Integrated approach on heat transfer and inactivation kinetics of microorganisms on the surface of foods during heat treatments—software development

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Abstract

The objective of this work was to create a software application (Bugdeath 1.0) for the simulation of inactivation kinetics of microorganisms on the surface of foods, during dry and wet pasteurisation treatments. The program was developed under the Real Basic© 5.2 application, and it is a user-friendly tool. It integrates heat transfer phenomena and microbial inactivation under constant and time-varying temperature conditions. On the basis of the selection of a heating regime of the medium, the program predicts the food surface temperature and the change in microbial load during the process. Input data and simulated values can be visualised in graphics or data tables. Printing, exporting and saving file options are also available. Bugdeath 1.0 includes also a useful database of foods (beef and potato) and related thermal properties, microorganisms (*Salmonella* and *Listeria monocytogenes*) and corresponding inactivation kinetic parameters. This software can be coupled to an apparatus developed under the scope of the European Project BUGDEATH (QLRT-2001-01415), which was conceived to provide repeatable surface temperature-time treatments on food samples. The program has also a great potential for research and industrial applications.

Introduction

Studies on the bacterial spoilage of foods and on the survival and possible outgrowth of microbial pathogens are extremely important for the food processing industry. The major incidence of food contamination by microorganisms occurs on food surfaces during harvesting (e.g. fresh fruits and vegetables), slaughter of animals and further processing. As the surface of foods is the interface for environmental contamination, development of suitable surface heat treatments is important to reduce microbial content, thus leading to safer products with improved shelf life and quality.

In the last years, microbiologists jointly with food engineers have been applying sophisticated mathematical approaches to predict microbial loads on foods (see Ross & McMeekin (1994, 2002) for an overview). The development of precise and accurate mathematical models, able to describe the inactivation behaviour of microorganisms on the food surface under stress factors

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Nomenclature

a_w	water activity
$c1$	bias factor
C_c	variable related to the physiological state of the cells
Cp	specific heat (J kg^{-1} K^{-1})
D	decimal reduction time (min)
D_{sample}	characteristic dimension of the food sample (m)
$D_{water\text{-}air}$	diffusivity of water in air (m^2 s^{-1})
Evap	evaporation term
h	heat transfer coefficient (W m^{-2} K^{-1})
k	inactivation rate constant (s^{-1})
K_m	mass transfer coefficient (m s^{-1})
M	molecular weight (kg)
N	microbial cell density (cfu g^{-1})
Nu	Nusselt number
P_T	water vapour pressure at dew temperature (Pa)
RH	relative humidity
t	time (s)
T	temperature (K, °C)
Tu	turbulence intensity (%)
V	air velocity (m s^{-1})
x	space coordinate (m)
z	number of temperature degrees which leads to a 10-fold reduction of D-value (°C)
z_{a_w}	distance of a_w from 1 which leads to a 10-fold increase of D-value

Greek symbols

α	thermal diffusivity (m^2 s^{-1})
ΔH	latent heat of water evaporation (J kg^{-1})
λ	thermal conductivity (W m^{-1} K^{-1})
v	kinematic viscosity of air (m^2 s^{-1})

Subscripts

air	of the air
bot	at the bottom
eff	effective value
i	initial value
inf	at bottom surface
max	maximum value
ref	reference value
steam	of the steam
sup	of the support
sur	at food surface
top	at the top
water	of water

(e.g. high temperature, particular ranges of pH and water activity), is crucial if industries are to design efficient and reliable pasteurisation systems.

Diverse mathematical models have been suggested to describe the kinetic behaviour of microorganisms in foods. Zwietering, Jongenburger, Rombouts, and van't Riet (1990) referred and compared the most relevant models used to describe microbial growth. Xiong, Xie, Edmondson, Linton, and Sheard (1999) gathered the most widely used mathematical expressions for modelling thermal inactivation. The majority of research works in predictive microbiology deal with constant process conditions. However, Van Impe, Nicolaï, Martens, Baerdemaeker, and Vandewalle (1992), Nicolaï and Van Impe (1996), Van Impe, Nicolaï, Schellekens, Martens, and Baerdemaeker (1995) and Geeraerd, Herremans, and Van Impe (2000) were innovative in the way they approached the modelling of microbial growth and/or inactivation under dynamically changing temperature conditions.

There are several software applications (commercially available, or down-loadable free of charge from the internet) in the field of predictive microbiology. Examples, such as Pathogen Modelling Program (Buchanan, 1993), Food Micromodel (Anonymous, 1997), Food Spoilage Predictor (Anonymous, 1998) and Seafood Spoilage Predictor (Dalgaard, Buch, & Silberg, 2002), illustrate the potential of predictive microbiology to users with lack of comprehensive skills in mathematics. These applications focus essentially on kinetic models for microbial growth and on shelf life prediction, while the (currently still available) versions 6.1 and 7.0 of the Pathogen Modeling Program do include a range of pathogen (non-) thermal inactivation and irradiation models. Further development of accurate and versatile mathematical software dealing with the microbial inactivation on the surface of food products is needed.

The objective of this work was to integrate heat transfer models and microorganisms inactivation kinetics on the surface of foods during heat treatments. The models were incorporated into a software program, developed in a user-friendly environment. Based on the characteristics of the heating regime, the surface temperature can be estimated. As shown in Valdramidis et al. (2005b), acceptable predictions of the microbial content at food surface can be attained under certain circumstances. These studies were based on the researching effort of partners of the European project BUGDEATH (QLRT-2001-01415), with FRPERC as the coordinator. The need to obtain reliable data on relationship between bacterial death and the surface temperature of real foods lead to the design, construction and commission of

equipment under the scope of the project. The software application here presented simulates the results obtained in the rig apparatus (Foster et al., 2005) that will be marketed and commercially available.

Modelling methodologies

Heat treatments are the most common and effective procedures for controlling the survival of microorganisms in foods, and should be designed to provide an adequate safety margin against food-borne pathogens. A global model, that combines heat transfer and microbial inactivation kinetics, is of major importance to determine the level of microbial destruction during surface pasteurisation, under wet and dry heating regimes. This requires two modelling approaches: (i) an accurate modelling of heat transfer, to describe the phenomena induced to the food surface by the thermal process, and (ii) modelling microbial inactivation behaviour under such temperature conditions.

Heat transfer model

The temperature history at the surface of the food product can be estimated considering a one dimensional heat transfer model, i.e., the product is assumed to be a flat plate of infinite length and width, and with two different boundary conditions being applied on each side of the plate. The surface temperature results from the combination of different heat transfer phenomena: conduction, radiation, convection and evaporation/condensation of water or steam (Kondjoyan et al., 2005; Kondjoyan et al., 2005a).

Inside the product, conduction is the relevant phenomenon, and the temperature T at each position (x) and time (t) can be calculated according to Fourier's second law:

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T(x,t)}{\partial x^2} \tag{1}$$

where α is the thermal diffusivity of the food.

On the topside of the food product, the boundary condition can be expressed by:

$$\lambda \left(\frac{\partial T}{\partial x}\right)_{\text{top}} = h_{\text{eff}}(T_{\text{air or steam}} - T_{\text{sur}}) \tag{2}$$

being λ the thermal conductivity of the food product, and h_{eff} an external effective heat transfer coefficient, that accounts for the exchanges by convection, evaporation/condensation and radiation, and T_{sur} denotes the surface temperature. If the heating medium temperature varies with time, the values of h_{eff} are also time-dependent (Kondjoyan et al., 2005, 2005a).

When the radiation is neglected, the following equation allows the estimation of the external effective heat transfer coefficient in a dry environment:

$$h_{\text{eff}} = h + K_{\text{m}} \Delta H \frac{P_T - a_{\text{w}} P_{T_{\text{sur}}}}{T_{\text{air}} - T_{\text{sur}}} \tag{3}$$

in which h is the convective heat transfer coefficient and T_{air} is the air temperature; K_{m} is a mass transfer coefficient [estimated by the correlation $\frac{hM_{\text{water}}}{C_{P_{\text{air}}} M_{\text{air}}} \left(\frac{\alpha}{D_{\text{water-air}}}\right)^{-0.67}$, Holman (1983)] and ΔH is the latent heat of water evaporation; P_T and $P_{T_{\text{sur}}}$ are water vapour pressures at dew temperature of the heating air and at food surface, respectively, and a_{w} is the water activity at the surface of the food sample.

During a dry air decontamination process a_{w} is decreasing very fast. The theoretical determination of a_{w} requires the coupling of the heat transfer model to a water transfer model. A coupled heat-water transfer model was developed and validated under the rig conditions (Kondjoyan et al., 2005a, 2005b). Traditional experimental methods used to determine a_{w} cannot be used during decontamination treatments, as they require equilibrium conditions which give plenty of time for the product surface to rewet before measuring. Thus an indirect method, based on weight loss measurement, was developed to determine water activity during dry air decontamination. Values of a_{w} calculated by the coupled transfer model were in very good agreement with those obtained from weight loss measurements (Kondjoyan et al., 2005a, 2005b). Calculations of the coupled heat-water transfer were accurate, but very time consuming, and cannot be incorporated into the user-friendly model. To speed-up temperature predictions it was decided to stop calculating water diffusion inside the product. Therefore a_{w} was not predicted and had to be replaced by an evaporation term, Evap, which had to be fitted on experimental results. All experimental conditions considered in the rig during dry air decontamination were taken into account (i.e. 60 °C, 75 °C, 90 °C and 100 °C fast and slow decontamination treatments). It was shown experimentally that the variation of a_{w} was closely connected to that of the surface temperature of the product, T_{sur}. Plateau or increase of T_{sur}, led to plateau or decrease of a_{w}. To keep that connection between a_{w} and T_{sur}, Evap was supposed to depend on the relative humidity (RH) of an airflow which temperature would be that of the surface of the product. At the beginning of the heat treatment the air-flow was supposed to be saturated with water (Evap $= a_{\text{w}} = 1$), then its relative humidity would decreased as T_{sur} increased. For all the conditions the best fitting of Evap on meat was obtained for:

Initial conditions

$$\text{Evap} = \text{RH}(T_{\text{sur}_i}) = 1 \tag{4}$$

at the initial surface temperature T_{sur_i}.

Step by step variation

Slow ramping conditions

$$\text{Evap} = 1.4\text{RH}(T_{\text{sur}}(t)), \quad T_{\text{sur}} < 60\ ^\circ\text{C} \tag{5a}$$

$$\text{Evap} = (0.0167T_{\text{sur}} + 0.4)\text{RH}(T_{\text{sur}}(t)), \quad T_{\text{sur}} \geqslant 60\ ^\circ\text{C} \tag{5b}$$

Fast ramping conditions

$$\text{Evap} = 3\text{RH}(T_{\text{sur}}(t)) \tag{5c}$$

In Eq. (3), estimates of the convective heat transfer coefficient can be obtained on the basis of empirical correlations of dimensionless parameters, developed for different flux regimes. In the rig, turbulence intensity of the air, Tu, was measured and was found to be between 20% and 25% (Kondjoyan et al., 2005). The heat transfer value determined in such conditions agreed with the one calculated from a previous correlation obtained by Kondjoyan and Daudin (1995) on short cylinders:

$$Nu = \frac{hD_{\text{sample}}}{\lambda_{\text{air}}} = 1 + 0.0176Tu\left(\frac{D_{\text{sample}}V}{v}\right)^{0.5} \tag{6}$$

where Nu is the Nusselt number, D_{sample} the characteristic dimension of the food sample (e.g. diameter) and λ_{air}, v and V are the conductivity, kinematic viscosity and velocity of the air, respectively. This correlation was used in the present model to determine the heat transfer coefficient for different air-flow conditions.

If steam is used, the surface temperature of the food was assumed to be 3 °C below the steam temperature. This was experimentally verified in the BUGDEATH test-rig apparatus (see Foster et al., 2005).

Since the product is placed on a support, the boundary condition of the bottom side of the food can be written as:

$$\lambda\left(\frac{\partial T}{\partial x}\right)_{\text{bot}} = h_{\text{inf}}(T_{\text{sup}} - T_{\text{inf}}) \tag{7}$$

where T_{sup} and T_{inf} are the temperatures of the support and bottom surface of the product, respectively; h_{inf} is a coefficient which describes exchanges by conduction between the support and the product.

In situations where the product thickness remains above 0.5 cm, the exchanges between the bottom of the product and the support can be neglected.

Combining the previous equations and applying convenient numerical analysis methods, the surface temperature of the product can be calculated. Eq. (1) was discretised by a finite-difference numerical procedure, using the Crank–Nicholson method. The number of nodes and time step were chosen in such a way that the convergence of solution and speed of calculation were achieved. If dry air is considered, the effective transfer coefficient (calculated by Eq. (3)) was recalculated at the end of each time step, using the actualised values of the variables. A computer program, written in Basic language (REALbasic©, REAL Software, Inc., Texas, USA, Version 5.2), was developed for calculations.

For dry air decontamination treatments, results were less accurate when using the present user-friendly model than when using the coupled heat-mass model. An example of user-friendly model predictions is given in Fig. 1. For all the treatments the average difference between simple model predictions and IR measurements was ±2 °C. However, local differences of ±4 °C were noticed in some cases. The values of Evap, determined from relations 4 and 5 a–c, were similar to those determined from weight loss measurements (Fig. 1b). Thus, they could directly be introduced into the new inactivation model developed during BUGDEATH project, to take into account the effect of a_w on the thermo-resistance of bacteria.

Calculations of surface temperature were performed for air velocities ranging from 20 m s^{-1} (velocity of the air jet in the rig) to 5.0 m s^{-1} (air velocity commonly encountered in food factories) using: (i) the coupled heat-mass model and (ii) the simple model. Results

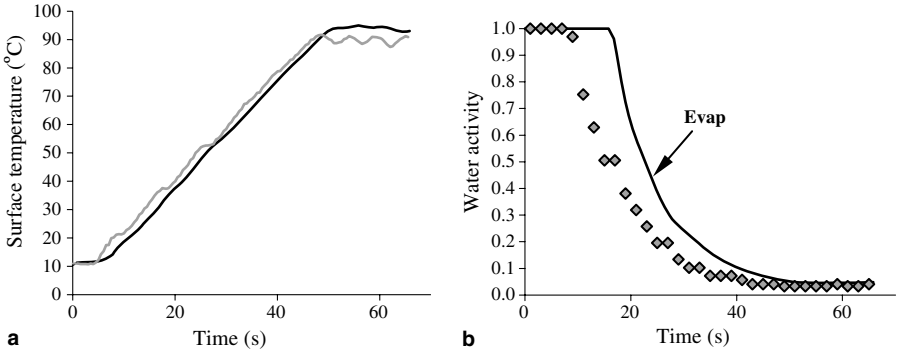

Fig. 1. Comparison between measurements (grey) and results issued from the present user-friendly model for the 90 °C fast treatment on meat samples: (a) surface temperature was measured using the calibrated IR sensor; (b) experimental a_w were determined from weight loss measurements (grey diamonds) and evaporation term came from correlations globally fitted on all experimental cases.

proved that air velocity had to be in between 15 m s^{-1} and 20 m s^{-1} to have an accuracy of ±2 °C on the temperature calculated by the simple model. As the simple model was mainly validated on meat, its accuracy would probably be less for other products. Despite these limitations the simple thermal model predicted the good trends for the variations of T_{sur} and a_w under a wide range of decontamination conditions.

Microbial inactivation models

The most widely used model to describe bacterial death or inactivation is based on the analogy with a first order chemical kinetics (see, for example, Schmidt, 1992). This model describes a linear decrease of the microbial content (expressed in a log scale) along the time. This is somehow restrictive, since in many situations a delayed decrease (lag phase or shoulder) is observed at the beginning of the inactivation process. Some models have been proposed to describe this tendency, such as modifications of logistic and Gompertz functions (Whiting, 1993; Bhaduri et al., 1991; Linton, Carter, Pierson, & Hackney, 1995). Geeraerd et al. (2000) developed a model that, besides the capability of describing the initial lag phase, has the advantage of dealing with time-varying temperature conditions, typical of pasteurisation heat treatments (come-up time followed by a holding temperature). This dynamic version of the inactivation model is of the form:

$$\frac{dN}{dt} = -k_{max}\left(\frac{1}{1+C_c}\right)N \tag{8}$$

where

$$\frac{dC_c}{dt} = -k_{max}C_c \tag{9}$$

N equals the microbial population (in absolute values), k_{max} is the maximum specific inactivation rate and C_c a variable related to the physiological state of the bacterial cells.

Changes in the numbers of the microorganisms with time can be calculated by combining Eqs. (8) and (9). When applying a model in time-varying circumstances, some implicit (so-called backstage) considerations are involved (Valdramidis et al., 2005a). These considerations are: (i) is there any growth possible during the come-up time?; (ii) what is the lowest temperature for inactivation?; and (iii) is there any affect of the heating history, for example an induced heat resistance? For the case studies considered in this research, the answers are, respectively: (i) no; (ii) 49.5 °C; and (iii) no. The last answer implies the hypothesis that the inactivation rate can be related with the *actual* temperature and surface water activity value solely, and that a relationship with the past temperature and water activity values does not need to be established (Valdramidis et al., 2005b).

The kinetic rate constant correlates to the decimal reduction time of the well-known Bigelow model, D, traditionally used to describe the heat resistance of microorganisms in thermal processes via the relationship $k_{max} = \ln 10/D$.

The kinetic parameter k_{max} is also affected by water activity, being particularly important in dry heating environments. In such conditions, a_w rapidly reduces to very (<0.2) low values (see Fig. 1b). If the Bigelow model is modified in order to include this a_w effect (Gaillard, Leguerinel, & Mafart, 1998), the following relationship emerges:

$$k_{max}(T, a_w) = \frac{\ln 10}{D_{ref}} \exp\left(\frac{\ln 10}{z}(T - T_{ref})\right) \times \exp\left(\frac{\ln 10}{z_{a_w}}(\text{Evap} - 1)\right) + c1 \tag{10}$$

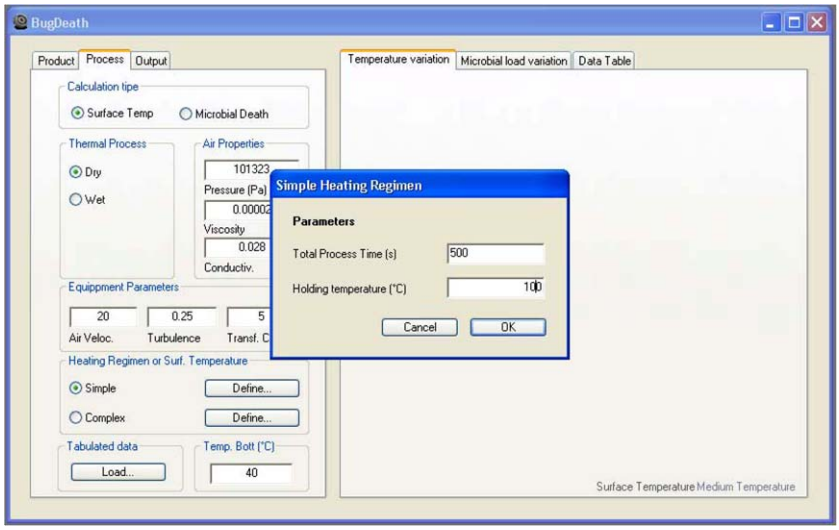

Fig. 2. Screen of Bugdeath 1.0 software—process.

in which D_{ref} is the decimal reduction time at the reference temperature, T_{ref}, z the conventional z-value, and by analogy z_{a_w} is the distance of a_w from 1 which leads to a 10-fold increase of D-value; c1 is a bias factor (see Valdramidis et al., 2005b).

To predict the change in microbial numbers at the surface of foods, T_{sur} (calculated on the basis of all considerations of heat transport) replaces the temperature T in the previous equation.

All mathematical models were validated on the basis of extensive experimental work, using two food products (i.e. beef and potato skin-on/skin-off) and two pathogenic microorganisms (i.e. *Listeria monocytogenes* and *Salmonella*), under the scope of the BUGDEATH project (Gaze, Boyd, & Shaw, 2005; McCann & Sheridan, 2005).

Kinetic parameters were estimated to produce accurate predictive models for reduction in microorganisms, that can be achieved on the surface of solid foods during surface pasteurisation treatments.

Software program

The Bugdeath 1.0 software is a user-friendly interface. Real Basic© 5.2 was selected as programming language, because it allows an easy implementation and performance using any personal computer (e.g. Pentium IV, 2.4 GHz, using Microsoft Windows 98® or Windows XP® operating systems from Microsoft Corporation©).

The user has to precise some process and product considerations in all the specific fields that appear in

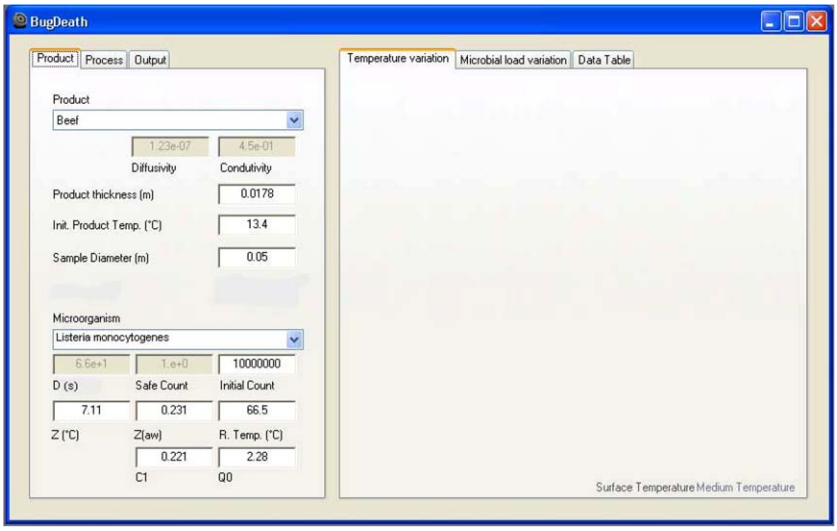

Fig. 3. Screen of Bugdeath 1.0 software—product/microorganism.

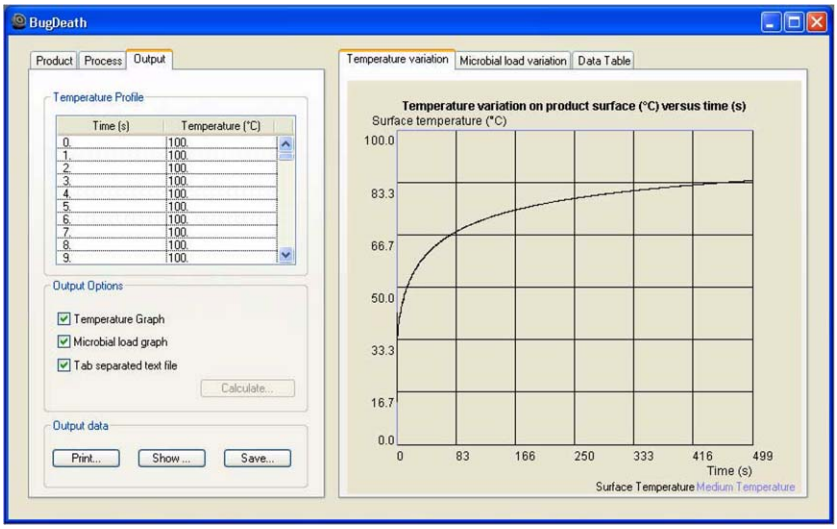

Fig. 4. Screen of Bugdeath 1.0 software—output/temperature.

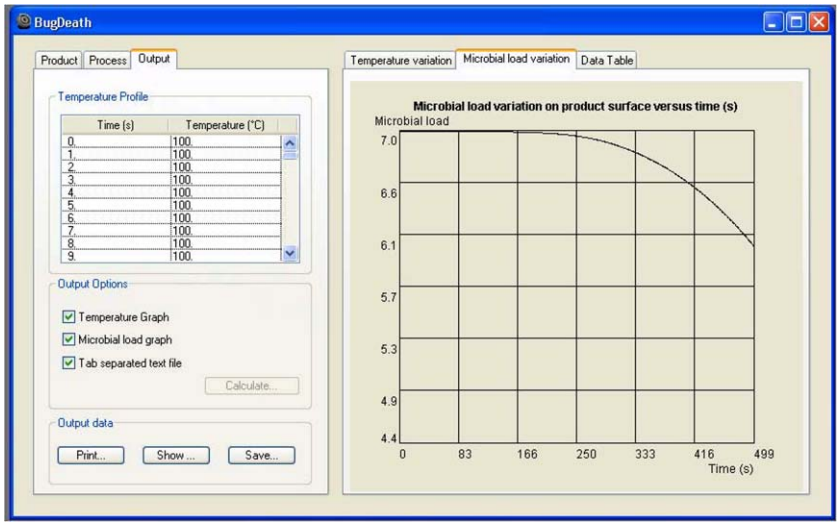

Fig. 5. Screen of Bugdeath 1.0 software—output/microbial load.

the screens. The first screen (as presented in Fig. 2) is related to the heating *process*. At this stage the user can decide between a dry or wet thermal process. The air properties and equipment parameters are linked to the choice and the values automatically display in the boxes. A pre-defined simple or complex heating regime can be chosen. It is possible to specify the total process time, heating time, holding temperature and duration of this stage, and final temperature. An additional option allows an input of time-temperature data of the heating medium. This can be done manually or by an input file. The values are automatically displayed in a table.

Optionally, the surface temperature of the food can be read from a text file and the calculation of the microbial death can be performed independently from the temperature profile calculation.

In the second screen of Bugdeath 1.0 (Fig. 3), the user can select a *product* and a *microorganism*, from a list of available products and microorganisms. The program interconnects automatically to a database of thermal properties of the food and kinetic parameters of microbial death models, and displays those results on the screen in the other boxes. By input, the user can specify the initial temperature and thickness of the product. The sample diameter is a fixed value as it is related to the sample holder in the BUGDEATH apparatus. In relation to the microorganism, the program allows the definition of initial counts.

After all fields/boxes are filled in, the program starts calculating the surface temperature of the product as a function of time (equations presented in Section 2.1) and assesses the microbial content (equations in Section 2.2).

The preferred *output* can be specified in the third and last screen. By selection, the user can show predicted results of temperature history (Fig. 4) and microbial load (Fig. 5) at the food surface, in tables or graphs. The program also includes edit and file options, such as printing, exporting and saving jobs.

Table 1
Values of characteristic properties and parameters of the heat transfer and kinetic models used in case study

Context	Property/parameter[a]
Heat transfer	
Food (**beef**)	Thickness = 0.0178 m
	$D_{sample} = 0.05$ m
	Initial temperature = **13.4 °C**
	$\alpha = 1.23 \times 10^{-7}$ m^2 s^{-1}
	$\lambda = 0.45$ W m^{-1} K^{-1}
Heating medium (**dry air**)	
	$h_{inf} = 5$ W m^{-2} K^{-1}
	$T_{sup} = 40$ °C
	$V = 20$ m s^{-1}
	$Tu = 0.25$
	$v = 20 \times 10^{-6}$ m^2 s^{-1}
	$\lambda_{air} = 0.028$ W m^{-1} K^{-1}
Kinetics	
Listeria monocytogenes	$N(t = 0) = \mathbf{1.0 \times 10^7}$ cfu g^{-1}
	$C_c(t = 0) = 2.28$
	$D_{ref} = 1.1$ min
	$T_{ref} = 66.5$ °C
	$z = 7.11$ °C
	$z_{a_w} = 0.23$
	$c1 = 0.22$

[a] Thermal properties of air and water can be found in literature (Holman, 1983; Perry, 1984).

Case study

The following example demonstrates the use and potential of Bugdeath 1.0.

The aim is to predict numbers of *Listeria monocytogenes* that survive on the surface of beef placed in dry air at 100 °C for 500 s. The parameters and characteristics of the food and the heating medium regime are presented in Table 1. The values, which are to be specified by the user, are indicated in bold, while the non-bold values are automatically selected by linking to the database.

The predicted temperature at the surface of the beef (Fig. 4) increases till approximately 60 °C, during the first 40 s of the process. In the following 200 s, the temperature goes up from 60 °C to approximately 80 °C. During the remaining process time, the food surface temperature gradually achieves 83 °C.

The simulated values of microbial load at the food surface (Fig. 5) show that no inactivation occurs during the first 250 s. Then, microbial content suffers a 1-log reduction during the remaining process time.

Conclusions

Bugdeath 1.0 allows an easy access to predictive microbiology. Accurate predictions of microbial load at the surface foods surface during pasteurisation treatments in the rig apparatus can be assessed within the range of the process/product/microorganisms combinations tested during the development of the modelling methodologies. The simulations can be valuable to a wide variety of companies in the food industry for developing appropriate and safe processes. The software has also the potential of being exploited for educational purposes.

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