several assumptions and simplifications that inevitably had to made, may reduce the reliability of the prediction. As a consequence, to prove the reliability and for the future use of the model, a check on the validity of the model prediction is required.

Several papers report on model validation of baking processes (for example Zheleva and Kambourova, 2005; Zanoni *et al.*,1993; Lostie *et al.*, 2002; Thorvaldson and Janestad,1999). However, their research is mostly focused on the heat and mass transfer phenomena during baking and misses the link with product quality. Some studies did consider quality aspects and parameter estimation. For example, Lostie *et al.* (2003) studied the effect of volume expansion, and Zanoni *et al.* (1995) reported about brownness development. Our challenge was to extend and put the previous work on a firmer basis by validation of the combined model for heat and mass transfer and a series of qualities.

The aim of this work is to evaluate the current model for the formation of bakery product quality (Hadiyanto *et al.* 2007a), and to adapt parameters in the model where necessary. Because the baking model is a sequential model, in the sense that the heat and mass transport is not influenced by the product transformations, the validation can also be done in a sequential way; starting from heat and mass transfer related measurements, then the state transformations and finally the quality measurements. The model is calibrated against experiments with constant operational conditions and subsequently the validity of the model to predict quality for dynamic baking operations is tested.

2. Materials and methods

2.1. Experimental set-up for baking

2.1.1 Dough preparation

Dough was prepared from a mixture of 500 g flour (C1000 bread mixture for white and ciabatta, with composition per 100 g flour : 50% starch, 8.6% protein, 5% fat, 2% yeast, 0.5% salt) and 300 g water in a dough mixer (Inventum BM20) at medium speed for 3 minutes and 37^{o}C. Then the dough was kneaded for 5 min and the product was placed on the baking plate for 30 min to rise at room temperature. The initial weight of the dough and the height of the formed sample were measured before the sample was put in the oven. The initial size of the dough was the same for all experiments with diameter 0.08 m and height 0.04 m, the initial weight was 250 g.

2.1.2. Equipment set-up

An overview of the baking equipment is shown in Figure 1. The domestic oven was expanded with an external microwave source, which can provide an adjustable power. A monitoring and control system for oven and microwave heating was developed in Labview. An impression of the user interface is given by Figure 2. This control system monitors the temperatures and allows for a dynamic operation of the convective and microwave heat sources. Here, input trajectories for convective and microwave heating were based on four intervals of piece-wise constant heating input for the oven and microwave system.

Temperatures in the oven and in the product were measured with optical temperature sensors using an optical slip ring (OSR) with multi probes (FISO Technology, Sainte-Foy, Quebec, Canada). The OSR system with four fiber-optic sensors is mounted on the oven and makes it possible to measure the temperatures during processing on a rotating table. The maximum temperature for the sensors was 250^{o}C and the accuracy 1^{o}C.

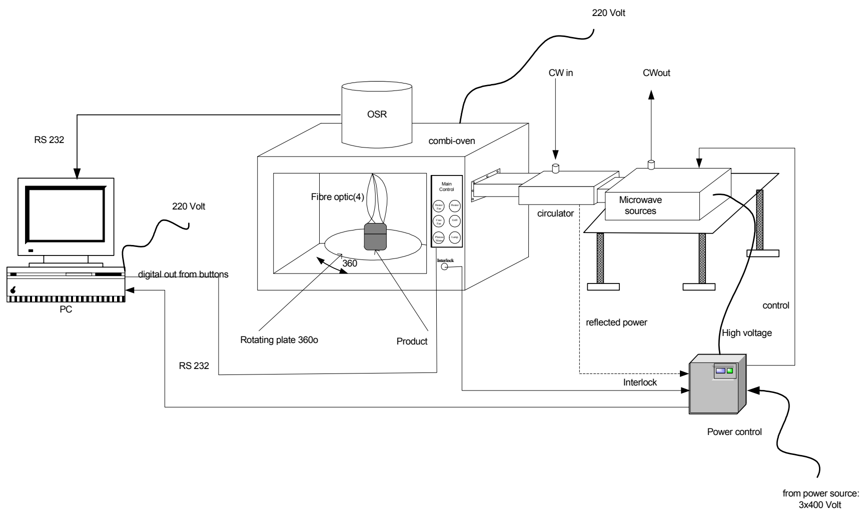


Figure 1. Equipment overview for baking

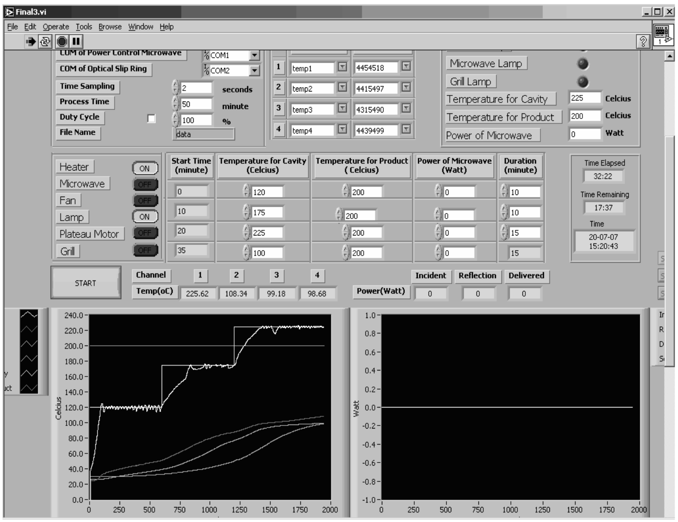


Figure 2. Users interface for the monitoring and control system for baking experiments

2.1.3. Baking experiment

Conventional oven baking was performed in the oven at a controlled temperature level (standard value was 200 °C) and time (standard 30 minutes). The oven was preheated for 10 minutes to reach the setting temperature before the dough was placed in the oven. To follow the development of the product formation during baking, several bread samples with the same initial properties were baked for different time periods.

Other experiments were performed for a combination of convective and microwave heating with an adjustable microwave source. For experiments with constant microwave input the dissipated power level was set to 100W.

2.2. Quality analysis

The color of the bread product was measured with a Minolta chromatometer (CR-200, Japan) using the *L*, *a,* and *b* color scale (Hunter method). Triplicate measurements were done at different positions on the bread surface and bread crumb, and then the mean value was calculated. The color change (ΔE) compared to a calibrated reference was calculated from equation 1 where the reference color is represented by L_0, a_0 and b_0.

$$\Delta E = \sqrt{(L - L_o)^2 + (a - a_o)^2 + (b - b_o)^2} \qquad (1)$$

A texture analyzer for food products (TA-XT Plus, Stable Micro Systems Ltd., Surrey, UK) was used for the instrumental analysis of the bread crust and crumb. Samples of crust and crumb with size 20 x 30 x 30 mm were subjected to a compression test using the SMS P/2 probe (test speed 1.7 mm/s, distance 6.2 mm). The measurements were done 2 hours after baking.

From the resistance the probe encountered during penetration a force-deformation curve was constructed. An example is shown in Figure 3. Penetration of the crust occurred at about 3.8 s after the probe touched the sample surface and the force-deformation reached a maximum load of 370 g. These peak values are used to represent the crispness of the product surface(Dogan and Kokini, 2007).

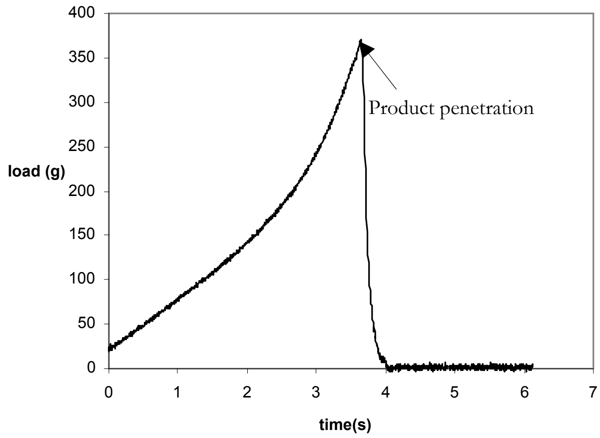


Figure 3 Example of load-time curve from texture measurements

The weight loss during baking was determined by weighting the product before and after baking. The relative weight loss was calculated as

$$w_L = \frac{w_o - w_f}{w_0} \tag{2}$$

Where w_o and w_f denote the initial and final weight of product, respectively. Similarly, the volume extension (e) was obtained by measuring the height of the bread product before (h_0) and after (h_f) baking and is calculated as:

$$e = \frac{h_f - h_0}{h_0} \tag{3}$$

3. Model development

Calculations for the product were done using a 2D spatial model, since the sample breads were much longer than they were wide. As the bread samples are symmetric, it satisfies to do the calculations for a half cross-sectional area. The geometry of the cross-sectional area of the product is given in Figure 4. The evaluated center and surface locations are indicated by point 1 and 2. A symmetry boundary was applied along the center plane and flux boundary conditions were used along the surface of product. The bottom of product is contacted with plate, where it gives conductive heating to the product.

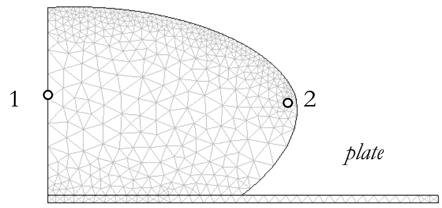


Figure 4. The product domain for simulation. Point 1 and 2 represent the center and surface points of the product for which the results are discussed (height 0.04 m, radius 0.04 m).

The model is a combination of three sequential processes: heat and mass transfer, product transformation and translation to quality, which are explained separately in the following sections. It was described in more detail in Chapter 3 and it is repeated here in brief form only. The symbols are explained in the appended notation list.

3.1. Heat and mass transfer

Energy balance

The energy balance covers heat conduction, evaporation and condensation heat, and convective heat transport due to the fluxes of water vapor and CO_2 (eq. 4). The second term is due to the change of product height.

$$\rho_s c_p \frac{\partial T}{\partial t} + \frac{\rho_s \lambda}{1+e}\frac{\partial e}{\partial t} = \nabla.(k\nabla T) - \lambda I_v - \nabla(m_v H_v) - \nabla(m_c H_c) \qquad (4)$$

Mass balances

The mass balances for liquid water, water vapor and CO_2 gas are given in Eqs. 5-7. The changes of liquid water in the product are the result of the rates of diffusion and evaporation (I_v). Water vapor is considered as an ideal gas which is in equilibrium with liquid water. The vapor concentration is a function of the rates diffusion and evaporation rate as well.

$$\rho_s \frac{\partial W}{\partial t} + \frac{\rho_s . W}{1+e}\frac{\partial e}{\partial t} = \nabla \phi_w - I_v \qquad (5)$$

$$\rho_s \frac{\partial V_v}{\partial t} + \frac{\rho_s . V_v}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_v + I_v \tag{6}$$

$$\rho_s \frac{\partial V_c}{\partial t} + \frac{\rho_s . V_c}{1+e} \frac{\partial e}{\partial t} = \nabla \phi_c + I_c \tag{7}$$

The flux equations

Flux equations for Eqs. 5-7 are:

$$\phi_w = \rho_s D_w \nabla W \tag{8}$$

$$\phi_v = \rho_s D_{vc} \nabla V_v - m_v \tag{9}$$

$$\phi_c = \rho_s D_{vc} \nabla V_c - m_c \tag{10}$$

The convective mass fluxes of water vapor (m_v) and CO_2 (m_c) depend on local pressure differences, kinematics viscosity (ν) and permeability (κ) of the product:

$$m_v = -\frac{\kappa}{\nu} \frac{V_v}{V_v + V_c} \nabla P \tag{11}$$

$$m_c = -\frac{\kappa}{\nu} \frac{V_c}{V_v + V_c} \nabla P \tag{12}$$

Hereby the pressure in the product is the sum of partial water vapor pressure and CO_2 pressure which follow from the gas ideal law.

Constitutive relations

Water vapor and CO_2 are considered as an ideal gas and balances are derived from Fick's law. The liquid water concentration and water vapor pressure are assumed to be in local equilibrium described by an experimentally derived sorption isotherm (Weijts, 1995) (Eq 13).

$$\frac{P_v}{P_{sat}(T)} = \frac{1.05W}{0.09 + W} \tag{13}$$

The evaporation rate (I_v) can be eliminated by combining Eqs 4, 5 and 6 with Eq 13. For the production of CO_2 by yeast or baking soda the empirical expression proposed by Zhang and Datta (2006) is used:

$$I_c = R_{CO} \rho_s \exp\left(-\frac{\left(T - T_{ref}\right)}{\Delta T_{CO}} \right)^2 \tag{14}$$

With R_{CO} is the CO_2 production at T_{ref}, and ΔT_{CO} determines the width of the Gaussian shape function.

The change of product size is represented by the relative extension (*e*) and is caused by the increasing pressure in the gas cells in the dough due to the release and expansion of water vapor and CO_2 from baking powder or yeast (Fan, Mitchell and Blanshard, 1999; Zhang and Datta, 2005). Hadiyanto *et al.*(2007a) considered bread as a Kelvin-Voigt visco-elastic material for which the rate of deformation is proportional to the pressure difference between the internal product pressure (*P*) and the ambient pressure (P_{atm}) minus the elastic strain. A similar expression was proposed by Lostie *et al.* (2002). The two parameters involve in this expression are viscosity (η) and the elasticity (*E*) of product.

$$\eta \frac{de}{dt} + Ee = P - P_{atm} \tag{15}$$

Initial and boundary conditions

The initial values for heat and mass transfer are given by:

$$T(0) = T_0 \qquad W(0) = W_0 \qquad e(0) = 0 \quad P_c(0) = P_{amb} - P_v(0) \tag{16}$$

The boundary conditions of model are given by Eq 17-19. At the boundary, the evaporation is mainly caused by the moisture gradient due to convective heat.

- Fluxes at the surface

$$k\nabla T = h_c(T_{oven} - T_s) - \lambda.\rho_s.D_w \nabla(W_s) \tag{17}$$

$$D_{vc} \nabla V_v = h_v(V_{ext} - V_{v,s}) \tag{18}$$

- Symmetry at the center of the product

$$\nabla T = 0 \qquad \nabla W = 0 \qquad \nabla V_v = 0 \qquad \nabla V_c = 0 \tag{19}$$

The weight loss in the model was determined by calculating the average water content of product, as:

$$w = \frac{\int W \, dV}{\int dV} \tag{20}$$

Where V is volume of product considered for the model calculations

3.2. Product Quality model

3.2.1. Brownness

The Brownness of bakery products is mainly the result of the Maillard reaction which produces melanoidins (m_e) as coloring compound. The Maillard reaction can be approximated as a zero order reaction of which the reaction rate depends on the temperature and the water content (Van Boekel,2006; Hadiyanto *et al.*. 2007a). In the rate equation 21, k_{me} is the Maillard reaction constant and To=363 K.

$$\frac{dm_e}{dt} = k_{m_e} \frac{\exp(9a_w)}{2.10^3 + \exp(11.3a_w)} . \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{To}\right)\right] \tag{21}$$

Hadiyanto *et al.* (2007a) used equation 22 to establish the non-linear correlation between the amount of melanoidins and the degree of brownness.

$$brown = 1 - \left(1 - brown_0\right)\exp(-k_{br}\ m_e) \tag{22}$$

Where $brown_0$ is the initial brownness of the dough and k_{br} is a brownness scaling factor. Both k_{me} and k_{br} are empirical values and therefore these two parameters will be adjusted by fitting the model in experimental data estimation.

3.2.2. Crispness

Crispness and softness of bakery products is related to the texture of the product during consumption and are complicated sensory qualities, depending on the product rigidity/elasticity and structure. However, to have an indication of the relative performance of these attribute in the total framework of the model, we propose to simplify the system and link the degree of crispness and softness only to the amount of gelatinization (α) and the difference between the product temperature and the glass transition temperature of the starch in the product ($\delta T = T_r - T_g$). The glass transition temperature depends on the moisture content and the sugar/starch ratio (S/Z) for which an empirical relation (Eq. 23) given by (Hadiyanto *et al.*, 2007a) is available.

$$T_{g/m} = 457.1 - 396.32\left(\frac{S}{Z}\right) - 853.21W + 716.76\left(\frac{S}{Z}\right)W + 430.27\left(\frac{S}{Z}\right)^2 + 778.44W^2 - 1424.71\left(\frac{S}{Z}\right)^2 W^2 \tag{23}$$

A schematic mapping is given in Figure 5.

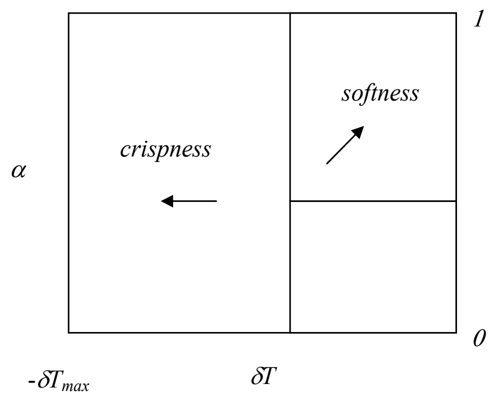


Figure 5 Mapping of crispness and softness to the degree of gelatinization (*a)* and the difference (*δT)* between product temperature (T_r) and glass transition temperature (T_g).

Products with a negative value for δT are crispy products and crispness reaches a maximum normalized value (crispness=1) when all water is evaporated which occurs for $\delta T = -\delta T_{max}$. For the degree of crispness between $\delta T = 0$ to $\delta T = -\delta T_{max}$ a linear expression is used. The parameter, $-\delta T_{max}$ will be adapted to fit the maximally encountered texture range.

$$crispness = \begin{cases} 0, & if \quad \delta T > 0 \\ -\delta T/\delta T_{max}, & if \quad -\delta T_{max} < \delta T < 0 \\ 1, & if \quad \delta T < -\delta T_{max} \end{cases} \tag{24}$$

4. Parameter estimation

The model described in section 3 has a large number of parameters. Deviation between model prediction and experiments can be the result of incorrect or suboptimal values of any of these parameters. Adaptation of all of these parameters is an enormous task, and would be virtually impossible anyway, given the lack of experimental spatial profiles for the temperature, moisture content and pressure. In addition, the large numbers of parameters probably imply a strong correlation between parameters, and hence limited reliability and physical meaning of the obtained numerical values of the parameters.

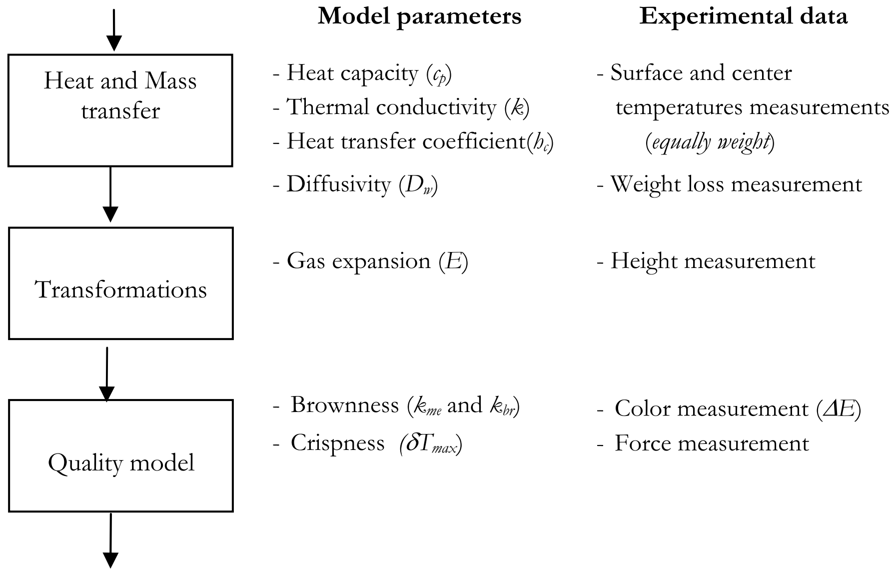


Figure 6. Step wise parameter estimation procedure

For the parameter estimation procedure it is assumed that part of the available parameters can be reliably extracted from independent experiments reported in the literature (e.g. kinetic information) while others have to be estimated more accurately. The focus of the parameter estimation is on the group of parameters that is involved in the expressions for product quality, which are based on qualitative product knowledge. The temperature at the surface and center and the overall mass are accurately followed experimentally, so that some of the parameters from literature (for which often a range of values is given) can be improved. The parameters selected for estimation are listed in column 2 of Figure 6.

The parameter estimation procedure is based on minimization of the sum of the squared differences between the measured values and model prediction values. Because of the hierarchical dependence of the model, the parameter estimation can be performed in sequential bocks. The estimation started with heat and mass transfer related data, followed by an improvement of the state transformations and finally the quality related data (see also Figure 6). This step-wise procedure reduces the complexity of parameter estimation. Parameters and data for each sub model are evaluated sequentially instead of estimating all parameters at once. For the evaluation of the whole system at once it is difficult for parameter estimation procedures to satisfy all data at the same time and the calculations end mostly in local minima and correlated parameters.

The parameters were obtained from the experiment with fixed temperature, as summarized in section 5.1, and the calibrated model result was compared with the measurement data, and was also used to see how well it could represent the experiment with combined fixed temperature and microwave power (sections 5.2 – 5.6). In section 5.8 the calibrated model is used for its intended purpose to derive dynamical process conditions that guarantee a specific product quality. First, an impression is given on how sensitive the calculated process trajectories are for model calibration, and next the calculated trajectories are used in an experiment to validate the model in the environment for which it was intended.

5. Results and discussions

5.1. Optimized parameters

The results of parameter estimation are listed in Table 1. The obtained parameter values are compared to literature values. Thermal conductivity is 0.373 W/m K and corresponds to the values obtained by Jury *et al.* (2007) who reported thermal conductivity values for bread in the range 0.1-0.4 W/m K. The value of the heat transfer coefficient, which is strongly linked to the bread surface temperature, is 26.09 W/m^2 K and is close to the value obtained by Zanoni *et al.* (1995) and also in the range (20-50 W/m^2 K) for natural convection heating reported by Demirkol *et al.* (2006). This parameter depends on equipment characteristics (like air circulation around the product) and therefore may differ from oven to oven. Rask (1989) reported for bread with water content in the range 33-45% specific heat values between 2151-2626 J/kg K. The estimated the value from our experiments falls in the middle of this range.

Table 1. Estimated parameters value and literature references

Parameter	Estimated value	Literature/start value	References
c_p [J/kg.K]	2361.2	2151-2626	Rask,(1989)
k [W/m K]	0.373	0.1-0.4	Jury *et al.*(2007)
h_c [W/ m^2.K]	26.09	20-50	Demirkol *et al.*(2006)
		30	Zanoni *et al.*(1994)
D_w [m/s]	1.710^{-10}	1.3-3.5.10^{-10}	Karathanos *et al.*(1995)
k_{me} [-]	0.0039	0.0049	Hadiyanto *et al.*(2007)
k_{br} [-]	0.2241	0.23	Hadiyanto *et al.*(2007)
E [N/m^2]	1.09E6	1.5E5	Marcotte and Chen (2004)
δT_{max} [^{o}C]	138.9	150	Hadiyanto *et al.*(2007)

The parameters for the quality model are also presented in Table 1. For the Maillard reaction *(k_{mr})* and brownness constants *(k_{br})* are estimated from ΔE measurements. The obtained values for these parameters are slightly below the previously reported values, just as the maximum temperature difference for the glass transition temperature *(δT_{max})*. The estimated elasticity coefficient (*E*) is above the literature value for a cake type of product.

5.2. Evaluation of the temperature trajectories

Figure 7 shows the development of the temperature at the crust and in the product center for convective baking and the combination of convective-microwave baking. Both experiments show that the product temperature at the surface increases rapidly at the beginning. This implies that evaporation at the surface is quick and the surface temperature goes quickly towards the oven temperature. During the full baking time there is enough water available in the product center to sustain a water activity near 100% and therefore the product temperature in the center increases only slowly to the boiling temperature (100^{o}C). Application of combined microwave and convective heating enhances the water evaporation in the product and results in a faster temperature rise in the center than with only convective baking (compare Figures 7a and 7b).

The agreement between experiments and model is in line with the results reported in the literature (Thorvaldsson and Janestad, 1999; Zheleva and Kambourova, 2005; Zhang and Datta, 2006). However, there is systematic deviation between the model and the experiments. This indicates that there is potential for further model improvement; for example to include the temperature and moisture dependency of parameters for specific heat coefficient, thermal conductivity and diffusivity as shown by work of Lostie *et al.* (2003) and Zheleva and Kambourova (2005). Furthermore it should be noted that the gas permeability was assumed to be constant, which should actually be a function of the product porosity, which changes during the baking process.

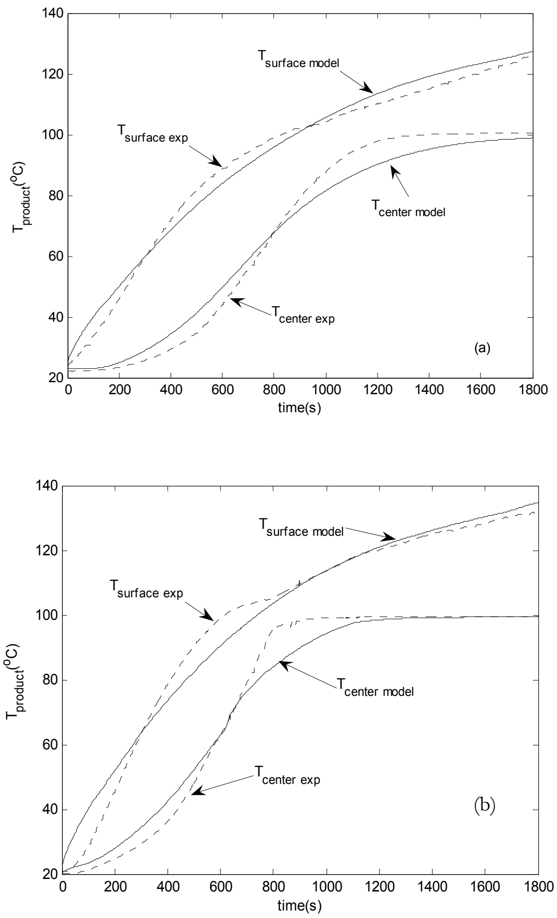


Figure 7. Product temperature during baking experiments (dashed line) and for model calculations (solid line) with convective heating (a) and the combination of convective and microwave heating (b).

5.3. Evaluation of Weight loss

The weight loss is due to the amount of water evaporated from the product during baking and depends on the baking processes. The weight loss for the two distinct baking operations is given in Fig 8. In total 10-20% of water is evaporated during baking. The weight loss for convective heating is small in the initial phase and increases exponentially after 900 seconds when the temperature in the product center exceeds 70°C. During combined heating baking water evaporation is enhanced. After already 600-700 seconds the temperature in the center of the product is around 70°C, after which the weight loss starts to increase. Microwave heat accelerates the evaporation of water in the product and might be used to control the water content inside the product.

There is a good correspondence between experiment and model after adjustment. However, the evaporation rate is overestimated for product temperatures in the range 70-95°C (600-1200 s), which is the same period where the temperature is overestimated by the model.

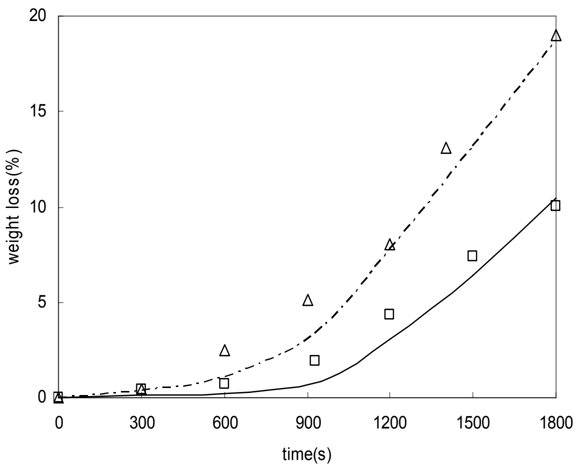


Figure 8 Product weight loss during baking with convective heating (□ : experiment; solid line: model) and combined microwave–convective heating (Δ: experiment; dashed line: model).

5.4 Evaluation of Height extension

The product size was measured for different baking times (see Figure 9). The size increases gradually until 1000 seconds of baking. The extension is result of the increase of internal pressure caused by the CO_2 gas production and the evaporation of water. Model predictions and experimental results are reasonably well. After 1200 seconds the size of product starts to decrease as a result of the decreasing pressure in the product and other non-modelled factors such as the change in gas permeability, but the results are not accurate enough to conclude that this is an essential effect.

Figure 9 shows that combined heating gives a faster development of product size, which is possible due to the increased water evaporation rate (see also section of weight loss). For convective heating at 200°C the product size increases up to 1.2 times above the initial size, while the microwave heating 100 W yields a size around 1.4 times above the initial size.

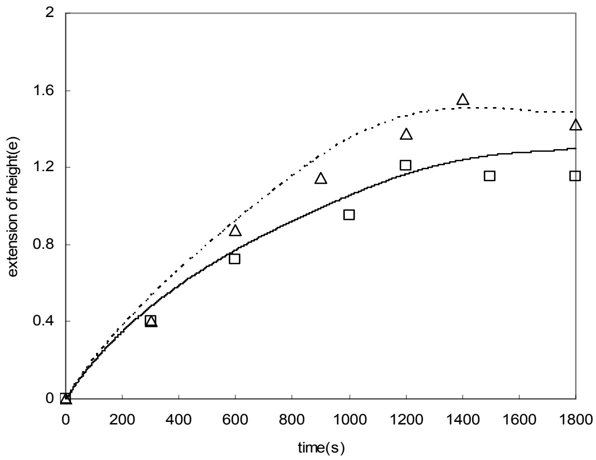


Figure 9. Height extension during baking with convective heating (□: experiment; solid line: model) and combined microwave–convective heating (Δ: experiment; dashed line: model).

5.5 Brownness development

Product brownness is mainly the result of the Maillard reaction. The intensity of the color, which ranges from pale yellow to very dark brown, depends on the intensity of this reaction (Henares *et al.*, 2006). Measured brownness values are in the range of ΔE = 24.35 for the initial dough color (pale), to ΔE = 67.12 for the highest value for a black product (Figure 10).

ΔE = 24.35 27.37 37.19 43.57 57.0 67.12

Figure 10. Formation of colour during conventional baking. The ΔE value is indicated

Figure 11 shows the correlation between the predicted brownness from the model and color measurement based on the Hunter method (Zanoni *et al.* 1995). The fair correlation implies that after parameter adjustment brownness is predicted satisfactorily and that the proposed relations (Eqs 21 and 22) can be considered valid.

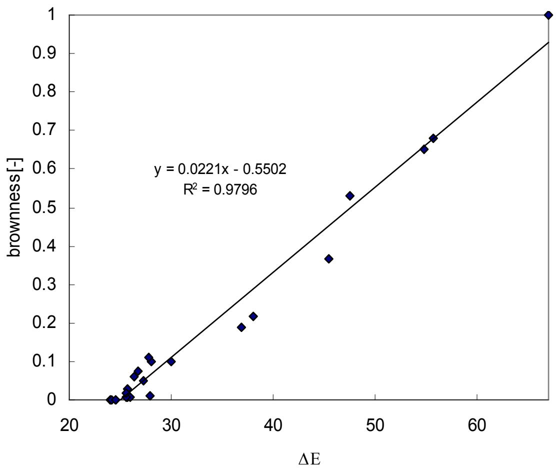


Figure 11 Correlation between brownness and measured ΔE values

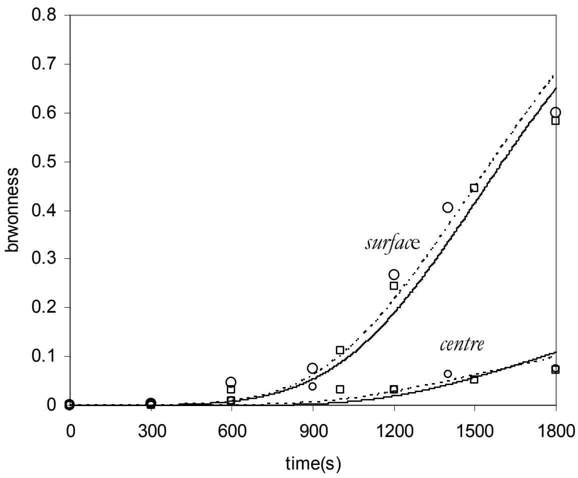


Figure 12 Color developments during baking in the center of the product and at the crust. Results for convective heating (□: experiment; solid line: model) and combined microwave–convective heating (O: experiment; dashed line: model).

In Figure 12 the brownness development during baking is given. The colour development for the surface is significant; in the center the colour changes are small. The difference in colour formation between convective and combined heating operations is minimal. These results are in agreement with the observations reported by Icoz *et al.* (2004) and Sumnu *et al.* (2001).

5.6. Crispness

The degree of crispness is in this study directly coupled to the maximum force required to break bread samples by the texture analyzer. Loads in the range 27 g to 512 g are linearly mapped to a crispness range from 0 to 1 (see Figure 13). The scaling is obviously dominated by one extreme loading, but the high correlation with the other measurements indicates that the use of the glass transition temperature in equations 23 as a predictor for the penetration force is a proper choice.

The crispness as a function of baking time is given in Figure 14. Compared to convective heating, the combination of convective heating and microwave gives only a small difference in crispness. This effect is result of the use of the microwave which generates heat inside the product and only partly affects the surface.

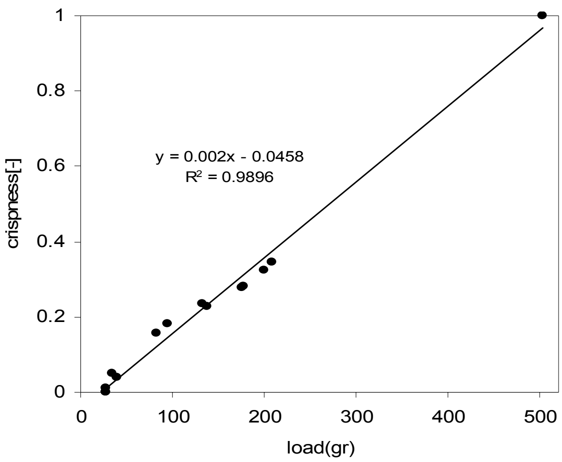


Figure 13 Correlation between crispness and load values

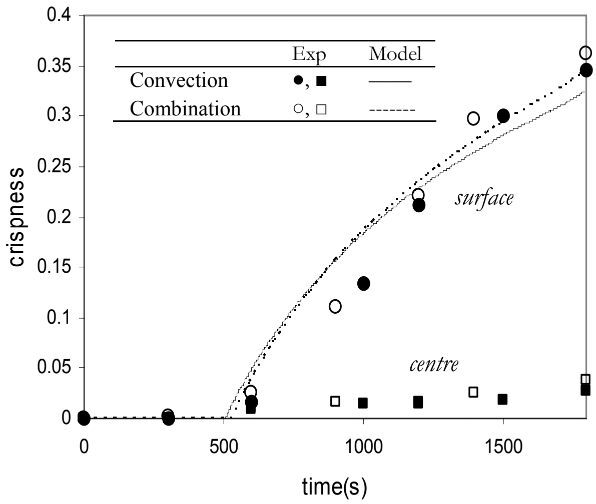


Figure 14 Crispness as a function of baking time. Experimental results (marker) and model simulation (line) for convective heating and combined heating inputs in the surface and center of product.

5.7. Accuracy

Although the model and the experiment have similar trends after parameter adjustment, the scattering of the data around the model prediction indicates that the prediction is not fully accurate. Table 2 contains an overview of the standard error after calibration for the temperature and product qualities over the discussed experiments together.

Table 2 Deviation between the experimental data and model prediction. The standard error of calibration is defined as $SEC=\sqrt{\sum(x_e-x_m)^2/n-1}$, where x_e is experimental data, and x_m is model data and n the number of data points

Quality	**SEC *)**
Brownness	5.0%
Crispness	6.5%
Volume extension	12%
Weight loss	1.1%
Temperature (°C)	5.2

5.8. Applying dynamic baking operations

In our previous work (Hadiyanto *et al.* 2007b) a model with un-calibrated parameters was used to find optimal heating strategies. In that work a nominal parameter set was used derived from literature.

It is interesting look at the sensitivity of the calculated trajectories to parameter changes. As an example, Figure 15 compares the input trajectories from the original parameter set and from the adjusted parameters obtained by the calibration in this work. The overall form of the trajectories is not affected by the calibration, but the exact trajectory is slightly affected by the new parameter set.

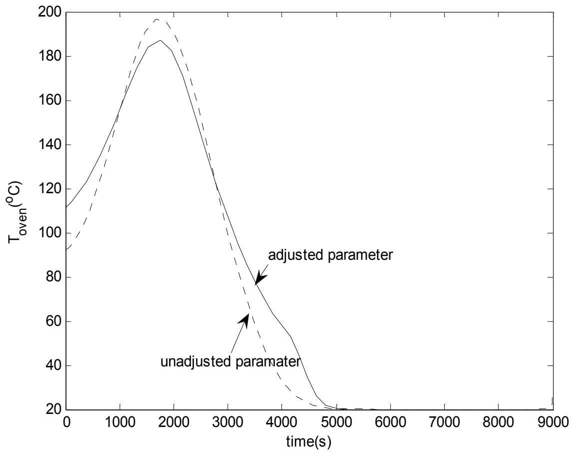


Figure 15 Example of heating input trajectories for a model with calibrated and with the nominal original parameters. The corresponded final quality for this input trajectory is brownness =0.8, crispness =0.65;

In the quality driven conceptual process design for which the model is intended the dynamic heating operations are an important component. Therefore, it is a good test to check the model performance for these kinds of dynamic inputs. This is more severe test, because the system is more excited than in the static operation used for the calibration. To this end dynamic heating operations as obtained are applied in an experiment, see Figure 16. Input trajectories for the experiment were calculated with the calibrated model by using control vector parameterization for four piece-wise constant intervals. Both convective heating and microwave plus convective heating were considered; the targeted quality values for the final product were brownness=0.8 and crispness=0.45. The recorded oven temperatures (Figure

16a and 16c), product temperatures (Figure 16b and 16d), and microwave input are shown and compared to the model values in Figure 16c.

Figures 16a and 16c show the planned and realized oven temperature and microwave trajectories. There are slightly deviations for planned and realized input trajectories. The reason for the difference is obvious; the oven has a heat buffering capacity (air, metal walls) and a resistance for heat transfer to the environment, which was not included in the model.

Figure 16b and Figure 16d show the product temperature according to the model prediction and measured during the experiments. The product temperature resulted from model prediction was calculated using realized (experiment) input trajectories. Overall, the predicted product temperature and measurements of both heating strategies have good agreement; though a slight deviation occurs in the phase where the center approaches the evaporation temperature. This difference is in line with the model-experiment differences as discussed in section 5.2. There is also significant acceleration of heating for the combined heating system during the first 15 minutes of baking; which results in a fast temperature rise and quick drying in this period.

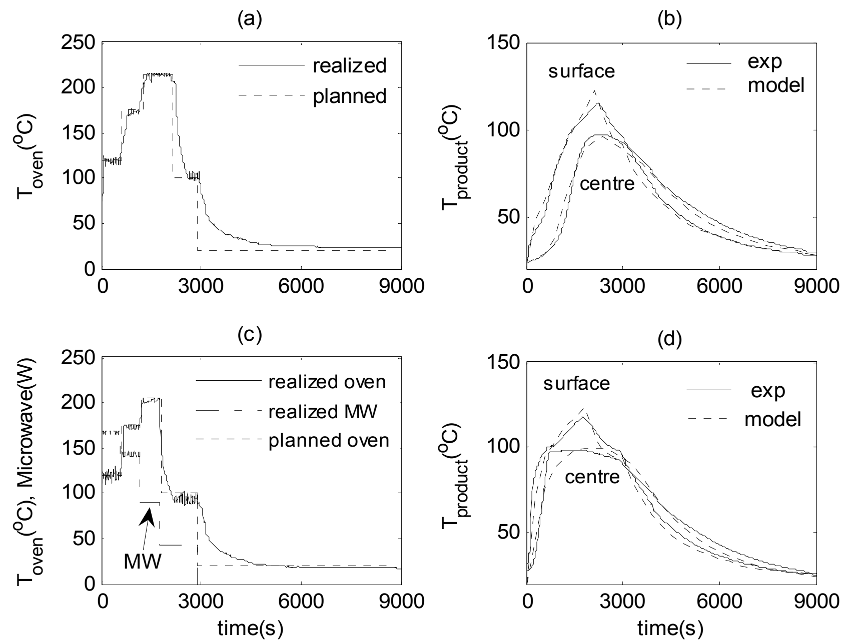


Figure 16. Experimental input trajectories for oven temperature (T_{oven}) and combination oven-microwave (*MW*) and the resulting product temperatures at the surface and in the center. a)

Convective heating, b) product temperatures for convective heating (solid line: experiment, dashed line: planned/model), c) combination oven-microwave, d) product temperatures for combination heating solid line: experiment, dashed line: planned/model).

The predicted and the measured qualities after baking are shown in Figure 17. The brownness values for convective and for combination heating are approximately equal. The crispness difference between the two heating methods is larger than expected. Most experimental values just fall within the prediction accuracy (see Figure 17 and Table 2), but nevertheless it can be noted that nearly all values are below the model prediction.

This might be partly attributed to the mentioned delay in oven cooling, but it is plausible that it is also related to the limited data set used for the calibration procedure. The model validation was only done for one temperature level (200°C) in combination with only one level for microwave power (100 W). During dynamic operation the system passes through a range of temperatures and microwave powers, and it is probable that the parameters have different values at these conditions. To improve the prediction for dynamic operations it would therefore be useful to extend the data set towards more temperatures and microwave power values.

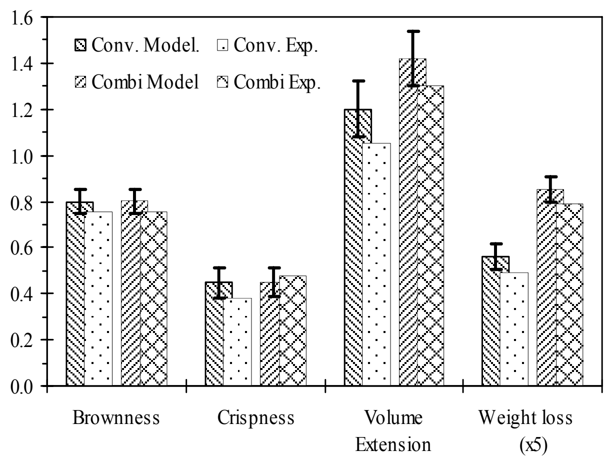


Figure 17. The comparison between model prediction (with expected uncertainty) and experimental measurement of final quality

6. Conclusions

A model for the prediction of baking product quality formation was calibrated and validated on the basis of a set of experimental data. The model is based on a combination of qualitative and partially quantitative information on transfer phenomena, phase transitions and product quality (Hadiyanto *et al.* 2007a). The most important model parameters were estimated from the experimental results in a sequential procedure for the different parts in the model: first heat and mass transfer related parameters, then parameters related to the state transformations and finally the parameters for product quality formation. This procedure is essential since optimization of all parameters at once is not successful due to the occurrence local minima and strong correlation between parameters.

The calibration set was obtained from baking experiments performed under constant baking temperatures and constant input of microwave power during 30 minutes and for a dynamic operation for 2.5 hours including a cooling period. The product quality was measured as a function of baking time at different positions (center and near surface) in the product.

With adjustment of the key parameters in the heat and mass transfer formulation, the model could predict the internal and surface temperatures well. The volume extension could be predicted well for most of the baking process, but still showed some deviation on the observed volume reduction in the final stage of the process. The product quality attributes brownness (based on zero order production of melanoïdines) and crispiness (based on the offset of the predicted glass transition temperature) could be well correlated with color and penetration (texture analyser) measurements, respectively. Moreover, it was shown that microwave heating hardly affects surface properties as color and crispness, but is an effective tool to control the water content of products.

The results for the dynamic validation experiments are within model accuracy and the differences between convective and combination heating could be clearly reproduced. However, the model slightly but consistently overestimates the quality attributes. This may well stem from the assumption that the model parameters are independent of the temperature. Further model improvement would probably require extension of the experimental data set to a range of temperatures, microwave powers, while measurement of the spatial gradients in temperature and moisture would enhance the value of the data set.

Nevertheless, the calibration and validation results show that it is possible with an integrated model, which encompasses the heat and moisture transfer and some important transformation, to predict the relative change and absolute value of some key product qualities, as function of the imposed process conditions. The main benefit is that such a model can thus be used to explore the all the degrees of freedom which are offered by the dynamic variation of process conditions and process design, and to directly show the consequences on the product quality attributes.

Acknowledgement

This research was financially supported by Graduate School VLAG, the Netherlands.

Annotations

Symbols	Descriptions	unit
a_w	Water activity	[-]
C	Other water binding components	kg kg^{-1}
c_p	Heat capacity	J kg^{-1}.K^{-1}
D_{vc}	Gas diffusivity	m^2 s^{-1}
D_w	Liquid diffusivity	m^2 s^{-1}
e	Extension of height	[-]
f	Fusion factor	[-]
E	Elasticity modulus	Pa
E_a	Activation energy	J mol^{-1}
G_0	Reference retrogradation rate	s^{-1}
I_v	Evaporation rate	kg m^{-3}s^{-1}
I_c	Production rate of CO_2	kg m^{-3}s^{-1}
h_c	Convective heat transfer coefficient	W m^{-2}K^{-1}
h_v	mass transfer coefficient	m s^{-1}
k	Thermal conductivity of product	W m^{-1}K^{-1}
K_g	Constant	[-]
k_{me}	Reaction rate of Maillard reaction	s^{-1}
m_v	Mass flux of water vapor	kg m^{-2}s^{-1}
m_e	melanoidins	[-]
m_c	Mass flux of CO_2 gas	kg m^{-2}s^{-1}
M_w	Molecular weight of water	kg mol^{-1}
P	Total pressure	Pa
$Pv_{,sat}$	Saturated pressure of water vapor	Pa
R	Gas constant	J mol^{-1}K^{-1}
R_{C0}	CO_2 generation rate	kg kg^{-1}s^{-1}
S	Sugar content	kg kg^{-1}
T_∞	Hypothetical temperature	K
U^*	Activation energy for product during recristalization	J.mol^{-1}
V_c	CO_2 gas concentration	kg kg^{-1}
V_v	Water vapor	kg kg^{-1}

W	Water content	kg kg^{-1}
Z	Starch content	kg kg^{-1}
T_g	Glass transition temperature	K
T_m	Melting temperature	K
T_α	Gelatinization temperature	K
S/Z	Ratio sugar to starch	[-]

Greek letters

α	Total degree of starch gelatinization	[-]
α_{max}	Degree of maximum starch gelatinization	[-]
λ	Evaporation heat	J kg^{-1}
ε	Porosity	[-]
υ	Kinematics viscosity	m^2 s^{-1}
ρ	Density of solid matrix	kg m^{-3}
κ	Permeability	m^2
η	Dynamic viscosity	Pa s
ϕ	Flux	kg m^{-2}s^{-1}

References

Demirkol, E., Erdogdu,F., and Palazoglu,T.K.(2006). A Numerical Approach with variable temperature Boundary Conditions to determine the effective heat transfer coefficient values during baking of cookies. *Journal of Food Process Engineering*,29,478-497

Dogan,H and Kokini,J.L.(2007). Psychophysical markers for crispness and influence of phase behaviour and structure. *Journal of Texture Studies*. 38,324-354.

Eliason, A.C., Larson, K.(1993). Cereals in bread making: a molecular colloidal approach. Marcel Dekker Inc, New York, USA, pp 328,351

Hadiyanto, Asselman, A., Straten, G. v., Boom, R. M., Esveld, D. C. and v. Boxtel, A. J. B.(2007a). Quality prediction of bakery products in the initial phase of process design. *Innovative Food Science and Emerging Technologies*, 8(2), pp. 285-298.

Hadiyanto, Esveld, D. C., Boom, R. M., Straten G. v. and v. Boxtel, A. J. B. (2007b). Product Quality Driven Design of Bakery Operations using Dynamic Optimization, *submitted*

Icoz, D., Sumnu G., Sahin, S. (2004). Color and texture development during microwave and conventional baking of breads. *International Journal of food properties*, 7, 201-213.

Jury,V., Monteau,J.Y, Comiti,J. and Le-Bail,A.(2007). Determination and prediction of thermal conductivity of frozen part baked bread during thawing and baking *Food Research International*,40(7),8*74-882*

Karanthanos,V.T, Kostaropaulos, A.E., and Saravacos, G.D.(1995).Diffusion and Equilibrium of Water in Dough/Raisin Mixtures. *Journal of Food Engineering*, 25,113-21;

Keskin, K.O., Sumnu, G., Sahin, S. (2004). Bread baking in a halogen lamp- microwave combination oven. *Food Research International*, 37, 489-495.

Lostie, M., Peczalski, R., Andrieu,J. and Laurent,M. (2002). Study of sponge cake batter baking process: II Modeling and Parameter estimation. *Journal of Food Engineering,* 55,349-357.

Marcotte, M and Chen,C.R. (2004). A computer simulation program for cake baking in a continues Industrial Oven. *ASAE/CSAE Annual International Meeting*, Ontario, Canada.

Ni,H and Datta,A.K.(2002). Moisture as related to heating uniformity in microwave processing of solids foods, *Journal of Food Process Engineering,* 22 , 367–382.

Rask, C. (1989). Thermal properties of dough and bakery products: A review of published data. *Journal of Food Engineering*, 9, 167-193.

Scanlon, M.G., and Zghal, M.C. (2001). Bread properties and crumb texture. *Food Research International*, 34, 841-864.

Sumnu, G. (2001). A review on microwave baking of foods. *International Journal of Food Science and Technology*, 36, 117-127.

Sumnu, G., Datta, A.K., Sahin, S., Keskin, O., and Rakesh, V. (2006). Transport and related properties of breads baked using various heating modes. *Journal of Food Engineering*, in press

Therdthai, N., Zhou, W., and Adamczak, T. (2002). Optimization of the temperature profile in bread baking. *Journal of Food Engineering*, 55, 41-48.

Thorvaldsson, K., and Janestad, H. (1999).A Model for Simultaneous Heat, Water and Vapour, Diffusion, *Journal of Food Engineering, 40*, pp. 167-172

Van Boekel, M.A.J.S. (2006). Formation of flavour compounds in the Maillard reaction. *Biotechnology Advantages*, 24, 230-233.

Weijts, F.G.M.P. (1995). Simulatie en optimalisatie van het bakken van biscuits. Landbouwuniversiteit Wageningen.

Zanoni, B., Peri, C., and Pierucci, S. (1993). A study of the bread- baking process I: A phenomenological model. *Journal of food engineering*, 19, 389-398.

Zanoni, B., Peri, C., and Bruno, D. (1995). Modelling of browning kinetics of bread crust during baking. *LWT*, 28, 604-609.

Zhang, J., and Datta, A.K. (2006). Mathematical modelling of bread baking process. *Journal of Food Engineering,* 75, 78-89.

Zheleva, I. and Kambourova, V. (2005). Identification of Heat and Mass Transfer Processes in bread during Baking. *Thermal Science*, 9(2), 73-86.

CHAPTER 8

Retrospection and Perspectives

1. Retrospection

There has been remarkable progress in the methods and tools for conceptual process design (CPD) in the past three decades. The conceptual phase of process design is not only important in the development of efficient production processes, but provides key competitive benefits with shorter product and process life cycles, flexible designs, and high efficiency for process operations. The major current part of activities in CPD concerns the production of chemical bulk products. However, there is increasing interest among food industries for developing new process design methodologies, driven by the need for attaining better product properties (defined by their quality and structure) in a shorter time, instead of process technology aimed only at process efficiency. Because of this interest this thesis introduces the concept of Product Quality Driven Food Process Design.

The specific research questions for this work defined in the introduction of this work were:

1. Are the current conceptual design methodologies applicable for food process design?
2. How to combine quantitative and qualitative knowledge on product qualities in a model?
3. Which contribution does dynamic optimization of transient processes give to quality driven food process design?
4. How do we deal with conflicting objectives in the process optimization and design?

This thesis discusses the potential applicability of conceptual process design frameworks for food production processes, with bakery production as example application. Reflection is given on the differences with the traditional approach for food process design, in which quality is the output, towards a quality driven approach (with quality as the input of the design process). Characteristics of product quality and processing units are treated as an integrated system by using quantitative and qualitative modelling, simulation and process optimization. The integrated approach for process design and operation, product properties and optimization delivers tailored design procedures and accelerates the identification of and development to new design solutions.

1.1. Product Quality Driven Food Process Design

The food industry requires flexible production processes to handle variations in product attributes and quality. Product quality as the main criterion for food process design is important as product quality ultimately should lead to consumer satisfaction and thus the success of product and process. The design approach proposed in this thesis approaches the design problem through a "reversed" reasoning procedure which starts from the required product quality, and from that proceeds towards the required process configuration. Successful design of food processes along this reversing approach requires a good understanding of the product's characteristics and possible processes conditions to form those products.

The design of food processes has to deal with multiple criteria and different design objectives. The specified criteria are consumer and market driven and simultaneously concern the high quality of products, microstructure, product and process safety, and process flexibility. These criteria are important for screening the design alternatives in the conceptual design level, but also specify from which point the design has to be started. The design procedure can be started from different points; it can either start from existing processes and products or it may be started for completely new products and processes. In addition it is important to take into account constraints imposed on the system by stakeholders as this can narrow the design space and thus will focus the design procedure.

The Delft Design Matrix (DDM) as systematic design procedure, developed for process design in the chemical industry, is based on an iterative design cycle, allowing process decomposition and product transformations. Even though the Delft Design Matrix seems applicable and flexible, it needs adaptation especially when it is applied to food process design. For example, process decomposition involves the decomposition of the design procedure in sub-blocks of design which reduces the complexity. The decomposition of food processes into small block of design will miss the integral picture of the whole processes, since the product quality can not be evaluated in the intermediate processes. The decomposition of food processes can be based on several criteria, i.e. on information from actors in the supply chain, on the process topology, on the total time of processing, on product quality specification and on product structure.

Determination of optimal operation strategies for product and process in the Product Quality Driven Food Process Design procedure is an extension of level four of the DDM (design of operational units). These optimal operation strategies are subsequently translated to unit operations; the other activity in level four of the DDM. By virtue of the procedure the identified unit operations will allow variations in the required product quality, thus increasing the flexibility of operation.

1.2. Predicting food product quality and transformations

Design of food processes implies dealing with the complexity of product(s) and transformation processes during the production process. Many food products have a complex structure, which determine the texture and taste experience. In addition, many process lines are used for the production of a range of products. The applied processes are essential in how the product structure develops during the time the product resides in the processing equipment. In many instances mass and heat transfer initiate transformations in the product, this finally leads to product quality formation.

In the process design procedure, (mathematical) models for process transformation and product quality were developed. This is considered of fundamental importance for food process design, especially when product quality is the basis of the design question. In order to be able to predict quality, all relevant aspects of the system behaviour, such as reaction kinetics, phase changes and corresponding process conditions, should be made explicit in the form of models.

To predict the transformations and product quality, a combination of qualitative and quantitative information from literature was used. The prediction is based on a combination of models for mass and heat transfer, product transformation and quality attributes. As knowledge on heat and mass transfer is well developed, this aspect was modelled in a detailed fashion, while other aspects are based describing the overall phenomena in a semi-empirical or fully empirical way.

The case under discussion (bakery production) shows how quality prediction can be used to improve the design of the process in terms of product quality. The qualities that have been considered for baking are crumb, crust, color, softness and crispness. The models for these properties were linked to the composition of the dough, process induced transformations and heating inputs. The transformations of starch are derived from the generally known behavior of polymers as a function of temperature and composition. Together with the glass transition, melting and gelatinization temperature, the degree of starch gelatinization is the main indicator for softness and crispness of the products. In storage the degree of gelatinization decreases by starch retrogradation, which results in stale products.

The Maillard reaction is the main reaction for color formation. The other phenomena such as protein network fixation, caramelization, carbonization and yeast fermentation do play a role, but they are less critical for design. Although only the main transformations were considered in the model, the quality prediction proved to be realistic and reliable, as was substantiated by the experimental validation work.

1.3. Optimization to determine operation strategy

Process optimization is important to identify better production processes, but also to identify possible alternative processing routes, different from existing ones. In addition, the optimized process may yield information about the behaviour of the product during processing, and as such may inspire product improvement or new product development. Finally, it may clarify the trade-offs between different quality factors in the final system (product + process) design. After the definition of the required final product quality, the processing strategies to achieve the product quality are calculated by using dynamic optimization. This optimization approach searches along a systematic way for the optimal conditions that a product has to meet during its transient time in the processing equipment. Currently available dynamic optimization methods were used in the search for the best solutions. In contrast to conventional design procedures, the search of the optimization procedures is not affected by *a priori* available engineering experiences and therefore the final solutions may yield unexpected, new process operation solutions.

The process optimization yielded the following results for Product Quality Driven Food Process Design:

- Different requested qualities are attained only through different heating procedures, which mean that product quality is indeed the essential starting point for design.
- The initial product properties determine for a large part the ability to achieve the required qualities.
- Using different sources of heat (multi-heating systems) increases the flexibility of bakery systems, or, in other words quality can be controlled by adjusting the process configuration.

In this work two approaches for dynamic optimization were used:

1. a method based on the calculus of variations using a gradient search method,
2. a method using control vector parameterization

Control vector parameterization in its simplest form (only a few parameters) yields switching functions. Even though control vector parameterization seems to be robust and easy to apply, the method based on the calculus of variations is regarded to be better in sense of achieved final objective value, because it converges closer to the solution by calculating and exploiting the gradient of the objective function to the input vector. However, the switching function is more likely used in the practice where it can be easily implemented as basis of operation.

Control vector parameterization with large number of parameter may large the computation burden. Therefore, in this thesis the standard control vector parameterization method has been improved. The adapted method reduces the computational load by starting with a coarse grid of only a few parameters, which is then iteratively refined at the most relevant locations during the operation. This method roughly halves the computational effort, while it yields an accuracy that is similar to that of the calculus of variation. The gain in computational efficiency is important for the optimization of the design and operation of any process system with complete processing line. In addition, it can also be used to identify critical quality control points in the production process, as these are the locations at which grid refinement occurs. This yields more insight in what factors and which process steps determine the quality of the product.

1.4. Design with multi-objective criteria

Product Quality Driven Food Process Design implies the handling of competing criteria and conflicting constraints. Not all of them can be satisfied at the same time and the final results of quality are described in terms of their trade-off. Feasible combinations of product quality are easily reached by adjusting the parameters of the input strategies. Unfeasible combinations of product quality yield deviations, which can be large or small depending upon the chosen utopia point, from the target values. Applying multi-objective optimization gives better understanding of what is good and not for the design of the production process.

The trade-off between two or more objective functions is represented by the Pareto front, which demarcates the feasible and unfeasible region. The Pareto front gives the decision maker information that there is not one single best solution for the competing objectives, but a set of solutions that come close to the (composite) goal. This set of solutions makes explicit how the preference for a specific product quality affects the other qualities. Moreover, the set of solutions on the Pareto front proved to be an important tool to extend the operational range of product qualities that can be achieved by using different heating strategies and different ways to prepare the starting materials. In the case of baking, the operational range was enlarged by applying multi-heating systems (process reconfiguration) and a shift of the feasible area was obtained by manipulating the initial water content (different preparation of the starting materials).

2. Perspectives

2.1. Application to other food products

The main issue in this work is how to design process operations and processing systems, led by the required quality of food products. The principle was demonstrated for bakery production, but it represents a general approach. In our view, it is also suitable for other problems in food process design. Knowledge about product quality formation is necessary, either mechanistic or descriptive, or a combination of both, as was applied in this work. The results show that even with extensive model simplifications the outcome can be significant.

In this thesis, a sequential model was used. The quality forming transformations in the product followed the results of the heat and mass transfer, but the transformations occurring did not have direct influence on the heat and mass transfer processes. A major advantage of this approach is that calculations for the sequential steps could be separated. However, in more complex food products with stronger interaction between mass and energy transport, transformations and product quality formation, the calculation task becomes more complex. For spatially inhomogeneous products, advanced Computational Fluid Dynamic (CFD) calculations may be required to obtain reliable prediction. These applications request advanced algorithms and significant computational power. With the developments in ICT (computer technology) these problems become feasible in the next years.

2.2. Supply chain design

Industrial food process design more and more comprises the full supply chain in which several actors as feedstock suppliers, producers, distributors and retailers and consumers are involved. The quality of products can gradually change in the supply chain and can be affected by the different actors. Since the quality is evaluated at the end-point, i.e. at the moment of consumption, strategies for quality control throughout the complete supply chain have to be considered. Analogous to this thesis work, the total chain has to be optimized with the final quality at the point of consumption as objective. By doing so, the whole production chain from feedstock to consumer preparation can be effectively optimized. However, because the system boundaries are significantly wider, the complexity of the design will increase, and hence the constraints by computation power. Thus, it is expected that process decomposition into smaller blocks will still remain necessary. In that case, the question how to stay close to the overall optimality will be an important issue for research.

2.3. Energy and other design aspects

In this thesis, the process design was optimized in terms of the product quality by adjusting process conditions and configuration. The process optimization was performed for a set of product qualities without any regard for the amount and type of energy that is being used in the process. From a consumer's point of view, this is mostly not a big point as long as the required product quality is reached. In contrast, the trend towards sustainable production, amongst others evidenced in raising energy prices and increasing governmental pressure to reduce energy consumption, becomes more and more important. Thus, the energy used during production may become a major aspect in food process design as well. This can be included in the design procedure developed in this work; it simply adds another criterion to the set of criteria used in the design process. Therefore, the application of multi-objective optimization for high quality and high process efficiency (e.g. by low energy consumption) may become even more relevant in the future. Thus we expect that product quality driven food process design will increasingly be an important and challenging area for future research and application.

A new trend in current process development is how to develop industrial processes for high quality products, efficient use of raw materials, minimal use of water and low waste. This trend is also a challenge for future development in food process design. The quality driven food process design approach has by its optimization background high potential to deal with these simultaneous requirements and can also help to find solutions when objectives seem to be conflicting.

Summary (English)
Samenvatting (Dutch)
Ringkasan (Indonesian)

Summary

Consumers evaluate food products on their quality, and thus the product quality is a main target in industrial food production. In the last decade there has been a remarkable increase of interest of the food industry to put food product quality central in innovation. However, quality itself is seldom considered as a starting point for the design of production systems. The objective of this thesis is to advance food process innovation by procedures for food process design which start from the product quality. The approach presented in this thesis is coined as Product Quality Driven Food Process Design.

The food industry has a limited tradition in systematic process design methodologies. **Chapter 2** gives a review on chemical process design methodologies and their potential applicability for food process design. The Delft Design Matrix, which combines the basic iterative design cycle, the product property difference method and the process decomposition method, provides a framework for flexibility in design and is able to decompose a complex problem into smaller parts. Food process design differs from chemical process design with respect to the criteria and design objectives. These differences arise from the quality demand (consumer preferences), the characteristic product microstructure, product safety and cost aspects. Nevertheless, the Delft Design Matrix is a useful framework to organize food process design procedures.

For design of food production systems, mathematical models have to be developed as a tool to simulate and explore the interaction between process design, operation conditions and product characteristics (**Chapter 3)**. A model for bakery applications was developed from a mixture of qualitative and quantitative knowledge, and assumptions that have been made to reduce the complexity. The baking model has three consecutive parts: mass and heat transport in the product, transformations concerning starch state transition and color, and the formation of quality attributes (color, softness, crispness and staling). The model for mass and heat transfer is based on laws of conservation and expressed in partial differential equations for spatial products. The starch state transition and color formation are a mixture of qualitative and quantitative information, while the product quality model is mainly based on qualitative information obtained from experts.

Chapter 4 presents the use of dynamic optimization as a tool for identification of baking strategies. The optimization methods use objective functions in which the final qualities are specified and places thus the product quality central in design. From the optimum operation strategies options for unit operation design can be derived. Two optimization approaches were

used: 1) calculus of variation and 2) control vector parameterization with a few switching functions. Optimization based on the calculus of variation gives overall a better result than using switching trajectories in terms of final achieved objective functions. The results illustrate that dynamic optimization procedures are versatile tools to generate design solutions. These search methods yield process solutions for which product quality can be realized more accurately and lead to more flexible production systems by generating a number of solutions from the specified final product qualities. Moreover, the results show the differences in required operation strategies for different final product attributes. Dough properties (dough water content and temperature) have significant effect on the operation strategy, and combining heating inputs (convective, radiation and microwave heating) improves the flexibility of the systems.

In contrast to the use of a few switching functions control vector parameterization can also be applied with fine grids, but the computational effort can be prohibitive while local minima are often encountered. In **Chapter 5** the efficiency of the control vector parameterization method with respect to computation time is significantly improved by applying a gradual refinement method. Starting from a low number of input parameters for a coarse grid, the grid is iteratively refined at time points for which the objective has a large sensitivity. This procedure halves the computational load while the obtained trajectories are hardly affected by local minima.

Not all combinations of product quality attributes can be obtained. Those combinations that are feasible can be easily achieved by single-objective optimization. However, combinations of quality attributes that cannot be obtained can only be approximated. A feasibility grid scan for product quality attribute combinations gives an indication of the feasible and non-feasible areas. As explained in **Chapter 6** the optimal approximations for product specifications in the non-feasible region are always on the border of the feasible and non-feasible area. Interestingly, the border can be evaluated by using multi-objective optimization to obtain the so called Pareto front. The Pareto front indicates that there is no single best approximation but a set of approximations representing different weighing of the various criteria. This set can be considered for the design. The application of a different process layout (multi-heating strategy) enlarges the feasibility area of design, while a change in formulation (dough water content) could shift the feasible area as well. In this way a wider range of bakery products can be produced.

The model presented in Chapter 3 was validated with bread baking experiments. As expected some parameters had to be adjusted when the model was confronted with real data (**Chapter 7**). The model, calibrated with data for constant operating conditions, was then validated by comparing the predictions for an independent set of data obtained from an experiment with dynamic operation. Although the model was developed in a straightforward way by combining qualitative and partially quantitative information, it predicts the quality of bread remarkably well. This gives confidence in the underlying understanding of the phenomena in the products and their interaction, and qualifies the model for use in dynamic optimization.

In the conclusion chapter (**Chapter 8)**, the approach of product quality driven process design is evaluated as a way of systematic thinking on how to improve or develop new processes from specified product quality. Major future challenges to follow market and economical developments are: (1) To apply the approach to other food products, (2) To use the methodology over the total production chain of food products from raw material supplier to consumer preparation and (3) To tackle design problems with a request for minimal use of energy and water, raw materials and minimum waste.

Samenvatting *(Dutch)*

Consumenten beoordelen voedingsmiddelen op hun kwaliteit, en daarom is productkwaliteit een van de belangrijkste criteria voor de verbetering van de industriële productie van levensmiddelen. Gedurende de laatste 10 – 15 jaar toont de industrie een toenemende belangstelling voor innovatie waarbij het de kwaliteit van het product een centrale plaats heeft. Toch is het opmerkelijk dat bij het ontwikkelen van productieprocessen het product geen centrale plaats heeft. Het doel van dit proefschrift is daarom de mogelijkheden van procesinnovatie uit te breiden met ontwerpmethoden die expliciet uitgaan van de productkwaliteit. De aanpak uit deze thesis wordt aangeduid met "ProductKwaliteit Gestuurd ProcesOntwerp".

De voedingsmiddelenindustrie heeft geen uitgebreide traditie in het gebruik van systematische methoden voor procesontwerp. **Hoofdstuk 2** geeft een overzicht van methoden die in de chemische industrie gangbaar zijn en de mogelijkheden om ze toe te passen in de voedingsmiddelenindustrie. De Delft Design Matrix combineert verschillende ontwerpmethoden (iteratieve procedure, productverschil methode en procesdecompositie), biedt mogelijkheden voor een flexibel ontwerpproces en maakt een complex vraagstuk hanteerbaar door het in kleinere stukken te verdelen. Bij toepassing van deze methode op de voedingsmiddelenproductie moet rekening gehouden worden met specifieke eisen van deze sector. Voorbeelden hiervan zijn de variëteit in consumenteneisen, de microstructuur in producten, productveiligheid en de kosten. Als hiermee rekening wordt gehouden blijkt de Delft Design Matrix toch een goede basis the bieden voor het ontwerpproces.

Voor het (conceptueel) ontwikkelen van productiesystemen worden wiskundige modellen gebruikt om de productieprocessen te simuleren en om interacties tussen het proces, de procesinstellingen en het product vast te kunnen stellen (**Hoofdstuk 3**). Een model voor het bakken van bakkerij producten is ontwikkeld door het combineren van kwantitatieve en kwalitatieve kennis, en een aantal aannames om de complexiteit hanteerbaar te maken. Het bakmodel bestaat uit drie op elkaar volgende delen: 1) warmte- en stoftransport, 2) transformaties voor het veranderen van de zetmeelstructuur en voor kleurvorming, en 3) kwaliteitsvorming (kleur, zachtheid/knapperigheid en verouderen van bakkerijproducten). Het model voor warmte- en stoftransport is gebaseerd op fysische behoudswetten en uitgedrukt in partiële differentiaal-vergelijkingen voor de ruimtelijke verdeling in de producten. De veranderingen in de zetmeelstructuur en kleurvorming zijn gebaseerd op kwantitatieve en kwalitatieve kennis, terwijl het model voor productkwaliteit voornamelijk op kwalitatieve kennis berust.

Hoofdstuk 4 betreft het gebruik van dynamische optimalisatie om dynamische bakstrategieën (met variërende verwarming gedurende de baktijd) te zoeken, waaruit procesontwerpen afgeleid kunnen worden. Deze optimalisatie maakt gebruik van doelfuncties waarin de gewenste productkwaliteit expliciet kan worden opgegeven. Daarom is deze techniek bijzonder geschikt voor 'productkwaliteit-gestuurd procesontwerp'. Twee technieken voor dynamische optimalisatie zijn gebruikt: 1) gebaseerd op variatierekening, 2) stuurvector parameterisatie van een beperkt aantal schakelpunten. Het resultaat laat zien dat dynamische optimalisatie een krachtige techniek is om tot een procesontwerp te komen. De oplossingen leveren dynamische bakprocedures als resultaat waarmee de productkwaliteit nauwkeurig bereikt wordt en welke flexibel is om aan een grote variatie aan eisen te voldoen. De eigenschappen van het deeg (watergehalte en temperatuur), en het gebruik van combi-ovens (oven-, magnetron- en grillverwarming) vergroten de flexibiliteit van het systeem. De optimalisatiemethode gebaseerd op variatierekening geeft betere resultaten dan de methode gebaseerd op het gebruik van schakelfuncties.

In plaats van stuurvector-parameterisering van een paar schakelfuncties toe te passen, kan stuurvector-parameterisatie ook gebruikt worden met een groot aantal schakelfuncties (fijn raster). Dat vraagt echter een erg grote rekencapaciteit, terwijl de oplossing vaak in lokale minima terecht komt. De efficiency van deze stuurvector parameterisering is in **Hoofdstuk 5** belangrijk verbeterd door met een grof raster te beginnen en dat iteratief te verfijnen op die plaatsen waar de gevoeligheid van de doelfunctie voor de procesomstandigheden het grootst is. Deze procedure halveert de rekentijd en is minder gevoelig voor lokale minima.

Ni*et al*le combinaties van aspecten van productkwaliteit zijn te realiseren. Combinaties die mogelijk zijn, kunnen zonder problemen gevonden worden. Combi naties die niet kunnen worden gerealiseerd kunnen alleen worden benaderd. Een haalbaarheids-scan voor haalbare en onhaalbare combinaties van productkwaliteitsaspecten kan een indruk geven van de haalbare en onhaalbare combinaties. De mogelijke beste benaderingen voor onhaalbare combinaties liggen dan op de scheidingslijn tussen het haalbare en niet haalbare gebied (het Pareto front). Er is dan geen unieke oplossing, maar er kan gekozen worden uit een aantal oplossingen, die verschillende afwegingen tussen de verschillende criteria vertegenwoordigen. **Hoofdstuk 6** laat zien dat een verandering van de layout van het proces (gebruik van een combi-over) het haalbare gebied vergroot, evenals een verandering van de productformulering (hier het watergehalte van het deeg).

Het model, dat in hoofdstuk 3 is gepresenteerd, is gevalideerd met broodbak-experimenten. Nadat een aantal parameters zijn aangepast op basis van deze experimenten heeft het model goede overeenkomst met het experiment (**Hoodfstuk 7**). Dit is een goed resultaat gezien het feit dat het model een rechttoe rechtaan combinatie is van kwalitatieve en kwantitatieve kennis. Het model voldoet ook redelijk voor de dynamische bakstrategieën. Een ander belangrijk resultaat van de validatie is dat nu een model beschikbaar is dat inzicht geeft in de processen die tijdens bakken van bakkerijproducten plaatsvinden.

In **Hoofdstuk 8** wordt de methode voor "productkwaliteit gestuurd procesontwerp" geëvalueerd als een systematische manier van denken voor het verbeteren en ontwikkelen van processen uitgaande van de productkwaliteit. Markt- en economische ontwikkelingen geven ook nieuwe uitdagingen voor verdere ontwikkeling van "productkwaliteit gestuurd procesontwerp": 1) toepassen voor een brede range voedingsmiddelen, 2) gebruik voor sturing van productkwaliteit over de gehele productieketen, 3) gebruik bij ontwerpvraagstukken voor de reductie van energie-, water- en grondstofgebruik en voor het minimaliseren van productieverliezen.

Ringkasan (*Indonesian*)

Konsumer mengevaluasi produk-produk makanan berdasarkan kualitasnya dan saat ini kualitas makanan dijadikan trend sebagai tujuan utama bagi industri-industri makanan dalam pengembangan prosesnya. Dalam beberapa tahun terakhir terjadi perubahan arah signifikan dalam inovasi di bidang kulaitas produk makanan. Akan tetapi dalam kenyataannya, kualitas produk belum di jadikan dasar atau patokan dalam desain proses makanan. Oleh karena itu, thesis ini memberikan kontribusi dalam mengembangkan lebih lanjut inovasi di bidang desain proses produk makanan dengan kualitas sebagai titik awalnya. Pendekatan yang diajukan dalam thesis ini adalah Desain Proses Makanan berdasarkan Kualitas Produk.

Metodologi desain untuk industri produk makanan saat ini masih terbatas. Oleh karena itu, **Bab 2** memberikan review tentang metodologi untuk desain untuk industri kimia dan potensial aplikasinya untuk desain proses makanan. Delft Design Matrix yang merupakan gabungan antara metode dasar, metode perbedaan karaketristik dan metode dekomposisi proses, memberikan fleksibilitas yang besar untuk desain proses bahan makanan, dimana metode tersebut mampu membagi problem yang kompleks ke bagian-bagian yang lebih kecil. Selain itu, desain proses bahan makanan berbeda dengan desain untuk produk-produk kimia dalam hal kriteria dan tujuan desainnya. Perbedaan-perbedaan tersebut yaitu konsumer evaluasi, mikrostruktur produk, safety, dan aspek ekonomi. Dengan demikian Delft Design Matrik menunjukkan potensialnya dalam prosedur desain untuk process bahan makanan.

Untuk desain sistem proses bahan makanan, model sangat diperlukan untuk dapat mensimulasikan dan memperoleh interaksi antara desain proses, proses kondisi dan karaketristik produk (**Bab 3**). Dalam thesis ini, model untuk bakery produk dibuat berdasarkan kombinasi antara kualitative dan kuantitative informasim dan beberapa assumsi juga dibuat untuk mengurangi kompleksitas desain. Model untuk baking dibuat dalam tiga bagian utama yang berturutan: perpindahan massa dan panas di dalam produk, proses transformasi untuk starch dan warna, serta pembentukan kualitas makanan (warna, keempukan, kerenyahan dan *staling*). Model untuk perpindahan panas dan massa berdasakan pada hukum-hukum konservasi dan dibuat dalam persamaan-persamaan turunan parsial. Starch transisi dan pembentukan warna merupakan gabungan antara kualtitaive dan kuantitative informasi yang disusun dalam persamaan-persamaan biasa sedangkan model untuk kualitas produk berdasarkan kualtitative informasi dan disusun dalam persamaan aljabar.

Untuk **Bab 4** membahas tentang kegunaan dinamika optimisasi sebagai alat untuk mencari optimal baking strategi. Optimisasi tersebut menggunakan kualitas produk akhir dalam fungsi objektifnya. Dari beberapa alternatif optimal operasi, kita memperoleh informasi untuk desain suatu unit operasi. Untuk keperluan tersebut, dua optimasi prosedur digunakan yaitu:1) Variasi kalkulus dan (2) parameterisasi vector kontrol dengan fungsi switching. Hasil yang diperoleh menunjukkan bahwa dinamika optimisasi merupakan cara yang efektif untuk menyelesaikan desain. Methode-metode tersebut menghasilkan penyelesaian proses dimana produk dapat dihasilkan secara akurat dan mendapatkan proses yang fleksibel. Selain itu, hasil riset juga menunjukkan bahwa strategi operasi tergantung pada kualitas produk yang diinginkan. Properti dari dough (adonan) seperti kandungan air dan temperatur juga mempunyai efek yang signifikan terhadap strategi operasi, dan kombinasi pemanas (konvektif, radiasi dan microwave) dapat meningkatkan fleksibilitas sistem. Optimisasi berdasakan kalkulus variasi memberikan hasil yang lebih baik dibandikan dengan fungsi switching.

Lain halnya dengan fungsi swicthing, parametrisasi vektor kontrol dapat digunakan untuk penentuan optimasi dengan jumlah grid yang relative tinggi, akan tetapi hal ini secara nyata berakibat pada meningkatnya waktu komputasi dan sering terjebak dalam lokal minimum. Dalam **Bab 5,** effisiensi dari parameterisasi vektor kontrol ditunjukkan dengan penurunan waktu komputasinya dengan metode refining. Dimulai dengan jumlah parameter yang rendah, kontrol dapat di refine untuk parameter yang mempunyai sensitivitas yang tinggi (lebih besar dari nilai batas). Metode ini mereduksi waktu komputasi sampai 50% dan input yang diperoleh sangat jarang dipengaruhi oleh lokal minimum.

Strategi operasi di area yang feasible untuk produk dapat dengan mudah di peroleh dengan optimasi satu fungsi yang diselesaikan secara simultan, akan tetapi spesifikasi di luar area sangat sulit untuk di peroleh. Untuk itu dilakukan grid scan untuk mendapatkan indikasi dimana area yang feasible dan tidak. Solusi yang bisa didapatkan untuk produk didaerah yang tidak feasible selalu berada di batas feasibel dan tidak feasibel area yang dikenal dengan istilah Sisi Pareto (Pareto front). Pareto front ini mengindikasikan bahwa tidak ada satupun hasil yang terbaik sehingga solusi dari desain dinyatakan dalam satu set solusi. Dalam hal ini juga ditunjukkan bahwa aplikasi dari kombinasi pemanas dapat meningkatakn flexibilitas processes dan kandungan awal dari adonan memberikan pergeseran untuk area yang feasible. Beberapa aspek ini dijelaskan dalam **Bab 6.**

Model yang telah dibuat di Bab 3 kemudian divalidasi dengan eksperimen untuk baking sebuah roti. Hasil dari validasi menunjukkan bahwa beberapa parameter dapat di prediksi dengan metode parameter estimasi **(Bab 7).** Meskipun model telah dibuat dengan cara yang mudah dengan menggabungkan informasi kualitatif dan kuantitatif, akan tetapi model tersebut dapat digunakan untuk mempredikasikan kualtias dari roti, demikian pula ditunjukkan dengan sistem operasi yang dinamik. Validasi model dapat digunakan untuk mengklarifikasi penggunaaan model untuk mengetahui fenomena di dalam produk dan beberapa interaksi yang terjadi didalamnya.

Pada Bab kesimpulan **(Bab 8),** pendekatan desain dengan berdasar pada kualitas produk dapat dikatakan sebagai cara berfikir yang sistematik terhadap bagaimana untuk meningkatkan atau membuat proses yang benar-benar baru dari kualitas produk akhir. Untuk rekomendasi ke depan, hal-hal yang perlu diperhatikan untuk mengikuti perkembangan pasar dan ekonomi: 1) penggunaan metodologi untuk produk lain,(2) Menggunakan metodologi untuk sistem produksi secara keseluruhan dari bahan awal sampai konsumer dan (3) Aspect lain seperti energy, limbah buangan dan minimal penggunaan air juga perlu diperhatikan.

Acknowledgement

The aim of life is appreciation; there is no sense in not appreciating things; and there is no sense in having more of them if you have less appreciation of them.
(Gilbert K. Chesterton)

This thesis is the end of my four year voyage to attain my PhD degree in the field of food process design at Wageningen University. During this voyage I have not travelled in a vacuum and there are some people who eased the way with words of encouragement and suggestions of different places to look to expand my work. Therefore, my last task is to acknowledge all those people that have contributed to the work described in this thesis.

A few lines are too short to make a complete account of my deep appreciation for my daily supervisor, Ton van Boxtel. Your patience and encouragement strongly motivated me to do this research. I learned a lot working with you, especially in relation to dynamic optimization and also how to improve and refine my manuscripts; which may have consumed a great deal of your time and gave impact on rescheduling your summer holiday. I would not be able to stand on the stage without your help. I look forward to welcoming you and Wietske to Indonesia to continue our zoo visiting tradition.

Next, I wish to gratefully thank Erik Esveld as my second co-supervisor. Your critical comments provided a valuable contribution to the first manuscript; I benefited a lot from our discussions, particularly for design methodology, feasibility area and process engineering aspects. Thanks also for restructuring our CPD. It took time, but, finally we made it accepted.

Gerrit, I greatly appreciate your valuable comments and critical corrections of the manuscripts that were essential for this thesis. I was gaining a lot of scientific aspects during our discussion. Thank also for being with me to finalize the thesis and apologize to interrupt your sabbatical activity. After all, it was a great opportunity to be a member of your staff.

Remko, thanks for your suggestions and comments on the manuscript, it significantly improved the quality of my writing. During your holiday time, you made nicely structure of paragraph from my scattering words of Indonesian-English. Thanks also for letting me join the PhD trips to Sweden and Denmark, I really enjoyed it.

Leaving the Systems and Control Group at Wageningen University will not be possible without conveying thanks to many people. Let me address to all AIO colleagues for your warm friendship, Bas, Zita, Dirk, Martijn, Tijmen, Djaeni. Special thank goes to Bas and Dirk for being my paranymphs. To former PhD student, Stefan, Timo and Ilse, who already left when I finished this thesis, thank for everythings. I wish you all success for your PhDs and future careers, many thanks to all of you. I want to express also my gratitude to the permanent staff; Marja, for your kind help; Hans, Karel and Gerard for the valuable discussion about technical optimization problems; Gerard, it was great experience to be your assistant in Signal and System Modeling practical; Rachel, who always helped me with MATLAB whenever I need; Kees, for helping to set up the equipment; Wilko and Johan, for your warm greeting.

There are number of student involved in this project, Anneke for your initial work on bakery modeling, thanks for that although we never met and knew personally. However, your works give good initial starting point of the whole CPD project. Andreas, Mei and Irene thanks for your works in setting up the practical experiments.

My special thanks also go to the Indonesian Embassy for the Royal Kingdom of the Netherlands, especially to Mr Muhadjir, Attaché of Culture and Education, for his support and friendship. We came to the Netherlands about the same time and now also finish at the same moment. It was a great opportunity to be your friend. Of course, there are still a number of people that remain to be mentioned.

Next, let me acknowledge Peter de Jong, Maarteen, Martijn and Erik for welcoming me at NIZO Food Researcher. It is great opportunity to be part of your team.

I would also like to extend my grateful to Prof Johan Grievink for discussion about the Delft Design Matrix during visit to your department. It was a great time for me to learn how the important a framework of design.

Living in Wageningen was a great experience with very nice surroundings, weather and people. I would like to thank the Indonesian students (PPI Wageningen) and their families in Wageningen for their friendship. Pak Pieter de Kam - Mbak Endah family, Pak Marco - Mbak Ina and Traa family (thanks for the BBQ we really enjoyed it), Pak Sharul and family, Pak Mumu and family and other Indonesian families, all of you have inspired me and my family to feel at home in Holland, we enjoyed all the activities that we had together. Many thanks are also addressed to Indonesian students who are coloring our life in Wageningen, especially when they always ready to accompany my family during my busy time: M' Widi, Ipung, and *Hoevestein groups*.

I would like to also thank my badminton and tennis fellows: Fadli, Putu, Wiratno, Dwiko, Djaeni, Helmi, Syafwan, Raymond, Helmi and Bambang. Of course, there is nothing more important than fun of our games.

Unquestionably, my family also played an essential role on this thesis. I would not be receiving the PhD diploma without the support of my beloved wife, **Adian** and my cute-little girl, **Adhelia**. Both of you always smiled whenever I was busy with my work and did not complain about not having a holiday this summer. I thank you for love, encouragement, and sacrifices throughout the past four years. I dedicate all this work to you, to honour your love and patience. *Ik hou van jullie*

My parents and parents in law, who are in Pemalang and Malang, have always put education as a first priority in my life, and raised me to set high goals for myself. They taught me to value honesty, courage, and humility above all other virtues. I have always needed to work hard to achieve my goals in life and they have always been there for me as an unwavering support. I dedicate also this work to them.

Of course, there are more people who have direct or indirect contribution to this thesis but too many to mention. Therefore, I wish you all the best and thanks. *Alhamdulillah.*

Wageningen, November 2007

Hadiyanto

Curriculum Vitae

Hadiyanto was born on October 28, 1975 in Pemalang, Central Java Indonesia. After completed his secondary high school (SMA 1 Pekalongan) in 1994, he pursued his bachelor at Chemical Engineering Department, Diponegoro University, Indonesia and graduated in 1998. He started his professional job as a process engineer at PT Pupuk Sriwidjaja, Palembang before he got back to Diponegoro University as academic staff in 1999.

In 2001, he was admitted to Wageningen University where he studied Food and Bioprocess Engineering and obtained his MSc degree in 2003. His final thesis was about *Lethal effects during sparging of microalgae culture in photobioreactor*. At the same year, he was appointed as AIO (PhD student) for period 2003-2007 at Systems and Control group, Wageningen University to work on project of conceptual process design for food production system under supervision Prof Gerrit van Straten and Prof Remko Boom. The results of the research are presented in this thesis.
Since September 2007, he is a Scientist at NIZO Food Researcher BV, Ede-The Netherlands. He can be reached on the email: *hady.hadiyanto @gmail.com*

List of Publications

Hadiyanto, R.M. Boom, G. van Straten, A.J.B. van Boxtel and D.C. Esveld. (2007). Multi-Objective Optimization to Improve Product Range of Baking Systems. *Submitted to Journal Food Process Engineering*

Hadiyanto, R.M. Boom, D.C. Esveld, G. van Straten and A.J.B van Boxtel. (2007). Control Vector Parameterization with Sensitivity Based Refinement Aplied to Baking Optimization. *Submitted to Journal Food and Bioproducts Processing*

Hadiyanto, R.M. Boom, D.C. Esveld, G. van Straten and A.J.B van Boxtel. (2007). Multi Objective Optimization for Dynamic Baking Processes. *Abstract for 27th Benelux meeting 2007*

Hadiyanto, R.M. Boom, D.C. Esveld, G. van Straten and A.J.B van Boxtel. (2007). Optimization of baking operation using refinement method. *European Congress of Chemical Engineering, 16-20 September 2007, Denmark*

Hadiyanto, R.M. Boom, D.C. Esveld, G. van Straten and A.J.B van Boxtel. (2007). Product Quality Driven Design of baking operation using dynamic optimization. *Journal of Food Engineering, submitted (under review)*

Hadiyanto, A. Asselman, R.M. Boom, D.C. Esveld, G. van Straten and A.J.B van Boxtel.(2007). Quality Prediction of Food products in the Initial Phase of Process Design. *Innovative Food Science and Emerging Technology, 8(2),285-298*

Hadiyanto, G. van Straten, R.M. Boom, A.J.B. van Boxtel and D.C. Esveld.(2007). Potential of Conceptual Design Methodology for Food Process Innovation. *Food Science and Technology International*, *accepted for publication*

Hadiyanto, A. Asselman,G. van Straten, R. Boom, D.C. Esveld and A.J.B. van Boxtel.(2005). Heat and Mass Transfer Phenomena of Baking process: product quality aspects, *Proceeding of Eurotherm 82 Conference, Poland.*

Hadiyanto, A.J.B van Boxtel and D.C. Esveld. (2004).Conceptual Process Design in Food Industry: Application for Bakery Products. *Abstract for the 2nd European Symposium on Product Technology (Product Design and Engineering), Groningen, the Netherlands*

Not related to this thesis:

M.J. Barbosa, **Hadiyanto**, and R.H. Wijffels.(2004). Overcoming shear stress of Microalgae cultures in Sparged Photobioreactor. *Biotechnology and Bioengineering,* 85(1),78-85

Overview of completed training activities

a. Discipline specific activities		**Year**	**Credits (ECTS)**
1. Reaction Kinetic in Food Science	VLAG	2004	1.4
2. System and Control Theory	SENSE	2003	6.0
3. Model Predictive Control	DISC	2004	1.4
4. An Unified approach to mass transfer	OSPT	2004	1.4
5. Sustainable Process, Product and Systems Design	OSPT	2005	1.4
6. Uncertainty analysis	SENSE	2006	4.0
7. 2nd European Symposium on Product technology, Groningen	EFCE	2004	1.4
8. Eurotherm 82, Numerical Heat Transfer Krakow	Eurotherm	2005	1.4
9. Benelux Meeting 2007	DISC	2006	1.4
10. ECCE-6 Copenhagen /Food Congress 2007	EFCE	2007	1.4
b. General courses, language use, presentation courses, statistics, e.g.			
1. Scientific writing	CENTA	2004	1.7
2. Scientific presentation	CENTA	2004	1.9
3. PhD week	VLAG	2004	1.1
4. DISC Summer school	DISC	2005	1.1
5. Career perspectives	WGS	2007	1.5
c. Optional			
1. Advanced Food Process and Production Engineering	WU	2003	6.0
2. Brainstorming week Process Engineering Group	PRE	2003/2006	2.8
3. Food Soft Matter	VLAG/PRE	2006	0.5
4. PhD Tours(incl. presentation)	VLAG/PRE	2006	1.7
5. Research proposal			6
Total			**45.3**

This project was carried out at Wageningen University, Department of Agrotechnology and Food Sciences, Systems and Control Group, P.O. Box 17, 6700 AA Wageningen, The Netherlands.

The research described in this PhD dissertation was financially supported by the Graduate School VLAG (Food Technology, Agrobiotechnology, Nutritional and Health Sciences).

Printed by Ponsen & Looijen B.V., Wageningen

Cover design by Hadiyanto