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A heat and mass transfer perspective of microbial behavior modeling in a structured vegetable food



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ABSTRACT

A mathematical model predicting *Escherichia coli* O157:H7 behavior was developed, depending on the applied thermal regimes, using a whole iceberg lettuce as a structured model food. The 3-D, transient model is based on energy and biomass conservation complemented by primary and secondary predictive notations, allowing one to virtualize the combined effect of bacterial growth and migration, under any possible handling and storage conditions.

Due to its flexibility and applicability, the model is a suitable tool to virtualize the bacterial contamination in fresh produce, from postharvest to consumer. Realistic cases such as external contamination or pathogen internalization are examined, following model validation. The complex combination of bacterial penetration and population level, for example, is highlighted which depends nonlinearly on bacterial diffusivity and operating temperature. While it is shown that, with variable thermal regimes, the total contamination level is practically equivalent if the cumulative thermal exposures are the same. The proposed procedure can be also applied to other food/microorganism pairs, provided that general

data on microbial generation and diffusion are available.

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1. Introduction

Mathematical modeling is a valuable tool to assist the predictive microbiology. A considerable hurdle in such modeling is the description of an *inhomogeneous* bacterial environment, when a realistic food definition is desired. In this way, a *structured food* can be speculated which includes both local bacterial diffusion and local pattern-forming diffusion limitations. As shown by Dens and Van Impe (2001), incorporation of microbial growth and migration notations into a Partial Differential Equations (PDEs) framework can lead to proper bacterial behavior modeling. Their vision is shared in the present paper.

A first attempt in exploiting the modeling potential and intertwining nature of microbiology and heat transfer in food science was carried out by Schellekens et al. (1994), by employing a commercial expert system to set up an integrated framework that could be used in virtual evaluation of composition and process effects on food safety. Then various approaches were reviewed by Lebert and Lebert (2006), while recently Warning and Datta (2013) reported

* Corresponding author. E-mail address: gianpaolo.ruocco@unibas.it (G. Ruocco). on the *interdisciplinarity* between microbiology and engineering.

The supporting role of modeling in food safety was confirmed by a number of comparisons with the associated experiments. Bellara et al. (2000) studied the growth of Escherichia coli in an inoculated substrate subject to conduction cooling, under controlled conditions. The dependence of Byssochlamis fulva growth on heat transfer in papaya pulp was speculated by da Silva et al. (2013) for a number of storage scenarios, but the occurrence of mold migration in that system was uncertain. Convective heat transfer and its effect on microbiology was addressed by Ben Yaghlene et al. (2009) with a simplified 1-D model, yet featuring a limited description of the bacterial growth (no lag time). Listeria innocua distribution in an inhomogeneous, structured food was studied numerically by Noriega et al. (2008), as it was affected by inherent oxygen availability, by means of a 1-D model. With reference to fresh produce, the influence of heat transfer and thermal regime throughout storage on the prediction of microbial behavior during the cold chain was studied by Hoang et al. (2012). The importance of combining physics-based modeling with the microbial kinetics to provide needed information at any time and location in the food during processing was recognized by Halder et al. (2011), but bacterial migration was left out again from modeling. Phyllosphere







contamination, depending on the applied conditions, did not receive adequate attention, as reported by Laguerre et al. (2013).

Fresh leafy vegetables are common examples of structured foods. Lettuce cultivars are not only amongst the most popular vegetables eaten raw, they are also involved in severe pathogen outbreaks world-wide: these systems need an improved description (Delaquis et al., 2007; Olaimat and Holley, 2012). A vast resource on leafy greens information, including both production and processing that would impact the retention of quality while ensuring the safest conditions, has been compiled by Erickson (2013), but to date no model has been found, in the available literature, encompassing said modeling elements and operating conditions.

Trying to fill this gap, in the present paper one such improved attempt is brought forth by exploiting a full 3-D model of a structured leafy food, to report on the bacterial behavior within the phyllosphere and in the various phylloplanes (leaves), along the entire handling chain. *General first-law equations* used in heat and biomass transfer have been employed, supplemented by a combination of *primary and secondary growth kinetics*, to deal with the bacterial growth rate and migration. In this way, the microbial behavior under a number of realistic handling situations can be virtualized from farm to table, following common occurrences such as external and internalized contaminations.

2. Materials and methods

2.1. Main model features and assumptions

E. coli growth and migration are considered to a fresh iceberg lettuce model during handling and storage. In lieu of a statistical treatment of phyllosphere tortuosity, a deterministic approach was preferred based on structural (connectivity) features such as interleaf contact points and thin insulating air interspaces, as purported in the following. *E. coli* grows and populates differently the leafy vegetable along each leaf and at different depths from surface (i.e., through consecutive leave layers inward or outward, depending on colonization direction) so that a population pattern will result within the whole sample (Dens and Van Impe, 2001) at any given storage time. *Four different aspects* have been encased in this model and discussed in this paper:

- 1. *Bacterial kinetics*, which depends on the temperature and bacterial cell population at any point in the phyllosphere.
- 2. *Bacterial migration*, which dictates biomass diffusion through the phyllosphere.
- 3. Structural features of the phyllosphere, in association with bacterial migration. Consisting in an ensemble of quasi-spherical leaf shells of given thickness (one inside the other), whole lettuce generally presents many random inter-leaf contact points and "entrapped" air pockets or interspaces (Fig. 1). Consequently, the bacterial population is expected to spread through the phyllosphere by exploiting the former, while its migration would be hindered due to the latter.

More specifically, contact points are employed in the present framework to simulate the function of open stomata, which generally allow for bacterial penetration through vegetable structures (Kroupitski et al., 2009). The number of such items, distributed pseudorandomly in the phyllosphere, has been the subject of scrutiny, in the model validation. In addition, adjacent leaves are insulated except at contact points, to simulate the presence of air interspaces which locally block the otherwise uniform pathogen spreading (Fig. 1).



Fig. 1. Close-up of an actual iceberg lettuce, with indication of specific structural loci.

4. *Thermal regime variability*, as any combination of time/temperature can be speculated to come up with indications of bacterial behavior and safety conditions of the sample, from harvest to consumer.

On the other hand, the following *simplifying assumptions* have been adopted, as they do not pose additional hurdles in the development of the model:

- 1. No thermal convection effect is considered between the external product's surface and the storage atmosphere;
- 2. No vegetable cells spoilage is allowed, as to alter the bacterial behavior;
- 3. The effects of respiration, transpiration or additional metabolic mechanisms are disregarded.

2.2. Governing equations

The governing equations in vector form and homogeneous properties for the *heat transfer* and *E. coli biomass kinetics and transfer*, following the approach of Golding et al. (1998) and the general procedure of De Bonis and Ruocco (2012), are therefore applied to a quasi-spherical lettuce model of average radius *R* (as shown in Fig. 2). With the spherical symmetry exploited, the PDE system yields for the distributions of temperature *T* (K), and bacterial cell population *x* (log CFU/g):

• Heat transfer:

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T \tag{1}$$

• Biomass kinetics and transfer:

$$\frac{\partial x}{\partial t} = D\nabla^2 x + S \tag{2}$$

The initial and boundary conditions, including those imposed by the structural features, are set as follow:

- Heat transfer:
 - an initial temperature is uniformly set at *T_i* in the phyllosphere;
 - depending on the simplifying assumption 1, the temperature is uniformly set at $T_e(t, r = R)$ on the external surface, depending on the applied thermal regime;

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