OPTIMISATION OF THERMAL PROCESSING CONDITIONS: Effect of Reaction Type Kinetics

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ABSTRACT

Food thermal processing conditions can be optimized in terms of final product quality retention. This optimization is possible due to the difference between the temperature dependence of quality factors and microorganisms or enzymes kinetics of thermal degradation or inactivation, respectively. All the available research in this field assume first order degradation kinetics for the quality parameters.

In this work the effect of reaction type kinetics on optimal thermal processing conditions and final quality retention is analyzed. Zero, second and reversible first order kinetics are taken into consideration. Assuming that the Arrhenius model is applicable, the main conclusion is that the reaction type kinetics does not have influence on constant optimal thermal processing temperatures for maximizing the final surface product quality retention. Optimal conditions for maximizing volume average quality retention are affected by the reaction quality thermal degradation kinetics and the differences between optimal constant temperatures depend on the kinetic parameters values and processing conditions and requirements. For reversible first order degradation kinetics, final quality retentions are analyzed as a function of processing conditions and kinetic parameters and the calculation of optimal processing conditions is discussed.

Key Words: thermal processing; quality; optimization; kinetics

1. INTRODUCTION

The optimization of thermal food processing conditions involves three main parts: 1) Identification of the design variables; 2) Identification of the process requirements and 3) Definition of the objective function (Norback, 1980). The most common objective function is the maximization of the final quality in terms of volume average or at the product surface.

The quality attributes thermal degradation kinetics is normally considered to be 1st order:

$$\frac{C}{C_0} = e^{-kt} = 10^{-\frac{t}{D}} \qquad (1)$$

where:
C_0 - initial concentration
t - time
k - reaction rate
C- concentration
D - decimal reduction time

The temperature effect on the reaction kinetics is usually described by the Arrhenius Law:

$$k = k_{ref}\, e^{-\frac{Ea}{R}\left[\frac{1}{T} - \frac{1}{T_{ref}}\right]} \qquad (2)$$

where: k_{ref} - reaction rate at the T_{ref}

T_{ref} - reference temperature
Ea - activation energy
R - universal gas constant

or by the Bigelow model:

$$D = D_{ref}\ 10^{(T_{ref}-T)/z} \qquad (3)$$

where: D_{ref} - decimal reduction time at T_{ref}
z - z-value

Several research works exist on this field. In particular Silva et.al. (1993) and Hendrickx et.al. (1993) developed regression equations for predicting optimal constant temperatures for maximizing final quality.
All the research in this field considers first order quality thermal degradation kinetics (Holdsworth, 1985).

The objective of this work is to study the influence of the reaction type kinetics for the quality parameter on optimal processing conditions for maximizing final retention.

2. MATERIALS AND METHODS

The quality retention was calculated for the situations described in Figure 1.
Figure 2 presents other common kinetic models and Figure 3 presents the dimensionless concentration, for the different reaction kinetic models, as a function of time assuming the same k_{ref} and Ea parameter values.
The objective function for the optimization procedure can be the maximization of the quality at the surface or in terms of volume average retention. Figure 4 presents the common objective functions.

3. RESULTS AND DISCUSSION

3.1 Surface Quality

Analyzing the objective functions for maximizing the product surface quality it can be concluded that, if the Arrhenius law is applicable and assuming the same k_{ref} and Ea parameters, the reaction kinetic model does not affect optimal processing conditions.
Figure 5 presents the final surface quality retention as a function of processing temperature for the case study described in Figure 1. Independently of the quality thermal degradation kinetic model the optimal sterilization temperature is 110°C.
Although for reversible first order kinetics an optimal processing temperature can be theoretically calculated, if the reaction rate and the final equilibrium concentration are relatively high the optimal quality retention is not significantly different from other retentions obtained with non-optimal processing conditions.

3.2 Volume Average Quality

Analyzing the objective functions for maximizing the product volume average quality it can be observed that there exists a difference between the 1st order (simple or reversible) and the second or the zero order kinetics. Optimal processing conditions, for the same k_{ref} and Ea parameters, may be different depending on the kinetics.
Figure 6 shows the final volume average quality retention as a function of processing temperature, for the same case study of Figure 5, for 1st order and 2nd order kinetics, and for two different target F_o values. It can be observed that for an F_o value of 15 min a difference of 2.5°C in optimal temperatures for 1st and 2nd order kinetics exists.

Reversible first order:

$$\frac{C - C_f}{C_0 - C_f} = e^{-k\,t}$$

C_f - equilibrium concentration

Zero order:

$$C = C_0 - k\,t$$

Second order:

$$\frac{1}{C} = \frac{1}{C_0} + k\,t$$

Figure 2 - Other typical reaction kinetics.

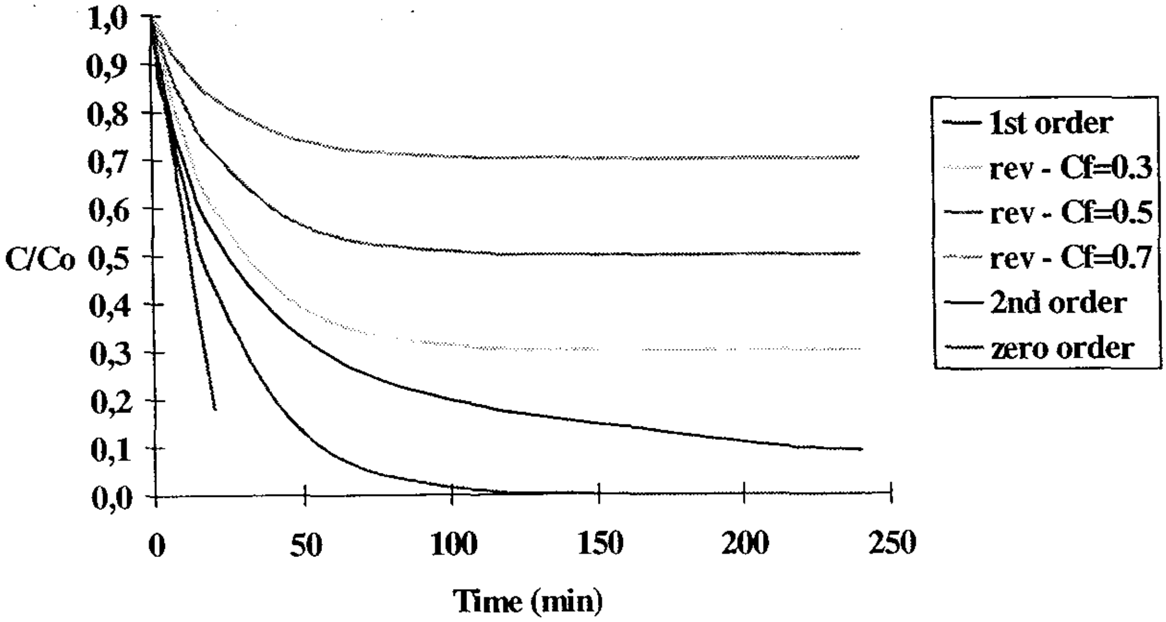

Figure 3 - Concentration as a function of time for different reaction kinetics at 120°C. ($k_{120°C}$=0.041 min^{-1})

4. CONCLUSIONS

The reaction kinetics does not affect optimal sterilization conditions for maximizing surface quality.

Optimal conditions for maximizing volume average quality retention are affected by the reaction quality thermal degradation kinetics. The differences between optimal constant temperatures depend on the kinetic parameters values and processing conditions and requirements.

When the quality parameter thermal degradation follows a reversible 1st order kinetics it may not be of interest the calculation of optimal conditions, because all the adequate processing conditions lead to equivalent final quality retentions.

REFERENCES

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FIGURES AND TABLES

type of process: sterilization of a conduction heating food in a cylindrical can
can dimensions: R = 4.36cm H/2 = 5.80cm
food properties: $\alpha = 1.7\times10^{-7}$ m²/s
$k_{120°C} = 0.041$ min^{-1}
Ea = 104.4 kJ/mol
process requirements: target sterility value at the geometry center for a microorganisms with a z-value of 10°C
F_0 = 3 or 15 min
process conditions: range of holding temperatures = 105 to 135°C
initial retort temperature = 20°C
Come-Up-Time = 0
surface heat transfer resistance = negligible

Figure 1 - Input data for the case studies simulation.

Surface:

1st order → $C_{surf} / C_0 = e^{-I_1} \ or \ C_{surf} / C_0 = 10^{-I'_1}$

reversible 1st order → $\dfrac{C_{surf} - C_f}{C_0 - C_f} = e^{-I_1} \ or \ \dfrac{C_{surf} - C_f}{C_0 - C_f} = 10^{-I'_1}$

zero order → $C_{surf} = C_0 - I_1$

2nd order → $C_{surf} = \dfrac{1}{\dfrac{1}{C_0} + I_1}$

$$\boxed{I_1 = \int_0^{t_f} k_{ref}\, e^{-\frac{Ea}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)} dt \quad \text{and} \quad I'_1 = \int_0^{t_f} \frac{dt}{D_{ref}\, 10^{(T_{ref} - T)/z}}}$$

Volume Average:

1st order → $(C / C_0)_{ave} = I_2 \ or \ (C / C_0)_{ave} = I'_2$

reversible 1st order → $\dfrac{C_{ave} - C_f}{C_0 - C_f} = I_2$

zero order → $C_{ave} = C_0 - I_3$

2nd order → $C_{ave} = \dfrac{1}{\dfrac{1}{C_0} + I_3}$

$$\boxed{I_2 = \frac{1}{V_T}\int_0^{V_T} e^{-I_1(V)} dV = \frac{1}{V_T}\int_0^{V_T} e^{-\int_0^{t_f} k_{ref}\, e^{-\frac{Ea}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)} dt} dV}$$

$$\boxed{I'_2 = \frac{1}{V_T}\int_0^{V_T} 10^{-I'_1} dV = \frac{1}{V_T}\int_0^{V_T} 10^{-\int_0^{t_f} \frac{dt}{D_{ref}\, 10^{(T_{ref} - T)/z}}} dV}$$

$$\boxed{I_3 = \frac{1}{V_T}\int_0^{V_T} -I_1(V)\ dV = \frac{1}{V_T}\int_0^{V_T}\int_0^{t_f} -k_{ref}\, e^{-\frac{Ea}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)} dt\ dV}$$

Figure 4 - Common objective functions.

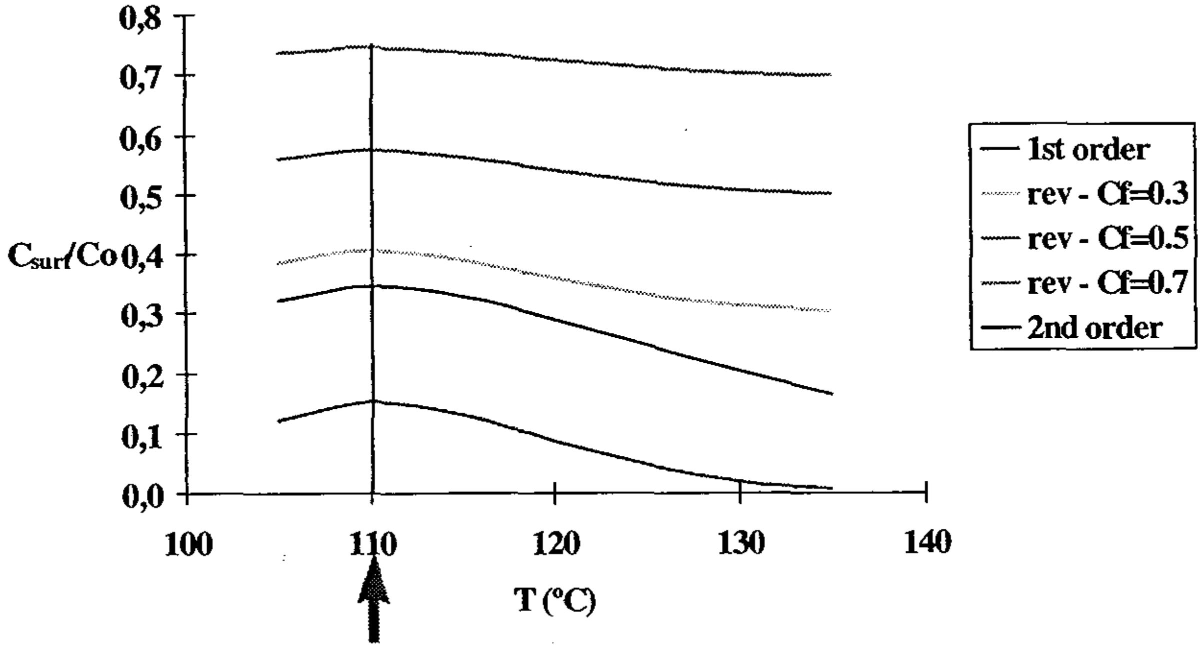

Figure 5 - Surface quality as a function of processing temperature for different reaction kinetics (case study described in Figure 1; $F_0=3min$)

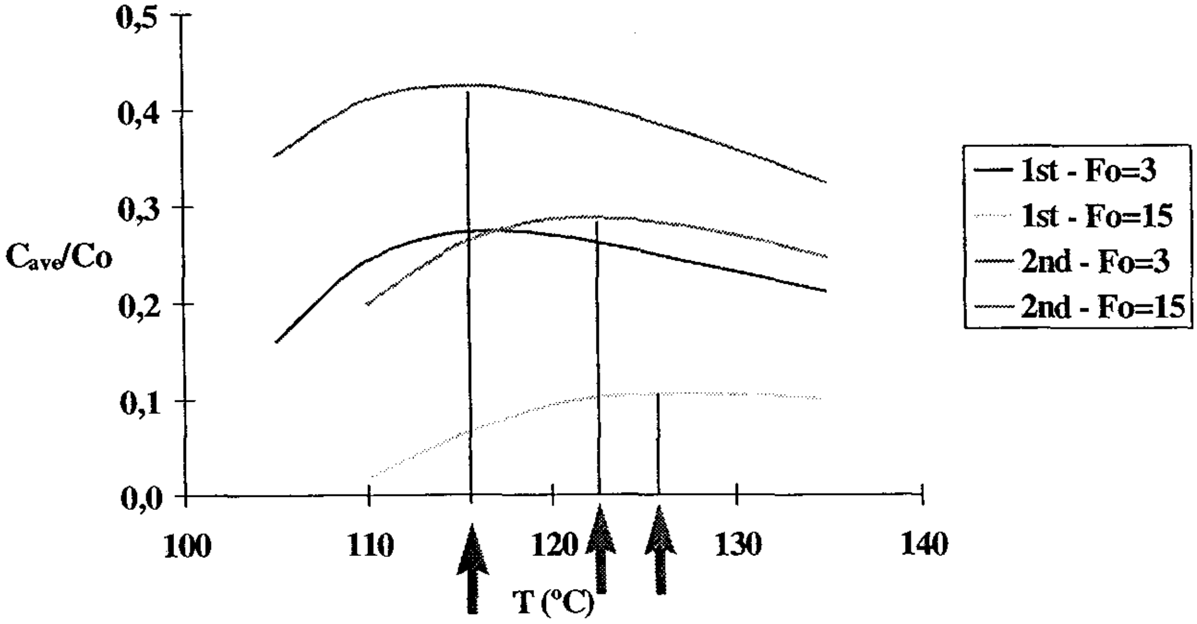

Figure 6 - Volume average quality retention as a function of processing temperature for different quality attribute reaction kinetics and target F_0 value.
(case study described in the materials and methods)