Current scientific practices and legal reality are discussed related to process modeling of food quality. Historically, microbial safety was the focus, using simple first-order kinetics, known as the $D$-$z$ concept. The impressive safety record of heated processed foods made this the standard in every food engineering textbook, and adopted by food safety authorities. However, procedures are empirically adjusted to prevent spoilage and extend shelf life. Points of criticism are: i) more advanced models and computational methods allow for better optimization, ii) too strong a focus on fitting experimental results rather than on predictive power of models, iii) choice of process targets and emerging targets, iv) new preservation technologies have a hard time to prove themselves when heating remains the legal bench mark, v) nutritional value, organoleptic properties, sustainability demand more attention nowadays. In conclusion, models for co-optimization of relevant quality attributes should become the focus rather than only safety; legal rules should be revisited.

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**Introduction**

Nowadays, predictive modeling is used to aid in product and process design and quality assurance. Such models are helpful to determine the most optimal processing conditions for high-quality food (e.g. [1,2]). Predictive modelling is basically an application of scientific insights by reducing complexity and making reasonable assumptions, resulting in mathematical equations that give quantitative results. While models are useful, they also have limitations that one should be aware of: they remain simplifications of reality. The concept of quality is a difficult one to model because it is ultimately determined by judgments of consumers. Nevertheless, several quality dimensions/attributes/indices can be objectively measured, such as nutritional value, shelf life, texture (‘bite’), and presence of micro-organisms. Thus, these aspects can be modelled, and should be co-optimized in fact to come to the best possible overall quality. The most important quality dimensions are that foods need to be:

- safe; this concerns microbial as well as chemical safety
- protected from spoilage (i.e. must have a certain shelf life), which is determined by chemical, physical, enzymatic and microbial changes taking place
- contribute to a healthy diet
- need to fulfill sensorial demands

The goal of this paper is to review what needs to be done to come to co-optimization of safety and quality and further integration of the safety dimension in quality optimization. This problem of co-optimization as such is well recognized in literature (e.g. [3–5]) but it seems that the historical heritage of quality modeling has led to a very strong focus on food safety, often forming even legal barriers to co-optimization. In other words, it sometimes seems that food safety has priority at the expense of quality. Several references claim that foods are actually overprocessed to make sure that it is safe (e.g. [6]). When it comes to co-optimization of quality, the question is how to find the right balance between these aspects, as some of them are contradictory, for instance, strong heating will make foods safe but will compromise nutritional value. The central question in this opinion paper is whether or not it is possible to optimize other food quality attributes than safety without compromising food safety, in other words: what is the room to maneuver? One hurdle is that legal limits act against co-optimization because these do not keep up with new scientific insights, let alone practical insights. In that respect, it is perhaps helpful to consider some historic developments.

**A short history on the modelling of microbial inactivation**

Modelling sterilization and $12D$ Clostridium botulinum concept for low acid foods (pH > 4.6)

The first modelling sterilization attempts in food science were published some 100 years ago [7,8] with the aim to...
achieve food safety with sterilized low acid foods. The so-called 12D concept was developed, meaning that a reduction of 12 log cycles of the target organism of concern, *C. botulinum*, should be obtained [4]. This first model was based on a linearized version of simple first-order kinetics, the well-known D–z concept, which can be found in every food engineering textbook. Hundred years ago, there were no calculators and computers but linear and semi-logarithmic millimeter paper and a ruler to plot points to produce a straight line, so it was a sensible thing to do in those days. However, nowadays we know that linear inactivation kinetics is rather the exception than the rule [9–11]). Consequently, models have been adopted that are able to capture the nonlinear nature of microbial inactivation using modern computer power. These should allow, in principle at least, to come to a more precise description of what is happening in practice. However, legislation is still adopting the old practices and new scientific insights are not automatically incorporated in laws and regulations.

The traditional way of calculating microbial sterilization is based on the (debatable) assumption that safety organisms of concern are the process target. The misunderstanding was based on the historic premise that an F0 of approximately 3 min at 121°C was required to achieve a 12D reduction of the presumed safety target organism, the most heat resistant proteolytic *C. botulinum*. This F0 of 3 min at 121°C was coincidentally also sufficient to control more heat resistant spoilage spores (approximate spore load 100/g) in conventional static retorting of glass containers or cans. From industrial practice it is known that the F0 of 3 min failed to prevent spoilage when rotary retort sterilization was used, or with more extreme spore loads. In essence, the volume of the cold spot and the heat resistant spoilage spore load are the relevant parameters and not the ‘12D’ concept based on the two parameter log-linear inactivation of *C. botulinum* [12]. A fluid dynamic simulation of static retort and rotary retort sterilization using the known heat resistance parameters and spore concentration of the true process bottle-neck organisms (e.g. *Bacillus thermohalodurans* IC4 and *Bacillus subtilis* A163) [6,11] versus the most heat resistant *C. botulinum* could test this hypothesis. Spores of mesophilic *B. thermohalodurans* IC4 would be an excellent, well characterized non-log-linear substitute for the currently used variable spore crops of pseudo log-linear thermophilic *Geobacillus stearothermophilus*.

*C. botulinum* can theoretically grow and produce toxin down to pH 4.6 in optimal media without heat treatment. In general, the legal requirement for sterilized low acid foods, as mentioned, is F0 = 3 min at 121°C, pH 4.6 or pH 7.0. However, to our knowledge no reported *C. botulinum* incidents in foods with a pH below 5.0 or with an F0 > 1 min at 121°C has ever occurred. A possible reason for sticking to pH 4.6 as the safe legal limit was that reliability of pH measurement in a factory environment had been traditionally so poor that a margin accumulating to 0.4 pH units could be imposed by quality control people. This straightforward window of pH 4.6–5.0 can be used to reduce heat treatment and optimize quality. There have been exceptions before to deviate. Concern in the USA about the *Clostridium* toxin stability of pasteurized processed cheese (a low acid food with pH 5.4–5.8) led to the predictive Tanaka model and subsequent improvement [13]

### 10’ 90°C requirement for pasteurization of refrigerated cooked extended shelf-life products

The safety process target of sous-vide refrigerated meals has become non-proteolytic *C. botulinum* even though there is no historic case for this [14]. Barker *et al.* [15] mentions that his group put spores in vegetables without competitive microflora, oxygen was removed, growth was demonstrated, and a safety risk was claimed. This resulted in a suggested inactivation heat treatment of 10’ 90°C, rather arbitrarily claiming to yield a presumed 6 D (decimal) reduction, ignoring the actual strongly non-log-linear heat inactivation of the organism (see [16], their Figure 3); this selected D-value was not even based on the most heat resistant strain [17]. In practice, this heat treatment may give some extension of the lag-time of psychrophilic spoilage spores [18]. This legal demand poses a big hindrance for introduction of mild preservation technologies. There is no substitute organism for the presumed target and a legal recommendation of 10 min 90°C cannot be met by an alternative technology. Peck [19] has recently raised doubts himself whether non-proteolytic *C. botulinum* or toxin producing *Bacillus cereus* are real safety issues for properly refrigerated foods. *B. cereus* does not produce sufficient toxin to cause disease. Non-proteolytic *C. botulinum* can only be significantly detected in sea food [20]. It is not present in other foods and, if incidentally present, the non-proteolytic organism will not be able to compete with the natural contaminating proteolytic spoilage microflora.

### 15’ 72°C Pasteurization of vegetative cells (in milk)

An important food in this respect is milk. Historic process target was *Coxiella burnetii* being the most heat resistant pathogen occurring in milk (and the causal agent of Q-fever). The question is whether this is actually a realistic target. (The most important transmission route for this organism is not even consumption of milk but air.) The recommended heat treatment (15’ 72°C) is claimed to yield a 5D reduction of this target organism, but reliable data are lacking (consequently, *C. burnetii* was not included in the review of [21]). The actual validation of milk pasteurization by heat is not done by taking the formal target organism *C. burnetii* but testing for inactivation of the heat labile, indigenous milk enzyme alkaline phosphatase (the enzyme itself has no effect on quality). The heat treatment is by far sufficient to inactivate the true pathogens of concern, e.g.
Psychrophilic Listeria monocytogenes or survival of STEC Escherichia coli (e.g. O157:H7). The latter is the big issue in trendy raw milk consumption, but the treatment is not sufficient to inactivate all relevant vegetative spoilage microorganisms or cold growing (psychrophilic) sporeformers. It is therefore not surprising that heat pasteurized milk has an excellent safety record under refrigeration conditions. In practice, milk receives a more severe pasteurization to extend its shelf-life, an important reason being inactivation of the milk-indigenous enzyme lipase. Without this inactivation, lipase will very quickly, in homogenized milk, lead to formation of fatty acids, giving a rancid, soapy off-flavor. The extra pasteurization gives also additional protection to the more heat resistant Mycobacterium paratuberculosis with a non-confirmed association with Crohn’s disease [22]. The lowered prevalence of allergy after raw milk consumption [23,24] warrants effort to allow validation of safe non-thermal processes.

The examples given so far demonstrate that thermal processing conditions do not have to aim so much at safety but rather at spoilage and shelf life targets, because then inactivation of pathogens is automatically included. However, legislation is still based on these microbial safety targets. It leads to rather strange discussions when new technologies are introduced such as high pressure and PEF, where legal authorities require inactivation of alkaline phosphatase in milk, while new technology aims to inactivate pathogens but not enzymes. Another concern is the lack of microbial preservation physiology knowledge. How to deal with a $D$ reduction demand if prehistory of cells can lead to $4D$ differences in process susceptibility between heat and high pressure [25] and vice versa.

More detailed criticism is on the modeling of microbial inactivation. While it made perfect sense to go for the linearized $D-z$ concept 100 years ago, it is nowadays a piece-of-cake to handle nonlinear behavior. However, the $D-z$ concept is still the standard in textbooks and legal requirements. It is sometimes defended by stating that it has led to perfectly safe foods. While this is true, it may also be that other food quality attributes are in danger. Suppose, for instance, that a food manufacturer lowers the pH of a food to make sure that the food remains safe, but has to add more sugar to compensate for the sour taste, the higher sugar content may compromise the nutritional value and contribute to another societal safety issue, namely that of obesity and diabetes. If more accurate nonlinear models would provide the opportunity to reduce damage to important safety issues, this could help to focus not only on safety but on health or quality in general. In the scientific literature, there is now ample recognition for the mostly non-linear activation of microorganisms and in fact there are now quite a few models available that account for this. A recent development is the online availability of various mathematical models [5,26]; see also Refs. [27,28] for a critical discussion on this. Table 1 attempts to give an overview of what has been discussed so far.

**Modelling chemical and physical quality attributes**

Next to the microbial condition of foods, other quality aspects are equally important, notably nutritional value. Processing affects not only micro-organisms but also nutritional value and chemical safety; examples are protein damage due to blockage of lysine in the Maillard reaction, formation of acrylamide, loss of vitamins, and many more reactions [1]. Models based on chemical kinetics are used in this respect (e.g. [1,29]). Temperature dependence is usually described by the semi-empirical Arrhenius equation, or the more fundamental Eyring model. Other more empirical models are also possible [30,31]. Recently, the Eyring model was updated to make it applicable to chemical reactions, enzyme inactivation and microbial inactivation, accounting for stochastic

| Table 1: Summary of major legally prescribed heat treatments of foods, safety and processing targets |
|------------------------------------------------------------------------------------------------|
| **General legal heat treatment requirements** | **Adequacy** | **Official microbial target/ validation substitute** | **True targets** | **Suggested modeling approach** |
| 15°–72°C Milk pasteurization | Safety = OK | Coxiella burnetii Alkaline phosphatase (only for heat processes) | Spoilage flora STEC E. coli | Weibull |
| 10°–90°C refrigerated foods with extended shelf-life | Safety = OK but need is questionable | Non-protective C. botulinum | Psychrophilic spores, for example, B. pumilis enzymes | Arrhenius |
| 3°–121°C ambient stable low (pH > 4.6) acid foods | Safety is OK, but heat treatment is insufficient. In practice, equivalent to 8–10° 121°C | Proteolytic C. botulinum Geobacillus stearotherophilus (not reliable) | Heat-resistant mesophilic spores, for example, Bacillus sporothermodurans, Bacillus subtilis | Lag time extension? |

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behavior of micro-organisms and proteins/enzymes [32]. The concept was applied to thermal as well as PEF treatment [33,34]. Modeling of chemical and physical quality parameters is more straightforward than that of microbial inactivation. While microbial death is a complex process, a chemical (for instance, vitamin degradation) or a physical change (e.g., protein denaturation) is usually simpler and therefore easier to describe with mechanistic models [29]. As an example, we modelled the degradation of vitamin C using kinetic parameters obtained from Corradini. The mathematical details can be found in Appendix 1 (Supplementary material). Figure 1 shows a temperature profile more or less similar to a treatment of 10 min at 90°C (corresponding to a heat treatment of cooked extended shelf life products) and two heat treatments at 80°C, which is hypothesised to be enough for sufficient microbial stability.

The right part of Figure 1 clearly shows that the two treatments at 80°C give substantially less ascorbic acid loss than the one at 90°C. Obviously because the thermal load is much less, while the safety risks are supposed to be equal in the three cases. It remains, of course, a simulation, but it shows the potential of co-optimization of quality loss.

Predictive power of models
A major criticism on the modeling approaches in food science is that the focus is strongly on fitting rather than on prediction; [35] calls this ‘retrodiction’, a term that nicely indicates that a model is then evaluated for its ability to fit already existing data. Authors thus typically fit a model to data, but do not evaluate how such a model would behave in its ability to predict new observations. Ultimately, a model should be judged on its capacity to predict when it is used for optimization. Other measures than ability to fit results are then needed. Prediction intervals need to be constructed (rather than confidence intervals that only show how confident one can be in a mean value). Information criteria such as the Akaike criterion (AIC), the Bayesian information criterion (BIC), the Widely Accepted Information Criterion (WAIC), predictive posterior checks (PPC) are more appropriate to indicate how uncertain future values can be [35]. This is especially relevant considering the biological as well as the experimental variation when dealing with foods and micro-organisms, which will impact the precision of prediction in a negative way. Figure 2 shows a simple example of the linear D-value model (Figure 2a) and nonlinear regression using the nonlinear Weibull model (Figure 2b) of inactivation of microbes with 95% confidence and prediction bands (the regression was done following a Bayesian approach [35]. The fit using the Weibull model is obviously much better. Figure 1c shows the uncertainty according to both models for predicted values of log S (S being the survival ratio log N/N0) at time = 15 min. Two things are obvious: i) the predicted values are quite different and ii) the uncertainty is much larger with the linear D-value model. Another way of showing that the use of a certain model leads to different results is by calculating the time needed for, for example, 5D inactivation for the micro-organism shown in Figure 1; this would be 18.5 min when using the linear D-model, and 17.5 min when using the Weibull model, so there is

![Figure 1](https://example.com/figure1.png)

**Figure 1**

Simulated degradation of vitamin C ([C6H8O6]+[C2H6O6]), ascorbic acid (C6H8O6) and dehydroascorbic acid (C2H6O6) as a function of time. The first temperature profile (blue) is based on industrial experimental data. The red and purple curves are assumed profiles for a proposed reduction of a still safe heat treatment.
Bayesian regression analysis of heat inactivation of Listeria innocua at 60°C, pH 7.5 (data from Miller, 2009, Combase). logS = survival rate = log \((N/N_0)\), time in min. Dark grey area represents the 95% confidence interval for the mean, the light grey area the 95% prediction interval for new observations. A: log-linear model, B: Weibull model, C: density profiles showing uncertainty in the predicted value at \(t = 15\) min for both models (solid line for the nonlinear Weibull model, dashed line for the linear D-value model, the vertical lines show the mean of the distribution for logS at \(t = 15\) min).

Bayesian inference has indeed a difference that could have an effect on quality: 1 min more heat load may damage other quality attributes. Once again, this is just a simple example, it may be obviously different in other conditions and other microorganisms.

Admittedly, the uncertainty with the Weibull model is still quite large, but it goes to show that the quality of prediction is a factor of importance. Choice of models should therefore be part of optimization criteria. More emphasis should be put on attempts to reduce uncertainty. However, it needs to be acknowledged that variation is a natural phenomenon. Den Besten et al. [11] also underline the importance of variability, and show that the efficacy of a heat treatment depends largely on the presence of a minor fraction of microbial cells with an extreme heat resistance. Nevertheless, uncertainty due to model choice is something that can be improved upon. In this respect, it may also be remarked to pay due attention to model parameters. They should have preferably a physical/biological meaning, so that they can be interpreted accordingly. Also, the more parameters the better the fit but the worse the uncertainty that comes with it [35].

**Optimizing food quality and safety**

When it comes to optimizing food quality, a compromise must be sought between safety and quality. Common industrial practice in the past century has been to focus mainly on food safety as the first measure, perhaps at the expense of other quality attributes, notably nutritional value. Of course, there is attention for this in literature, see, for example, [36]. In fact, the UHT process widely used in dairy processing is a result of this: considering the widely differing temperature sensitivities of microbial and chemical reactions, it led to the idea that at temperatures around 150°C microbial inactivation requires only a few seconds, while such times are too short to cause chemical damage. With liquid products this is easily achievable. When it comes to further optimization of food quality, future research should really focus on the co-optimization of food quality indices and models are very useful in exploring that. A major problem to deal with is variability and the effect of food components on microbial as well as chemical and physical reactions. Most experiments are done with model foods, for example, they are simplified in terms of composition and structure in order to understand a particular behavior. While this is perfectly reasonable, the danger is in extrapolating the results to real foods and one should be very careful with that. Describing such dependencies on food composition and structure is also a major challenge in modeling. Models can be used in this respect in various ways:

- Modeling microbial inactivation as a function of processing
- Modeling chemical changes as a function of processing and storage
- Modeling microbial growth as a function of storage

Co-optimization requires the combination of such modeling exercises to find the right balance between safety and other quality attributes.

**Conclusion**

This opinion article ends with the invitation to think differently in terms of co-optimization of quality. To paraphrase a saying of Einstein: “We need to find new ways of thinking to deal with the problems caused by the old way of thinking”. There is probably a lot of unpublished industrial information to confirm and challenge our opinion and it would be good to share that knowledge, also in the face of an increasing resistance to processed foods (e.g. the NOVA classification). But also for food scientists in academia, it is an invitation to think differently about how to combine several quality aspects, how to model that, how to deal with variation. Finally, it is an invitation to legislation to make it easier to incorporate new insights from science into rules and regulations, so that there is room created for innovation. In any case, we hope that future efforts in modeling will have a broader scope and do not focus only on one dimension of quality.

**Declaration of interests**

Nothing declared.

**Appendix A. Supplementary data**

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.coifs.2020.02.001.

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