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Quality Modelling

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INTRODUCTION

What is Quality?

In one way or another, all research and technological efforts in agriculture are related to quality. Massive efforts have been conducted to produce quality, to maintain quality as good as possible, and in the long run, to improve the quality of our lives. It is, however, amazing that this ever-present and always important quality is so ill defined. It differs from person to person, from situation to situation, from product to product. In working with quality of agricultural produce, researchers are implicitly and often unknowingly involved in the field of psychology, and the changing behaviour and desires of man. Furthermore, the behaviour and decisions of individual consumers with respect to acceptability and actually acceptance, is strongly affected by the economic boundaries and market situation in which that particular consumer operates. So, when conducting research on product behaviour and properties, it is necessary at least to realise that these three areas (product, psychology and economics) each affect quality, or rather acceptability, in a specific and mutually independent manner.

So, we have to grasp the meaning that quality has for each individual consumer, how he translates his observation of the product and how he evaluates his perception. This whole process will eventually result in an acceptability of the product by an individual consumer for an individual purpose (fulfilling expectations MacFie 1995, 1996, Sloof et al. 1996).

For research on quality, acceptance, product behaviour and consumer behavioural patterns targeted at practical applications in production trade and processing of food products, this individual perception and evaluation of quality has to be extended to include group behaviour, both with respect to the product as to the consumer. That is the realm of consumer and market research and is well out of the scope of this lecture. Nevertheless, to provide some information to consumer and market research, and to provide some guidelines for product research, for food production, for trade and for processing, it would be very advantageous to uncouple these three interacting fields that are associated with what is normally called quality.

Also for modelling product behaviour, with respect to quality for users and consumers, it is essential to have at least a fundamental notion what quality really is, and which product properties determine the quality assigned by the consumer to a product. In other words, what is allowed and what is to be avoided when modelling product behaviour in terms of quality and acceptability.

So, a more philosophical view on quality was developed with the sole purpose of determining how and what to model when describing food quality as objective as possible (Tijskens et al. 1994b, Sloof et al. 1996, Wilkinson et al. 2001). Meanwhile, it turned out to be a satisfactory theory for quality in general. The central and crucial aspect of the viewpoint is the decomposition of evaluation and appreciation into a more (although not completely) objective assessment of quality called the assigned quality that is valid for the majority of consumers and users. The more subjective appreciation in term of acceptability is postponed to the market and consumer part of the acceptance chain.

What is modelling?

The ultimate goal of modelling is to provide reliable predictions of occurrences that did not yet take place, for any product, from any source and in any situation. In the formulation of Rickert (2001): *Models can be regarded as a repository for past research since they collate and integrate information from past research.* This goal, although agreed upon by every modeller and every user of models, is however at the present time far out of reach and far away from being fulfilled by the present technology in modelling. Oh yes, modellers have achieved major progress in mathematics, modelling techniques and modelling tricks during the past few decades, from the early seventies of past century (Thornley 1976, 1990, Edelstein-Keshet (1988), Keen and Spain (1992), Brown and Rothery (1993) up to the 21st century. What technology can deliver at the moment, is a fairly accurate mathematical description of the behaviour of a product or commodity in conditions not too far away from the conditions at which the tests have been conducted and at which the results have been gathered based upon which the model is so-called validated or calibrated.

For modelling the quality behaviour of our food from the growing site through the different handling sequences, the distribution chain, storage, processing up to the final consumption and the final judgement of consumers, that situation is not different. A vast number of models, submodels and applications have been built and many of them have been reported in detail. Most of these models are very valuable for exactly that but only that application: predicting the future behaviour of a product in circumstances similar to the test circumstances. These are the so-called dedicated models. From the moment on, the application is extended to fairly new circumstances, the sometimes huge task of developing, creating and calibrating new models has to be taken up again. In terms of efficiency of resource utilisation, this approach seems efficient in the short span of time, in the long run, however, this approach is not very efficient or satisfying. Moreover, in terms of understanding of the problem at hand and generating knowledge this approach generates only circumstantial understanding.

To achieve the ultimate goal of modelling quality: predicting future behaviour of any product and its quality from any source in any circumstance while generating more knowledge about the process under study, we need to and have to include all available knowledge, fundamental as well as practical, that is at our disposal. The results of this kind of approach are the so-called fundamental (or rather fundamental oriented) models. These do indeed generate more knowledge and understanding, and can direct scientific research to those areas where information and understanding seems to be lacking.

Fundamental models and disciplines

Fundamental oriented models can be built in many ways and within many scientific disciplines. Disciplines, however, are a result of the deep-rooted urge of man and scientists to bring some order in our view and perception of the world. Nature on the other hand, does not have or need disciplines at all. Processes occurring in nature "naturally" comply with the laws of nature. The ultimate drive of science is to detect and understand those laws, and to convert the understanding of these laws into some practical application to increase the quality of our lives. So, within the realm of each discipline, the same laws of nature will be present and known in one form or another. The direct consequence is that in modelling and understanding processes of nature, it does not really matter which particular discipline is used as a framework, as long as its rules are used consistently and thoroughly. For myself, being a chemist by education, the choice of kinetic modelling was self-evident.

The general rules of kinetic modelling are summarised and described in van Boekel and Tijskens (2001). The rules of discipline and the laws of nature in the area of chemistry were all discovered and formulated in the early days of chemical discoveries and theories were formulated. They are now a standard part of textbooks on chemistry, physical chemistry, kinetics and enzyme kinetics (Fersht 1984, Chang 1991, Whittaker 1994 etc). Although this knowledge is available for such a long time, when building empirical models old-fashioned style, this knowledge is the first information that consistently is **not** used at all. Every time new data need to be analysed, mathematical and statistical relations are invented and tested, and the model with the statistical best fit to the data at hand is chosen to represent the behaviour of that system, without including any expert knowledge whatsoever. Modern science is based on the most important rule of all: the repeatability of a process. That is in the same conditions the same process will occur with the same rate. In making models, we should use this very basis of science and search for process rate constants that are true constants for any condition encountered. In other words, rates constants of processes will be the same for the same processes, no matter what the conditions are.

Some general rules can be drawn up when modelling the complexity of interacting processes that occur in nature. When targeting at modelling interactive processes, it is of utmost importance to apply the old Roman rule “divide et impera” (divide and rule). In modern terminology, that is problem decomposition. Having used this technique almost unconsciously for several years in developing process oriented models, a young information technologist devoted a major part of his PhD thesis to develop a more consistent, understandable and applicable system in that respect (Sloof 1999, Sloof 2001). Still, the process of detecting possible and plausible mechanisms in rather unstructured data is apparently quite a difficult task for most people. In my opinion, that is what makes a modeller a good modeller, rather than the necessary requirement of mathematical skills or product expertise.

Another general rule for developing process-oriented models is the consistent application at all cost of the laws of a particular discipline. Adapting mathematical equations, whether at the level of differential equations or at the level of functions or analytical solutions of these differential equations, invariable changes the fundamental nature of a model into an empirical one. Changes are only permitted at the level of developing appropriate mechanisms. Changes at a mathematical level inevitably prevent any further development along fundamental lines. Process oriented modelling offers not only the advantage of an increased understanding of processes and interactions. It also ensures also a reusability of models and above all the transferability of parameter values to all kinds of different situations and conditions the product is used at. And that is the ultimate goal of modelling altogether: providing a prediction of future behaviour of products from any provenance, from any growing conditions and in any circumstance during the food supply chain.

Based on these ideas, using the vast knowledge product experts have on the occurring processes and the applicability of the laws of disciplines, modelling product behaviour, and modelling food quality is not difficult at all, it only takes a lot of time and effort. The reason this technique has not been used consistently in every case is the idea that our food is too complex to be described by these simple principles.

Colour

For many products, colour is the only attribute that can be perceive by consumers / buyers without touching or eating the product. In itself it has not directly a quality attribute, but it is strongly related to the physiological maturity. For many products it is, therefore, used as a general quality and maturity indicator.

The colour of many products changes in a sigmoidal pattern from (mostly) a dark green colour to a bright red colour (tomatoes, cherries), a yellow colour (banana, cucumber, apple, leafy vegetables, melon) or any other colour typical for that product (e.g. brown for nuts). Sometimes a green colour is considered good quality (vegetables), sometimes the final colour is (tomato), and sometimes an intermediate step is related to quality (banana).

The sigmoidal pattern is often describes by the logistic function (Tijskens & Evelo 1994a, Schouten 1997). In the simplest form, this logistic behaviour could be traced back to the following (autocatalytic) mechanism:

$$G + R \xrightarrow{k_r} 2 \cdot R \qquad \text{eq 1}$$

G stands for green of chlorophyll, R for red or decay products, and k_r is the reaction rate constant. This results in the following set of differential equations:

$$\frac{dG}{dt} = -k_r \cdot G \cdot R, \quad \frac{dR}{dt} = k_r \cdot G \cdot R \qquad \text{eq 2}$$

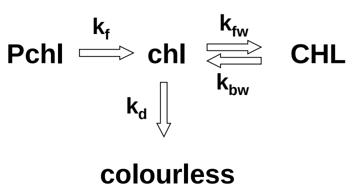
At constant external conditions (mainly temperature), an analytical solution can be obtained by integration and converting into a normalised description ($R_0+G_0=1$):

$$G = \frac{1}{\left(\frac{1}{G_0} - 1\right) \cdot e^{kr \cdot t} + 1} \qquad \text{eq 3}$$

Like any chemical reaction, the rate of colour development depends on temperature according to Arrhenius' law. In Figure 1, a simulated example is given for the development of red colour (e.g. of tomatoes) at increasing temperatures.
If one likes to think in terms of enzyme action, exactly the same analytical solution can be obtained from the mechanism:

$$G + E \xrightarrow{k_r} 2 \cdot E + R \qquad \text{eq 4}$$

where E is some enzyme, probably chlorophylase. Although these mechanisms describe adequately the colour development for a large number of fruits and vegetables, this mechanism is only a huge simplification of the processes occurring in real food products. Schouten et al. (2002) developed a more realistic physiological (but far more complex) model for green products (cucumbers) that comprises a colour precursor (Pchl) to chlorophyllides (chl) and chlorophyll (CHL). Both chlorophyllides and chlorophyll are the colouring compounds:



eq 5

In Figure 2 an example of the general behaviour is shown, indicating the initial increase in observed colour, generated by the conversion of colourless protochlorophyllide to coloured chlorophyllide and further to chlorophyll. The fundamental difference in colouring behaviour between cucumbers of apparently the same stage of development can now be attributed to differences in the initial state Pchl.

Firmness

Another quality attribute that is considered very important by consumers and buyers of many fruits and vegetables is firmness. What firmness really is can be discussed, and depends on the situation, the observer and the technical possibilities. Formally, firmness is the sensation of mechanical properties of the product that humans perceive when eating or chewing the product. As such, firmness is a purely sensorial attribute. In a wider sense, firmness is frequently measured objectively by compression equipment, and lately also non-destructively based on vibration resonance frequencies. In the case of firmness, however, a much larger discrepancy then in the case of colour, exists between sensorial firmness and objective firmness. Care has therefore to be taken to assure that objective firmness matches at least partially the sensorial sensation.

For many products, firmness decrease upon storage by a simple first order reaction:

$$F \xrightarrow{k_f} decay \qquad \text{eq 6}$$

which results in the well know exponential function, possibly adapted for an invariable end value F_{fix}:

$$F = F_0 \cdot e^{-k_f \cdot t} + F_{fix} \qquad \text{eq 7}$$

F represent the firmness, k_f the reaction rate constant of the firmness decay reaction. This invariable end value in firmness F_{fix} is both a solution to a frequently occurring problem, as well as the source of new problems at the same time. To understand more fully the meaning of this parameters, we have to reconsider what firmness (i.e. the textural property that we sense in our mouth, and that can be determined by objective mechanical measurements) really is and where it comes from. According to Tijskens et al. (1999) and Dijk & Tijskens (2000) firmness can be generated from 6 different sources:

1. turgor pressure inside intact living cells and the associated tissue tension ,
2. special compounds inside cells possibly generating strength (e.g. starch),
3. cohesive forces within a cell: chemical properties of the cell wall,
4. adhesive forces between cells: chemical properties of the pectin,
5. overall structure and shape of separate cells,
6. overall structure and shape of tissue: strength and distribution of e.g. stronger shaped vascular tissue.

In this summation items 1-4 represent the chemical and physical based forces and items 5-6 represent the histological and morphological ones (archestructure).

Depending on relative occurrence and relative importance of one of the mentioned items, a very diverse range of textural behaviour can be depicted, e.g.:

- with only tissue tension (turgor) as major item, products are soft and juicy, loosing texture upon processing, like fresh strawberries
- with pectin forces overruling, products are essentially crispy and juicy (rupture through cells; juice with contents comes out of disrupted cells), like fresh apples
- with cell wall forces overruling, products are essentially mealy and dry (rupture along cells; juice with contents stays inside intact cells), like sometimes in overripe apples
- with vascular tissue important, products are essentially tough and fibrous, like sometimes in asparagus

Depending on the type of product under study, the type of firmness generating compounds may be different and different combinations of theses compounds may be important. The end value often encountered in firmness decay (see eq. 7) may constitute that part of firmness generating compounds that does not change in the circumstances under study. But they may well change in different circumstances.

So we have to extend the mechanism of firmness change to account for these possible differences. For the sake of simplicity, let us assume that both firmness generating compounds decrease in time according a first order reaction, but with very distinct rate constants and temperature dependence.

$$F_1 \xrightarrow{k_{f1}} decay$$

$$F_2 \xrightarrow{k_{f2}} decay \qquad \text{eq 8}$$

$$F_{tot} = F_1 + F_2 + F_{fix}$$

which reduces to the analytical solution

$$F_{tot} = F_{10} \cdot e^{-k_{f1} \cdot t} + F_{20} \cdot e^{-k_{f2} \cdot t} + F_{fix} \qquad \text{eq 9}$$

When k_{f2} at a certain experimental temperature is so small that changes in F_2 can not be measured, the second term reduces to a constant, effectively generation the found solution with F_{fix} in eq. 7. With more compounds important for generating firmness, this type of equation can be extended to even more terms. In a simulated example (Figure 3), the change in observed end value clearly depends on the applied conditions, in this case on temperatures. This is the behaviour as found in the storage of apples at different CA conditions (Tijskens 1979) and in the enzyme activity of lipase in rapeseed during heating at different temperatures (Ponne et al. 1996).

Integrating the effects of CA conditions on all physiological activity, including a preferential accumulation of the firmness decreasing enzyme PG and different temperatures during storage and during shelf life, a comprehensive model was presented on the behaviour of firmness of apples (Tijskens et al. 1999).

Enzymatic effects

The mechanisms used until now, however, are most probably too simple. Reactions occurring in all living matter are in the majority of cases made possible by action of enzymes. And all kinds of things can happen with enzymes. We like to think about them as constant entities that do not change during the course of our experiments. Enzymes are, however, in a constant process of degradation and production (turnover). And not too much numerical data are available on that score. What has been studied in more detail is the inactivation of enzymes during heat treatments.

During the action of enzyme upon their respective substrates, increasing with increasing temperature, the enzyme starts at the same time to decrease in molar amount due to a conversion into an inactive form (e.g. by unwinding the protein backbone of the enzyme). The whole mechanism can (highly simplified) be represented by the following mechanism:

$$\begin{aligned} S + E &\xrightarrow{k_p} P + E \\ E &\xrightarrow{k_d} \text{decay} \end{aligned} \qquad \text{eq. 10}$$

In this mechanism S is some substrate, E some enzyme converting the substrate, k_p and k_d are the reaction rate constants of conversion and enzyme denaturation, respectively. Based on the laws of chemical kinetics, this mechanism can be converted into a set of differential equations, which can be solved at constant external condition like temperature (eq. 11). The property that is normally called enzyme activity and that can be measured readily, is E·kp. In Figure 4 an example is given for that behaviour. Note the different "optimal" temperature of the same enzyme, depending on the time of applying heat. The effect on the amount of remaining available substrate reflects the same behaviour (not shown).

$$E = E_0 \cdot e^{-k_d \cdot t} \quad , \; S = S_0 \cdot e^{\left(k_p \cdot E_0 \cdot \left(\frac{e^{-k_d \cdot t} - 1}{k_d} \right) \right)} \qquad \text{eq.11}$$

So, even a very small extension of an existing model formulation (in this case inactivation of the enzyme) can bring about a major change in the appearance of what we can and may observe in our products.

To mimic the normal 'turn-over' of enzymes, we could assume an additional constant production of enzyme (see eq. 12, 2nd reaction).

This enzyme 'turn-over' is frequently encountered in many enzymes in living material.

$$
\begin{aligned}
& S + E \xrightarrow{k_p} P + E \\
& \xrightarrow{k_f} E \\
& E \xrightarrow{k_d} decay
\end{aligned}
\qquad \text{eq 12}
$$

By including this constant enzyme production, starting from an initial amount of zero, the behaviour of available substrate resembles all of a sudden the often-encountered logistic function (Figure 5) that was used in the colour models. In Figure 6 the same simulation is presented, but now with a moderate initial amount of available enzymes. So a simple difference in available initial amount of enzyme can profoundly change the apparent behaviour of the substrate, e.g. firmness, from logistic look-alike to exponential look-alike without changing in itself the mechanism acting upon the substrate.

So, to develop models on physiological processes related to quality in our products, to develop reliable models on product quality originating from all different growing conditions and climatic circumstance from all over the world, applicable in all links of the food supply chain, we need not only to know how our property is changing over time, but also which enzymes are essential in that change, and how these enzymes behave themselves during growth and distribution. And that knowledge put a strong emphasis on a far better integration of preharvest and post harvest information in our quest for quality models applicable in the whole chains, for products from all over the world. The importance of this type of integration between preharvest growing conditions and postharvest storage behaviour is indicated in Tijskens et al. (2002a, 2002b).

Producing quality

A lot of research effort has been devoted over the years on the effects that growing conditions have on the post-harvest quality of agricultural and horticultural product. The majority of this research effort has, however, been devoted to typical preharvest attributes like mass, dry matter, vitality etc. The knowledge on how actually eating quality is grown, and the subsequent dynamics of quality change is very limited and fragmented. Part of the apparently incomprehensible variance in postharvest behaviour of quality of fruits and vegetables can possibly be attributed to differences induced by the growing conditions and the maturity at the moment of harvest. In a theoretical deduction, the possibilities of integrating preharvest information with postharvest product behaviour and quality development, the simple effect of maturity at harvest was indicated (Figure 7 and Figure 8) (Tijskens et al. 2002a, 2002b). One of the more confusing facts is that preharvest works and thinks in time since fruit set, while postharvest research invariably works with the time starting from harvest.

More effort and research should be devoted to unravel the mechanisms at work in quality production (including the enzymes and their dynamics) during the growth period as related to the mechanisms at work (again including enzyme dynamics) during the postharvest chain.

Storing quality

Within the chain, distinct links are recognised and defined, like e.g. transport, storage, distribution, retail etc. We like to see these links as very distinct and their actions as very different from one another. The storage period takes up so much time of a product's lifespan, whereas transportation and distribution is so quickly nowadays. For the produce that goes through the chain, all these links, however, trigger the same processes, already occurring in the product, but just at other circumstances of temperature, gas conditions etc. So, as far as the intrinsic product quality is concerned, storage is no different than transportation, distribution or cabinet display, provided all processes, occurring at the specific conditions of these links, are included in the integrated model. It can, however, take years of study and effort to find out which processes should be included as being important, and which processes should not. A good example of this line of reasoning applied to the firmness of Elstar apples can be found in Tijskens et al. (1999).

Another nice application build on the line of reasoning depicted, that is problem decomposition and building up complex application based on models of separate processes can be found in the work of Hertog et al. (1997) on modified air packaging. The concepts of respiration, packaging, storage decay, condensation, bacterial infection and keeping quality were combined into one application.

Keeping quality

Up to now, all examples were dedicated to product properties that determine for a large extend the quality assigned to a product. The problem of quality was decomposed into a part primarily connected with product properties, and a part that is more related to consumer preferences and wishes. These preferences and wishes of consumers were not taken into consideration.

One of the systems, halfway between total neglect of consumer preferences (product knowledge) and full attention to them (consumer and sensory science) is the system of keeping quality or shelf life. The system of keeping quality expresses the time a product can be kept, stored or handled while maintaining sufficiently high quality to be acceptable to the majority of consumers.

In that definition, there is already explicitly a double ground for uncertainty and doubt. What is defined as sufficient quality (or the limit of acceptance) and what is a majority of consumers? But a far larger problem is posed by the implicit problem: how do consumers integrate multiple quality attributes of products into one single acceptance? This problem will be dealt with in a separate lecture in this conference.

Assuming that the limit of acceptance is known for a large group of consumers or users of a product, and assuming all attributes of the product change according the same mechanism, a single equation for keeping has been deduced, that is independent of the actual mechanism with which the attributes change (Tijskens & Polderdijk 1994, 1996).

$$KQ = \frac{KQ_{ref}}{\sum_{i=1}^{n} k_i} \qquad \text{eq. 14}$$

where n = the number of attributes that are important for determining the acceptability of the product, and KQ_{ref} is the keeping quality at reference temperature. KQ_{ref} strongly depends on the active mechanism. For exponential (first order) mechanisms, it is

$\ln\left(\frac{Q_l}{Q_0}\right)$, where Q_l is the quality limit applied, and Q_0 the initial quality.

In Figure 9, two examples are shown for tomato, a chilling sensitive product and for lettuce, a chilling insensitive product.

The effects of changing quality limits for different groups of consumers or for different regions are worked out in Tijskens et al. (1994). The dynamics of keeping quality of produce during storage and transport is worked out by Hertog et al (1998).

Eating quality

When considering the eating quality of agricultural products, more issues come into play then just the properties and attributes of the product. Expert panels can judge, at least they are trained to, the properties and attributes of products. Naïve consumers, whether trained or not, always refer simultaneously to both the properties of the food and the suitability of the product for his particular purposes. Is the quality that I assign to that product in agreement with the price I paid for it? Are there more products to chose from? When you are starving, even a hard dry crust of bread can be of an exceptional good taste. So, for consumers the intrinsic properties of a product are only a part, and sometime only a small part of the acceptance. In that respect, in some circumstances, any criterion whether physiological, psychological or economic may be considered as the major indicator of quality. But that does not reflect the quality of the product itself, but the "fitness for use" of that particular product in that particular situation. In short, we are dealing with a combination of intrinsic properties and situational behaviour of consumers and economic factors. So, we enter in the world of psychology, behaviourism and economics.

Modelling this kind of interactive and complex issues is up to now conducted exclusively based on empirical relations and postulated combinations. The knowledge in psychology is simply not well enough advanced, mainly due to the immense difficulties in obtained reliable data, to allow a fundamental approach. Molnár (1995) has proposed an empirical model to describe overall quality by weighted combining individual product attributes.

The system depicted up to now, based on thorough problem decomposition into the constituting processes, is gaining lately more and more interest of behavioural and sensory science. With proper dedication using intelligent experimental set-up, in due time more insight can be and will be obtained on consumer behaviour, preferences and buying habits.

In the area of economics, the situation is even worse: if we look at the viewpoints on economics, poured out over us in almost every news flash on radio and TV, the main point communicated on economics is that it is completely based on belief and trust, without virtually any knowledge on the processes governing the whole thing. It is therefore not surprising that knowledge of the economic factor in the acceptance of food products by buyer and consumers is very limited indeed. Considerably more effort should be dedicated during the coming decades to understanding the true nature of economics, what processes govern that, and how that interact with consumer behaviour If we really want to conquer the world for global sourcing and deliverance, not only the process of quality assignment, the behaviour of product properties and quality attributes should be known and understood, but also the response of mankind towards its environment and surroundings.

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Figures

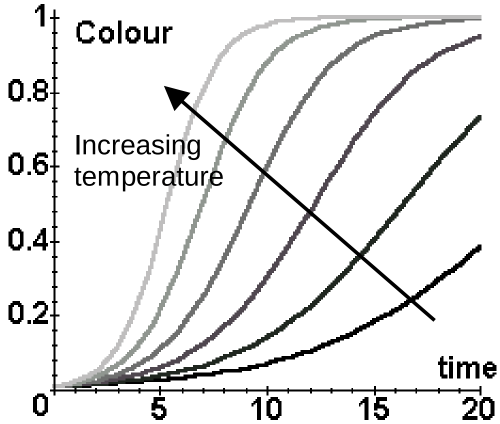

Fig. 1. Colour development according autocatalytic mechanism.

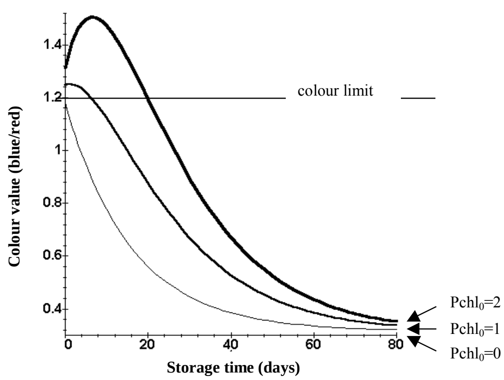

Fig. 2. Colour behaviour for of three cucumbers differing in $Pchl_0$ only (based on Schouten et al. (2002)).

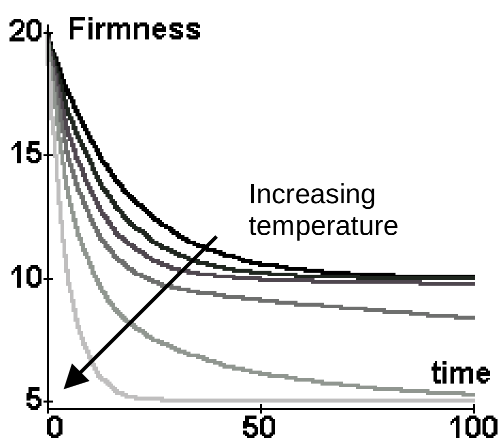

Fig. 3. Example of multi-component firmness at different temperatures

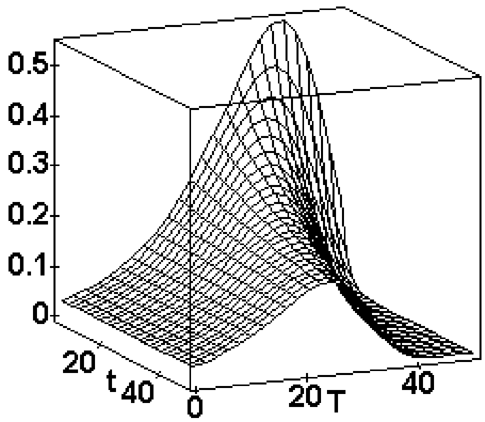

Fig. 4. Example of enzyme activity with increasing temperature.

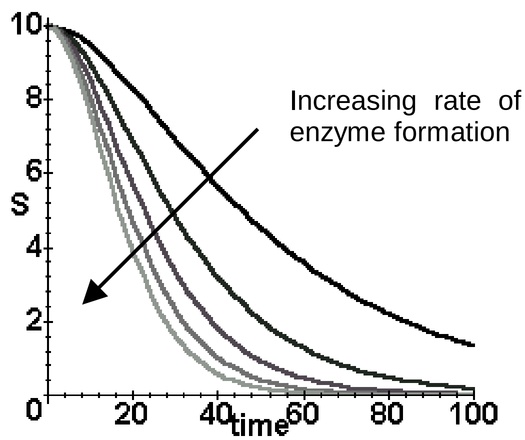

Fig. 5. Behaviour of substrate under the action of an enzyme exhibiting 'simple' turnover. Initial amount of enzyme = 0.

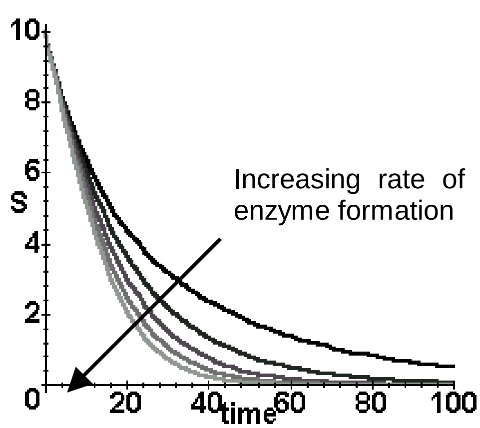

Fig. 6. Same simulation as Figure 5, but now with a moderate initial level of enzyme.

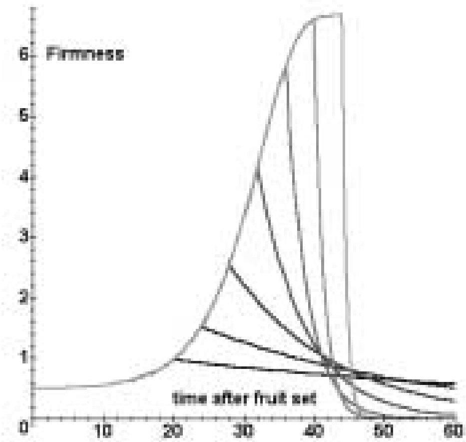

Fig. 7. Development of firmness during growth and decay after harvest at different stages of maturity (dark line= 20 days, light line= 40 days).

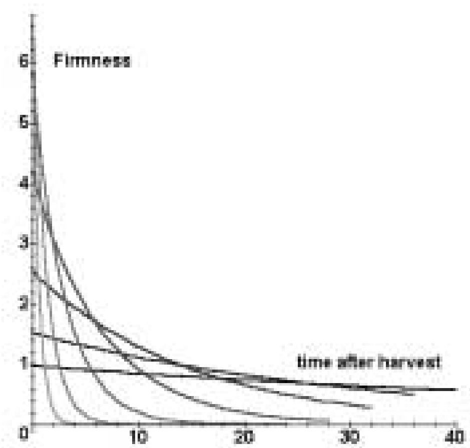

Fig. 8. The same behaviour of firmness as in Figure 7 during postharvest storage, counting time from the moment of respective harvests.

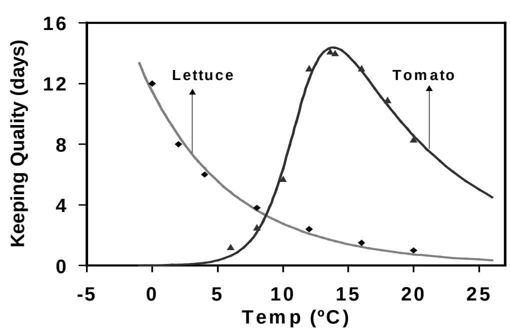

Fig. 9. Keeping quality of tomato and lettuce as a function of storage temperature.