
QUALITY CHANGE AND CONDITIONING MODELS, TWO FACES OF A COIN

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Abstract

The aims of Modelling in Food Processing: predict safety and quality of products, mark critical points of the production process, optimize quality and cost, and to facilitate the combination of research results in different domains of the supply chain, and structured data acquisition, cannot be reached but in a combination of congenial modelling of product quality and processing steps.

Advanced approaches to quality change model design in microbiology are described in short, with special attention to a general formulation of deterioration reactions. The importance of the subsequent domains of unitization, conditioning and logistics is shown with respect to optimization of product quality regarding energy usage, investment, and environment. Methods for the elaboration of the progress of deterioration reactions in chain operations towards risk analyses, to statistical information, or to design and operational aspects of chain processes or equipment are indicated.

Hopefully more interest and funds will be invested in the development of user-friendly conditioning models.

Full quotation of experimental data is a necessary step for a satisfactory development of models.

Introduction

For the application of quality change kinetics in consumer safety and quality change prediction, in design and operation of supply chains, product change rate models must be combined with product conditioning models. Probability calculus forms the link to statistical models, which allow the evaluation of chances for safety hazards and quality failures. The combination only with conditioning models allows predictions of the development of product quality in a chain process, either as product risk analyses directed towards determination of maximum allowable time-temperature loads, or to stepwise evaluation of links to get information on the effects of conditioning on the distribution of quality in each link. The results of actions for improvement by design or operational measures can be predicted and evaluated.

Microbiological deterioration models have attracted the interest of Health Protection Agencies and considerable funding. Much less public attention is paid to biochemical/physiological quality loss, which is the responsibility of the industry. Still less interest is given to the development of user-friendly product conditioning models. Combined models of deterioration reactions and time-condition development draw on product science, process technology, an refrigeration engineering, indicated as Refrigeration (or Storage) Technology, which reaches in the domains of logistics, economics, and environment.

The interfacing fields of research between the model spaces of microbiology, biochemistry/physiology, and conditioning (Refrigeration Technology) need activation to bridge the gap in the interest of optimisation of quality against cost. They are barely recognised as key subjects by research contractors.

Quality Change Kinetics.

Deterioration reactions can be attributed to physical, (bio)chemical/ physiological, and microbiological processes, the rate of all depending on physical conditions (temperature, humidity, atmosphere composition) of the products, moving in supply chains.

General deterioration reaction kinetics

Temperature appears as the most important single driving force for deterioration, which explains the great attention devoted to its influence on quality development and decay. Humidity and atmosphere composition play a supporting role.

Temperature

The application of the physico-chemical reaction model together with Arrhenius' concept of reaction rate has proved to be satisfactory for general application ie. estimation of Quality Life (Storage Life, Shelf Life, Keeping Quality) of foodstuffs, fresh and frozen, (Kuprianoff, 1956) (Thorne and Meffert, 1978) (Labuza, 1982) (Spiess 1988) (Meffert 1990) as well as on specific quality attributes, including microbial counts (Tijskens *et al.*, 1996), single and in combination, independent (Tijskens, 1995) and interfering (Tijskens, *et al.*, 1994), and also in statistical terms (Spiess, 1988) (Meffert, 1990) (Tijskens and Wilkinsaon, 1996).

Model approaches were developed also for the case of oscillating temperatures (Schwimmer *et al.*, 1955) (Salvadori and Mascheroni, 1995).

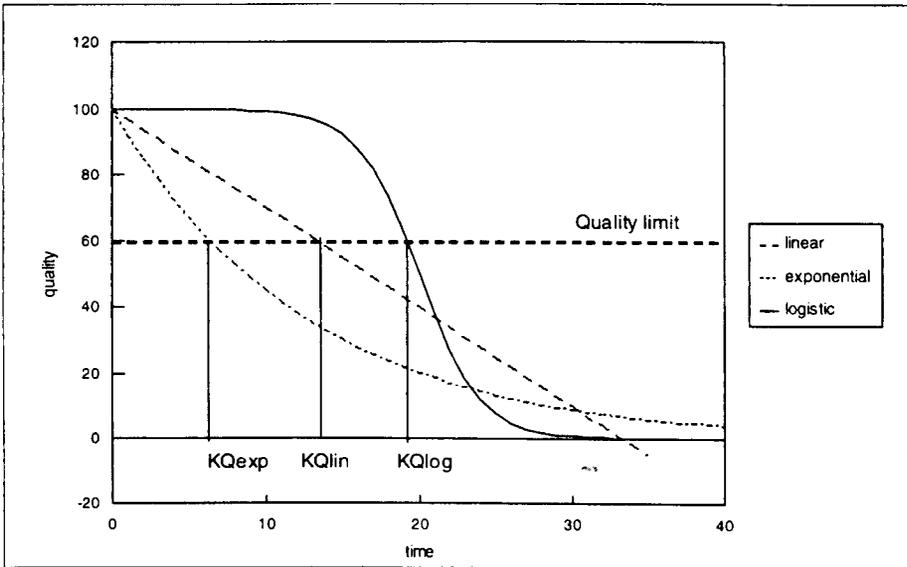


Figure 1: Course of the quality indicator in time for the most important reaction mechanisms.(Tijskens, 1995)

Figure 1 shows the course of quality attributes in time, table I the characteristic magnitudes, for different reaction types in a common formulation. Note, that the choice of reaction type of order is a question of scale for the quality attribute, and that in the initial phase, the reaction order is not significant for the course.

The generic physico-chemical model for Quality Life under influence of decay reactions in parallel, following Arrhenius' approach for temperature dependency, runs (Tijskens 1995):

$$QL = \frac{QL_{ref}}{\sum_{i=1}^n k_{ref(i)} \exp\left(\frac{E_a(i)}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right)} \quad (1)$$

with: QL(T)	Quality Life at prevailing temperature	days
n	number of independant decay reactions i	
k _{ref(i)}	reaction rate constant of reaction i at reference temperature	1/h
E _i /R	Activation Energy of reaction i / gas constant	K
T _{ref}	Reference temperature	K
T	Prevailing temperature	K

The power of this approach has been demonstrated with old and new experimental data for Quality Life, even for additional influences from atmosphere composition (Polderdijk *et al.*, 1995) and stochastic distribution of qualities (Zwietering, 1993) (Nicolai *et al.*, 1995) (Tijskens and Wilkinson, 1996), temperatures (Nicolai *et al.*, 1995), temperatures and times (Spiess 1988).

The essential simplification, non-interfering processes, resulting in one quality judgement, implies no order of importance for the decay reactions.

The approach may be less accurate in a large temperature range.

A simplified model was also developed for mixed physiological and microbiological deterioration, considering a bacterial count as initial quality attribute. (Tijskens *et al.* 1996)

$$QL = \frac{\ln\left(\frac{Q_o (B_o + Q_o - Q_{lim}) k_b + k_q}{Q_{lim} (k_b B_o + k_q)}\right)}{(B_o + Q_o) k_b + k_q} \quad (2)$$

Modified atmosphere conditions appear to affect the pre-exponential factor, which determines the reference quality life rather than the exponential increment, which stands for the temperature influence. (Polderdijk *et al.* 1995)

Table I
Quality change reaction kinetics and Quality Life (Tijskens 1995)

Reaction Type	Quality Function QF	Quality change -dQ/dt	Quality Life (QL) t
General biochemical 0 - Order linear Michaelis-Menten	$Q_i - Q_{lim}$	$k(T)$	QF/k
1st Order exponential	$\ln(Q_i) - \ln(Q_{lim})$	$k(T) \cdot Q$	QF/k
Logistic	$-\ln\left(\frac{Q_\infty - Q_{lim}}{Q_i C_{hu}}\right)$ $C_{hu} = \frac{Q_\infty - Q_i}{Q_i}$	$k(T) \cdot Q \cdot \left(1 - \frac{Q}{Q_\infty}\right)$	QF/k
Microbiological	$\ln(B) - \ln(B_i)$	$\frac{\mu(T) \cdot B}{}$	$\frac{\ln\left(\frac{B}{B_i}\right)}{\frac{\mu(T)}{}}$
Waterloss	$M_i - M_{lim}$	$m_{spec} \cdot WVPD$	$QF/m_{spec} \cdot WVPD$

Where:

- $k(T) = k_0 \cdot \exp(-a/T)$
- $= k_{ref} \cdot \exp(b \cdot (T_{ref} - T))$, with $b = a/T \cdot T_{ref}$
- $B =$ microbial count
- $\mu = (c \cdot (T - T_{lim}))^2$
- $m_{spec} = \text{kgW} / (\text{kgP} \cdot \text{WVPD} \cdot t)$

NB: For $dQ < 0.1 \cdot Q_i$ the reaction order is not important. It is also a matter of subdivision of the quality scale (see fig.1)

It appears that very different decay mechanisms can, with appropriate choice of parameters, be modelled in a uniform way, which follows from a simplification from the original Arrhenius equation for a restricted temperature range:

$$QL(T) = QL(TT) * \exp(b * (TT - T)) \quad (3)$$

with:	QL(T)	Quality Life at prevailing temperature	days
	QL(TT)	Quality Life at Target Temperature	days
	b	exponential increment of the Quality Life	1/K

Based on this concept and in line with an earlier proposal (Thorne and Meffert 1978) a subdivision of perishable foodstuffs can be given with regard to Target Temperatures (TT) - maximum for frozen and chilled products based on legislation (UN, 1991), minimum for chilled and fresh products on recommendations (IIR/IIF 1979) (Thompson 1996), Quality Life at Target Temperature, and the exponential increment of the Quality Life with temperature. The differentiation of product groups (2 frozen, 3 chilled, 5 chilled and fresh) by Target Temperatures, Quality Life (5): less than 3 days, 3 to 7, 7 to 14, 14-30, more than 30 days, and temperature sensitivity=exponential increment (4): less than .05, .05 to .15, .15 to .25, larger than .25 1/K, allows the choice of through-flow times and required conditions for perishable products in supply chains. (Meffert 1990)

Chain modelling

The generalised model facilitates the application of the Chemical Engineering chain reaction concept on supply chains, by modelling the chain as a cascade of reaction vessels, which represent the links (stores, transport equipment, retail facilities) as reaction vessels with residence/ through-flow times and temperatures. The total conversion of a Quality Attribute then is:

$$\underline{Q / Q_i = 1 - \prod_{i=1}^n \left(\frac{1}{1 + Da(i)} \right)_n} \quad (4)$$

with: $Da = k * V / v = k * t$

and: $k = 1 / \text{Quality Life (T)}$
 $t = \text{mean or maximum residence time per link}$

(Broetz, 1956) (Levenspiel 1972) (De Jong 1996)

The simple reactor cascade model holds for mean values of temperatures and residence (through flow) times, and does not consider quality distributions in the feed.

A detailed approach, using probability calculus can describe the progress of quality change during the links of a cold chain for frozen food by convolution of the distribution functions for quality, temperature and residence time. Stepwise convolution is applicable on arbitrary distributions, described by suitable classes of quality, time and temperature. The procedure has been described for frozen food (Spiess 1988) and for chilled products, including the choice of equipment and operational measures. (Meffert 1990)

Humidity

The moisture content of the surrounding atmosphere affects the Quality Life of a product in two ways:

- Relative Humidity conditions the product (surface) with respect to skin resistance against transpiration and as a medium for microbial activity.
- Water Vapour Pressure Deficit is the driving power for waterloss (Weight loss - Carbon loss) (Van Beek & Meffert 1981)

Products can be divided into groups of skin resistance. (Fockens and Meffert 1972) (Becker and Fricke 1995)

In a first approach the water vapour pressure in a hold may be taken as constant. Then WVPD depends on the local temperature.

Cowell gave an analytical solution for the distribution of water vapour concentration in packages. (Cowell 1960)

Atmosphere composition (Controlled-CA, Modified-MA)

Modified atmospheres around the product influence biochemical, microbial and physiological decay. In Modified Atmosphere Packaging (MAP) the source properties (O₂ consumption; CO₂ production) of the product must be balanced by the permability of the package material. In Controlled Atmosphere Storage or Transport, the balance is maintained artificially by machinery and controllers.

As far as concentration differences between macro- and microclimate are to be maintained, the source/sink properties of the products and the resistances of package materials with respect to gas exchange have to be considered. Both obey the Arrhenius model of temperature influence, but match only in a limited temperature range, the "temperature window". A safety device is recommended which opens the package if the safe temperature is exceeded. (Exama 1993) (Sharp 1993)

Conditioning models

Whereas Quality Change Models evidently can be formulated uniformly in simple expressions, the chances for such a development of conditioning models are less promising. Modelling a field of conditions, steady or transient, is not so much a problem of formulation but of solving a four dimensional set of variables (including time) by computational procedures.

Thermal models on an analytical base were developed more than 100 years ago, but only operationalised as FDM or FEM with the support of powerful computers. (Cleland, 1990) These computational thermal models are in need of input generated by models of air movement, which are available in a basic form as CFD, a troublesome, and time and equipment consuming procedure. (Wang 1991) (Van Gerwen and Van Oort, 1990). New approaches by LGA (Lattice Gas Automata) are in development and need further validation. (Van der Sman, 1997). Simple, direct formulations on experimental base, have been proposed (Meffert 1976) (Heap 1985) (Meffert and Van Beek, 1988) need more theoretical support and broader validation against generic models.

Conditioning models for products in refrigerated holds are designed for steady and transient conditions, most of them of generic nature, complex and time consuming to implement for practical situations (Hasse *et al.*, 1996). A principal problem is presented by the relation between macro-climate (the hold) in micro-climate (the product). The macro-climate is results from design and operational factors of the refrigeration system, the microclimate follows as determined by stowage, package and product properties.

Steady conditions.

Most conditioning processes develop slowly, and can be treated as quasi-steady processes, provided the parameters are suitably chosen.

Temperature

In storage and transport operations there is no such thing as a storage temperature. In all cases one has to deal with a temperature field in space and time. The temperature field in space can be described by a range and a distribution function.

Temperature range

A direct approach relates the temperature range of products (DT_p) in a refrigerated hold directly to heat load, air circulation and thermal properties of the system. (Meffert, 1976).

$$DT_p = A*Q_e + B*Q_i \quad (5)$$

Where: Q_e = external heat load W
 Q_i = internal heat load/product heat generation W
 $A = N1/F*(c_p^*r)$
 $B = N2/F*(c_p^*r) + N3*X^2/N*V*1(1-2/Bi)$

and $N1, N2, N3$ = coefficients, taking account for air distribution around and percolation through the product arrangement in the hold.

For practical purposes, if the overtemperature in the product can be neglected, the relation can be simplified (Heap 1985).

$$DT_p = CC*DT_a \quad (5a)$$

Where: $DT_a = (Q_e + Q_i)/PHI*(c_p^*rho)$

With: CC Configuration Coefficient
 F Air flow m³/h
 c_p^*r Volumetric specific heat Wh/m³

The Configuration Coefficient stands for the lumped influence of the configuration of the system on the air distribution which governs the product temperature range. The Configuration Coefficient can be derived from experiments or model calculations. For a number of cases, values could be calculated from experimental data. These are compiled in table III. More information could be supplied, if relevant experimental data were reported from the numerous temperature measurements, especially on retail cabinets.

Temperature distribution

The distribution of product temperatures within the range can be modelled by **Weibull Distribution Functions** for rare events, known from reliability studies and Particle Size Distribution Analysis. The double exponential function can, due to the scale and the shape parameter, be adapted to represent a large range of distributions, from exponential via quasi-normal to sharp peaks.

The distribution has a fixed lower limit, which is physically given by the controlled delivery temperature of the cold air from the cooler. (Meffert, 1993, 1995)

Table III
Configuration Coefficients for selected systems, experimental data

System	Conf.Coeff.	Observations	Ref.
Storage Fruit cold store	7 -14		1)
Transport Reefer containers	1.5-6		2)3)4)
Reefer vehicle	3.1/3.3	with/without air chute	5)
Distribution Retail cabinets	2 1.5-3	island freezer multi deck chillers	6) 7)

- Ref.: 1) Meffert, DKV-Tagungsbericht 1992, Band III, p123-135
 2) Heap, Proceedings 1985-5, p201-206, IIR/IIF Paris
 3) Meffert, Proceedings 1993-3, p509-518, IIR-IIF Paris
 4) Meffert, Proc.19th Int.Congr.Refriger. Vol.II, p559-566
 5) Bennahmias and Labonne, Proceedings 1993, p241-256
 6) Nordtvedt and Noordvang, 1995, Proc.19th Int.Congr.Refriger., Vol.II, p744-751
 7) Axell and Fahlen, 1995, Proc.19th Int.Congr.Refriger. Vol II, p673-680

Residence times and distributions

Residence times in supply chains have been investigated for frozen foods (Spiess 1988), and for horticultural produce (Rudolphij, 1988).

Storage

Residence time distributions in storage of frozen foods appear to depend on the production. Non-seasonal products show a skewed (to short keeping times) and bell-shaped distribution, to be modelled by an Erlang-function:

$$dF/dt = t/t_{max} * \exp(-t/t_{max}) \quad (6)$$

The residence time distribution of seasonal products appears flat:

$$dF/dt = \text{constant (Spiess 1988)} \quad (6a)$$

This type of distribution can also be described by **Weibull Distribution Functions**:

$$F = 1 - \exp(-(t-t_0)/SCP)^{SHIP} \quad (7)$$

The two parameters, one for scale and one for shape determine the positioning, together with $(t-t_0)$ sometimes referred to as the third parameter, determine position and shape of the Distribution Function F and of the derivation dF/dt in a general way over a wide range. (Meffert 1993)

Product temperature ranges in storage and transport equipment can be estimated by the model given in a previous chapter. Attention has to be paid to the effect of partial loads on the range and distribution of product temperatures. (Meffert, 1971)

Product temperature distributions in case of delivery air temperature control are satisfactorily described by Weibull Distribution Functions. (Meffert 1995)

Transport

Transport of refrigerated goods represents special cases with regard to the residence times. These appear as blocks, from full load, one residence time to batches per stop at increasing time steps. The effect of partial space occupation on temperature range and distribution needs special consideration. (Spiess *et al.*, 1977)

Retail

The retail links of back-up storage and display cabinets can be treated in the way described above, provided relevant data on residence times and air-temperatures available for the type of equipment and operation under consideration. Unfortunately, grand distributions of product temperatures in retail cabinets do not allow conclusions on temperature distributions depending on operational and design factors.

Transient processes

Warming up and cooling down processes have been investigated since mid-19th century, which resulted in solutions for selected problems in mathematical or graphical models: Tables and graphs in terms of Biot- and Fourier-numbers.

The introduction of computational data processing resulted in general calculation schemes of which the Finite Differences Method (FDM) and the Finite Elements Method (FEM) are widely applied (Cleland 1990).

The course of local temperatures in time and temperature distributions at certain times in bodies with known boundary conditions and thermal properties can be predicted by more or less time consuming calculations. Both groups of data and calculation procedures are subject of ongoing refinement (Nesvadba 1995)

During cooling or heating processes the water vapour pressure tends to take the value of the macro-climate, which means that the product is meeting a WVPD related to the surface conditions, Water activity and saturation temperature, explaining why most products, especially those with a small skin resistance for water diffusion profit from fast cooling processes (Fockens and Meffert, 1972).

Applications

The combination of deterioration models and conditioning models and further integration with system models for practical application in product quality control in supply chains requires knowledge of time-condition (temperature, humidity, atmosphere composition) loads throughout the chain. Quality Management in the logistic model space is strongly determined by inventory management and delivery frequency.

The integrated models can be used for two main purposes:

- For Public Health Protection: to guarantee safety for the consumer. Date marking requires knowledge of the worst time-temperature load.
- For consumer protection: to know the chance, that an unsatisfactory product reaches a consumer.

In both cases the results are useful for the evaluation of design and operation of the chain as a whole and per link, as well as of equipment and procedures in the links.

Solutions for both cases can be developed to the design of optimal distribution systems, with appropriate organisation and equipment. With appropriate additional input, these can be directed towards cost (energy and investment/maintenance) and environmental optimization.

Storage, Transport

The needs for modelling quasi-steady storage and transport conditions can be satisfied with existing means, from simple specific to highly sophisticated generic models. Unfortunately the choice cannot draw on an objective comparison of different approaches.

Transshipment

The transfer of refrigerated goods in the interfaces between links of cold chains need special attention for two reasons:

- the chances of partial warming up,
- the need of reconditioning in the following link (this is neglected in many cases, especially in standardisation of transport and retail equipment)

The development of temperatures in units of product can be modelled analytical as well as by computer. Both ways are not adapted to the needs of the chain operators, who are in need of simpler information. (Meffert, 1976)

The prediction of extreme temperatures is not too difficult. The distribution of temperatures requires more computations. Modelling in statistical terms may be hampered by lack of computer capacity, but means are available for estimation.

Chain calculations can be performed for:

- the average time-temperature load, using mean residence times and temperatures,
- the maximum load, using maximum times and temperatures, for hazard analyses,
- the statistical load, consideration of the time, temperature and quality distribution in each link of the chain, eventually estimated by a general distribution function (Weibull).

Chain performance testing and monitoring by time-temperature measurement needs quality change and thermal models for interpretation of the principally local measurements with regard to the influence on the batch. The choice of time-temperature indicators relies on the match of an indicator with a (group of) product(s). (Taoukis 1991) (Beyer 1994) (Van Loey 1996)

Discussion

Various models for product quality change, have been elaborated by approaches from different disciplines, following single or lumped quality attributes. The users and databanks are confronted with a lack of compatibility and user-friendliness.

Generic models can handle different quality definitions and deterioration processes. The fundamental base as well as the broad application qualifies the Arrhenius model for the temperature influence on reaction rates as a general standard. This would greatly simplify the use of generalised models supported by appropriate databanks.

Less uniformity in model approach can be expected in the domain of conditioning. The combination of CFD-models with FDM- or FEM-models is troublesome, time and cost intensive. A new approach by LGA has opened interesting perspectives. Evaluation of different models, and simplifications, at the hand of the results of verification experiments has hardly been attempted, in spite of indications that with less effort a satisfactory approach might be reached. (Wang 1991)

The effective and efficient combination of the two model spaces is not only important for the implementation of predictive quality modelling, with effects on equipment, process and organisation design and operation, but also for a practical consequence of quality control: Temperature Monitoring.

Temperature Monitoring needs a basic model which relates local measurement to the distribution of product conditions, otherwise neither mean nor extreme temperatures can be estimated.

Given the importance of the combination of Quality Change Models with computerised thermal models and the integration of these in logistic and environmental systems, one would expect greater efforts from research establishments and contractors.

Distribution problems of time and temperature conditions can be mastered by the general application of Weibull functions.

For risk predictions, the real maximum time-temperature loads must be known. However, the statistical significance should be considered. For this purpose, local temperature measurements have to be related with temperature distributions, a limiting product unit has to be defined. Such procedures require large computer capacities.

Decision Support System (DSS) for strategic (concepts for production and distribution networks), tactical (design or choice of equipment for the links), and operational (choice of conditions, trajectories, and products) must rely on combined models from different model spaces. For practical use on tactical and operational level, streamlined calculation would be preferable. Uniform expression for deterioration processes would simplify computations and databanks.

Conclusions

Models for different quality change mechanisms have developed to a state of uniform approach, which facilitates computation and databanking. The Arrhenius reaction rate model evidently covers the temperature dependency of very different quality change reactions and in addition also the diffusion rates of gasses in MA packaging.

Predictive quality change modelling can only deploy its full value for improving product safety and quality, definition of critical points, and optimization of equipment and operations, if accompanied by congenial conditioning models. Consideration of quality, temperature and residence time distributions, based on design and operational factors, is necessary to substantiate cost and benefit analyses.

The basic approach to conditioning models by CFD + FDM/FEM is troublesome, and time and cost intensive. New approaches to the combined heat and mass transfer problems are promising. Testing of simplified approaches is overdue.

Simple models for product quality, temperature range and distribution, related to design and operation factors, appear to cover experimental results with reasonable accuracy. They allow the analysis of main factors with regard to the management and monitoring of product temperatures by range and distribution in refrigerated spaces, based on technical and product parameters.

Generalization and simplification of approach could improve the acceptance of quality change models for supply chains of all groups perishable foodstuffs. The Arrhenius reaction rate model, the Weibull distribution model, and simple relations for range and distribution of temperature conditions are recommended. More elaborate and sophisticated computational models, especially those based on fluid dynamics, have not yet proved their additional value.

Chance calculations by stepwise convolution, however, do not require models for time and temperature distributions, but only a subdivision in meaningful classes of the distribution frequencies for time, temperature and quality.

Only with two equally fitting (=user-friendly) faces, the coin of Quality Change prediction can be minted for the sake of food quality assurance in supply chains.

Recommendations

The computational and experimental exploration of product temperature ranges and distributions in cold chains is overdue, in view of the development of monitoring instruments, which indicate local conditions only, transformed by the characteristics of the measuring probe and instrument.

Large and small storage facilities, especially display cabinets need closer attention with regard to the influence of design and operational factors on product temperature range and distribution, which does not exclude transport and storage equipment from further research.

Available models for temperature distributions should be assessed, with regard to user-friendliness, time and equipment requirements.

Research establishments and contractors should devote more attention to the combination of general quality change and thermal conditioning models.

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