A Computational Fluid Dynamics (CFD) Study for Heating Bacterial Culture Media and Effect of Natural Convection on Total Heat Flux

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***Abstract*—In the present study, a predictive model was developed for heating bacterial culture medias. One of the most common medium for microbiological studies, Plate Count Agar (PCA) was used in the experimental studies and non-linear partial differential equations for coupled heat and momentum transfer were solved by finite element model using COMSOL Multiphysics®. Temperature of PCA solution was recorded at three different positions and it was observed that the predicted temperature values were found to be in a good agreement compared to experimental ones according to root mean square errors calculated. Natural convection has shown a dominant impact on total heat transfer and the developed model was found to have convincing performance to explain the temperature variation during heating process and that is important to evaluate further processes like sterilization applied for microbiological studies.**

***Index Terms*—COMSOL, finite element approach, PCA agar, sterilization, temperature and velocity profiles**

I. Introduction

Sterilization is defined as a process aiming elimination/killing or removal of all microorganisms (including spores) from a medium or a material [1]. An adequate sterilization has a critical importance especially for microbiological studies. Buffer solutions to prepare dilutions, medium and equipments such as pipets and petri dishes should be carefully sterilized before use. Otherwise, the residual microorganism load may interfere with microbial load count studies and miss-interpretation could be unavoidable [2].

There are several methods used for the sterilization practices such as heat treatment, chemical treatments and disinfection, filtration, and radiation. Apart from these common techniques, there are some other methods achieving partial elimination of initial microbial load but not a complete sterilization. In this extent, freezing, drying and ultrasonic application are considered. Besides of these full and/or partial sterilization efforts, the main and most common method is the sterilization in an autoclave which is generally performed at 121 ℃ (15 psi pressure depending on the medium/material). Amount of the material to be sterilized and the way how the equipment placed in the autoclave chamber affect time required for a proper sterilization [2].

Vegetative cells of Bacillus and Clostridiums can be eliminated at temperature levels higher than 75-80 ℃, however, their spores can survive below 100 ℃. Thus, main target should reach to adequate temperature levels in order to kill even bacterial spores. As a result, in most cases the sterilization is performed at 121 ℃ for 15 min [3]. For instance, regular agars and broths, nutrient broth, Mac Conkey agar, brilliant green bile broth, Baird-Parker agar, potato dextrose agar and plate count agar are sterilized in described way above in an autoclave. It is emphasized that heating regime should be achieved for a successful and complete sterilization.

Volume of the medium to be sterilized, concentration of agar in the medium, the type of container and its wall thickness are effective parameters for the determination of time requirement for an adequate sterilization [4]. In the light of these facts, it is easy to be concluded that container size and properties, medium composition may result in variations in physical properties of medium (density, viscosity, thermal conductivity, thermal convective transfer coefficient, specific heat capacity) and thermal properties of container which cause changes in sterilization progressed and degree of sterilization. Another point is the temperature programme followed during sterilization. Temperature specified in heating programme of autoclave system is the chamber atmosphere, not the sterilizing medium in a container (generally glass bottle). Thus, temperature history of medium during sterilization should be expressed and validated, which is required for the evaluation of the sterilization efficiency, especially for microbiological analysis. In laboratory practices, it is generally tested using chemical and biological indicators. For chemical verification, indicator strips are used and color changes depending on temperature variation is monitored to decide the degree of sterilization is enough or not. However, the strip measures the temperature in the chamber not medium in the container. Regarding biological indicators, some microorganism spores are inoculated into medium in the bottle before sterilization and following the sterilization; few medium poured petri

Manuscript received March 28, 2019; revised August 2, 2019.

doi: 10.18178/ijfe.5.3.183-189

dishes are left empty and taken to incubation to see possible microbial growth in them for sterilization dependent problems. If it is, that means an inaccurate sterilization for medium used [4]. But here it is worth to emphasize that sterilization control by this way can be done after incubation of petri dishes (culture media) and in some cases it may be too late. Thus, it is required to follow temperature profile of the coldest point in medium from the engineering aspect.

In literature, there are some studies which investigated heat transfer process regarding fluids and other food materials using mathematical models. Lespinard and Mascheroni [5] studied the pasteurization of tomato puree in a bottle. In another study, pasteurization of solid model food prepared using potato was examined and model was developed by Marra, Zell [6]. Heat treatment of conserved liquid foods [7], effect of radio-frequency on some pathogens [8], pasteurization of fruit juices, milk and some other food material [9], [10], thermal treatments to solid-liquid model systems [11]-[15] were other previous published reports in literature in this regard. However, there is no any published study investigating the influences of medium and container properties on the efficiency of sterilization according to our best knowledge.

Thus, in the present study, (1) a predictive model has been developed and validated against experimental data to forecast the temperature variation in a bottle filled with PCA, (2) temperature variations of the PCA at three different positions have been figured out and compared to temperature in chamber, (3) magnitude of total heat flux by convection and conduction compared to heat flux total were investigated.

II. Material and Methods

A. Material

In the study, one of the most common medium (plate count agar, PCA) was selected and its solution was used. For that purpose, 22.5 g PCA (Merck) was completely dissolved in 1 L of boiling water. Chemical composition of the PCA is presented in Table I. Then, 500 ml of the solution was transfer in an autoclavable borate glass bottle (Fig. 1a). Before the temperature measurement, the bottle and the content were cooled at room temperature by continuous gently agitating to ensure a homogenous temperature distribution in the bottle and prevent the agar from gelling especially at bottle surface. When the temperature of PCA solution reach to 50 ℃, the bottle was immediately placed into a pre-heated water bath at 93 ℃ to heat it up. At the same time, as shown in Fig. 1b, temperature level at three different positions was monitored and their values were recorded for 5 s intervals, simultaneously.

TABLE I. Chemical Composition of Plate Count Agar (PCA)

Chemical compound	Concentration
Peptone from casein	5.0 g/L
Yeast extract	2.5 g/L
D(+) Glucose	1.0 g/L
Agar-agar	14.0 g/L

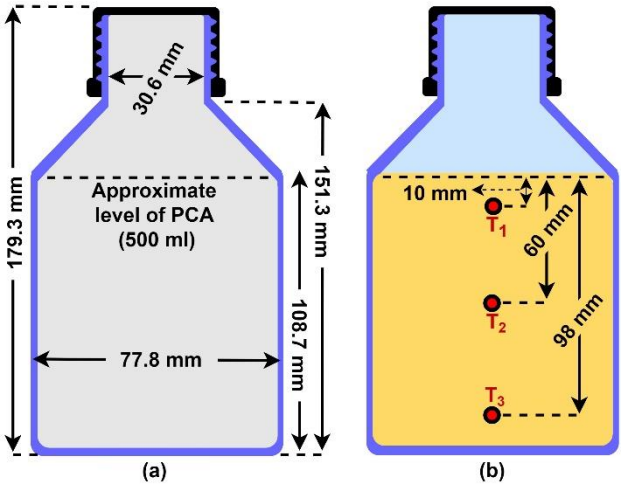


Figure 1. Shape and size of modeled bottle during computation (a), sensor locations on which temperature changes were monitored.

B. Model Description

The evaluated problem aims to describe the temperature change of a solution (PCA) containing agar in an autoclavable glass bottle. Effects of natural convection on the heating pattern were also included. The geometry were formed by three parts (glass bottle, liquid and head space) (Fig. 1). For glass bottle (silica glass) and headspace (water steam), the embedded equations in COMSOL Multiphysics® software were used to calculate physical and thermo physical properties (dynamic viscosity (μ), specific heat capacity (c_p), density (ρ)) (Eq. 1-3). Density of steam was calculated from the ideal gas law. Thermal properties of culture media were calculated using the equations presented by Choi and Okos [16] as a function of concentration of each individual compound presents in solution and temperature (Eq. 4-6).

$$k_{glass}\ (J/kg.K) = 1.38 \quad (1)$$

$$c_{p\ glass}\ (W/m.K) = 703 \quad (2)$$

$$\rho_{glass}\ (kg/m^3) = 2203 \quad (3)$$

$$\mu_{headspace}\ (Pa.s) = -1.42 * 10^{-6} + (3.84 * 10^{-8})T - (3.85 * 10^{-12})T^2 + (2.10 * 10^{-15})T^3 \quad (4)$$

$$c_{p\ headspace}\ (J/kg.K) = 1.36 * 10^4 - (9.04 * 10^1)T + (2.77 * 10^{-1})T^2 - (4.21 * 10^{-4})T^3 + (3.18 * 10^{-7})T^4 - (9.56 * 10^{-11})T^5 \quad (5)$$

$$\rho_{headspace}\ (kg/m^3) = 1.32 * 10^{-4} + (5.15 * 10^{-5})T + (3.90 * 10^{-8})T^2 - (1.37 * 10^{-11})T^3 \quad (6)$$

Dynamic viscosity of agar solution for the temperature higher than 45 ℃ was calculated as follows (Eq. 7) [17].

$$\mu_{liquid} = e^{\left[8.62 * 10^{-6}\, e^{\left(\frac{3.61 * 10^4}{RT}\right)} \dot{\gamma}^{(1.19 * 10^{-3}T - 1.35)}\right](1.70 * 10^2 C + 2.92)} \quad (7)$$

where R represent gas constant, T is temperature (K) and $\dot{\gamma}$ is share rate (s^{-1}). In the viscosity model was proposed for $\dot{\gamma}$ values between 1-200 s^{-1}, thus the value of $\dot{\gamma}$ was taken 1 s^{-1} when it was lower.

C. Governing Equations

The problem was described using transport equations as follows (Eq. 8-10) [18].

Continuity equation

$$\nabla \cdot \boldsymbol{u} = 0 \tag{8}$$

Momentum equation

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) = -\nabla p + \mu \nabla^2 \boldsymbol{u} + \rho \boldsymbol{g} \tag{9}$$

Energy conservation equation

$$\rho c_p \left[\frac{\partial T}{\partial t} + (\boldsymbol{u} \cdot \nabla) T\right] = k \nabla^2 T \tag{10}$$

D. Initial and Boundary Conditions

- Axial symmetry was considered at the center of the bottle in order to simplify the problem and reduce the computational load.
- The initial temperature of all geometry was accepted as 50 ℃ and uniform.
- For validation studies, the temperature of outer boundary of glass bottle was set to be 93 ℃ for the water level and the part above the water level was accepted as 45 ℃ (measured).
- For sterilization studies, the temperature of outer boundary of glass bottle was adjusted to autoclave chamber temperature with respect to time (Fig. 2).
- The initial velocity is the liquid is null and heat generation as a result of viscous dissipation is negligible due to very slow velocities. The no-slip boundary condition at the inner surface of bottle is accepted.

E. Model Solution and Validation

The predictive model consists of non-linear coupled partial differential equations for heat and momentum transfer. The equations have been solved by finite element method using COMSOL Multiphysics® software version 5.3a.

The experimental data were compared to predicted results for validation of the developed predictive model. A 2D asi-symmetrical geometry was created and meshed in COMSOL. Mesh sensitivity was performed, where mesh density was increased in a series of simulations until it had no further influence on solution [19].

To evaluate the accuracy of predicted data compared to experimental measurement, the root mean square error (RMSE) was calculated as follows (Eq. 11).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(T_P - T_M)^2} \tag{11}$$

where n is total number of samples, T_P and T_E are predicted and measured temperatures, respectively. After the evaluation of how well the mathematical model described the experimental data, it was concluded that the model had a satisfying performance to be used in sensitivity analysis.

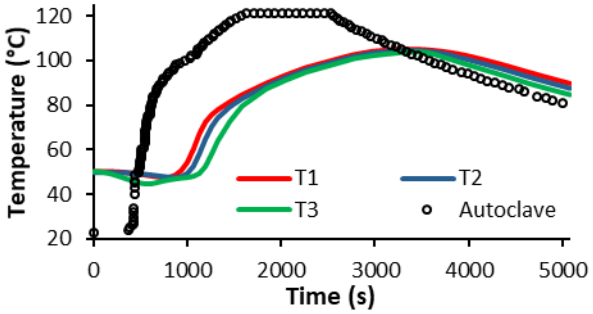


Figure 2. Autoclave chamber temperature with respect to time.

III. Results and Discussion

A. Temperature Profile of Medium in a Glass Bottle During Heating Process

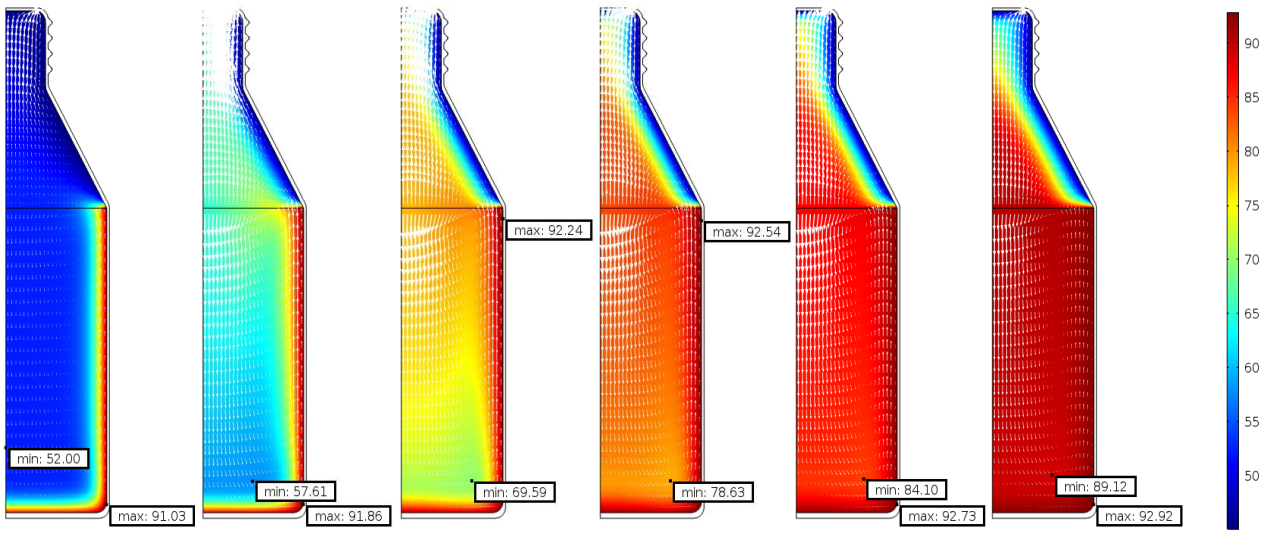


Figure 3. Temperature profile (°C) and minimum and maximum points in PCA medium in a glass bottle as a function of time for 100, 500, 1000, 1500, 2000 and 3000 s (left to right)

Temperature profile of agar medium was predicted by developed model. Fig. 3 represents the calculated minimum and maximum temperature levels and their locations in a glass bottle as a function of time for the

validation studies. As can be seen from Fig. 3, positions of minimum and maximum temperature points varied with time due to the effect of natural convection formed as a result of temperature dependent change in physical properties (density, viscosity) of medium.

It is clearly seen that temperature of medium next to inner surface of glass bottle equilibrated to almost its outer boundary layer and minimum temperature level located different inner part of agar medium was also close to that temperature level (Fig. 3).

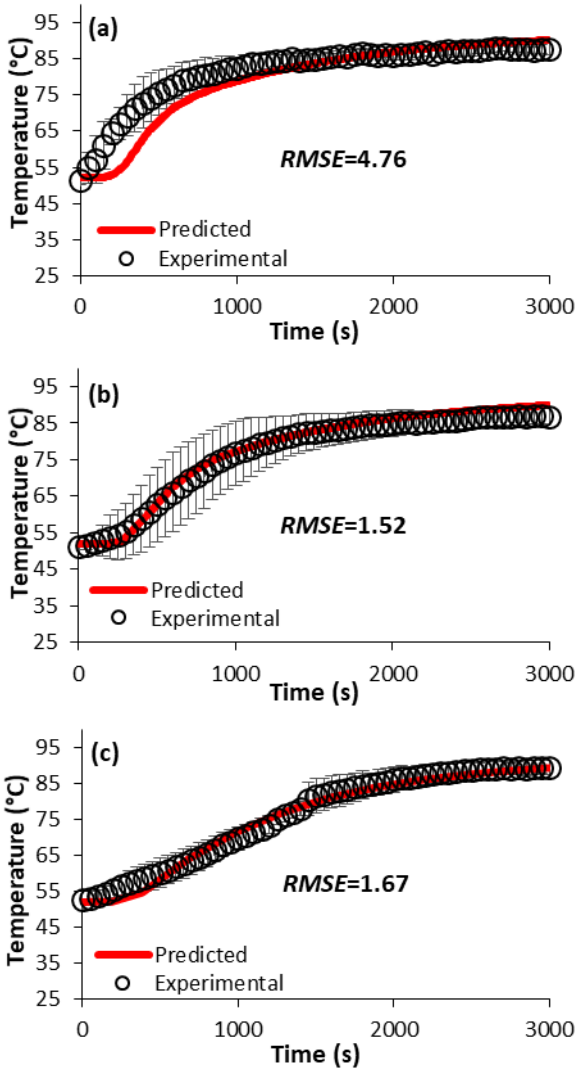


Figure 4. Temperature vs time at top sensor location (T_1) (a), middle sensor location (T_2) (b), bottom sensor location (T_3) (c).

Fig. 4a-c display the temperature change as a function of time at three different locations where sensors (as seen in Fig. 1b) collected data, as well as corresponding predicted data from developed model.

When Fig. 4 was examined, it can be seen that the RSME values belonged to middle and bottom sensor measurements and their predictions were lower than that calculated for top sensor one. In other words, the developed model showed better performance to explain the temperature variation as a function of time at bottom and middle of PCA medium compared to top one.

When the environmental temperature was adjusted to temperature belongs to autoclave chamber inside, none of the positions stated as T1, T2 and T3 could not reached to 121°C during the all sterilization process. However, the temperature at these positions achieved to reach 100°C and more than 8 mins, the temperature maintained above that critical threshold.

B. Natural Convection and Related Heat Flux during Thermal Process

In this system, heating throughout the glass bottle and PCA medium is dependent on natural convection occurred as a result of temperature dependent physical properties of medium. Change of velocity profile through arc length as a function of time and location were presented in Fig. 5a-c.

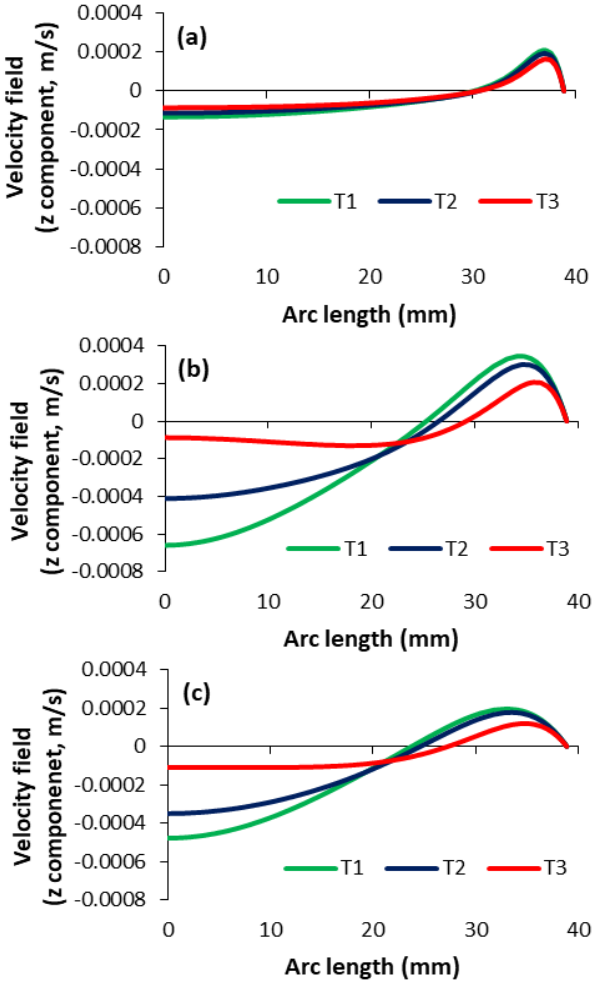


Figure 5. Velocity profile vs time and sensor location for time of 100 s (a), 1500 s (b), 3000 s (c).

As can be seen Fig. 5a, velocity gradient developed in positive direction at the region close to side surface of glass bottle at very beginning of heating process for all sensor locations, whereas its direction turned over to the negative direction and developed over there when region was closed to center of the glass. Similar trend was simulated and displayed in Fig. 5b-c, but development of velocity profile increased with heating time around 1500s,

and further heating was resulted in velocity decreased when time was getting close to 3000s.

Temperature profile started to develop at the region close to side surface of glass bottle at very beginning of heating process for all sensor positions (Fig. 6a-c). Temperature profile almost equilibrated for heating time of 1500s and almost equalized for heating time of 3000s (Fig. 6b-c). Trend for temperature profile development was coincident with that simulated for velocity profile, since at the very beginning of heating process weak velocity profile developed and that resulted in slow heat transfer in PCA medium.

However, simulation results indicated the presence of faster velocity profile meaning stronger convective flow and resulted higher heat flux and strong temperature profile development for heating time of 1500s. Finally, heating process closed to its end, temperature difference throughout the arc-length of glass bottle for all sensor locations almost disappeared, which limited the temperature dependent change in physical properties of agar medium and natural convection weaken.

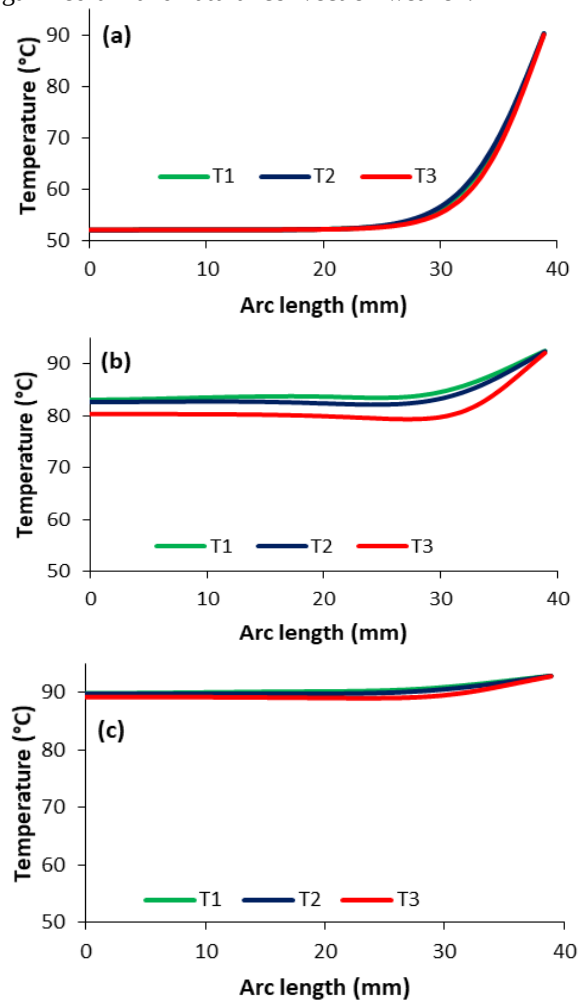


Figure 6. Temperature profile vs time and sensor location for time of 100 s (a), 1500 s (b), 3000 s (c).

C. Heat Flux Magnitude Contributions Taking Place During Heating Process

Fig. 7 displays the change in total heat flux magnitude as well as individual convective and conductive heat flux magnitudes as a function of heating time. It is clear that the convective heat flux was the dominant heat transfer mechanism during the heating of agar medium in a glass bottle heated in a water bath. Conductive heat flux was only pronounced at the very beginning of heat process, whereas it was almost negligible for the remaining part of process. This is agreed with the weak natural convection simulated for very beginning of heating process. For further part of heating, conductive effect decreased and almost disappeared, since convective heat transfer as a result of stronger natural fluid flow became pronounced.

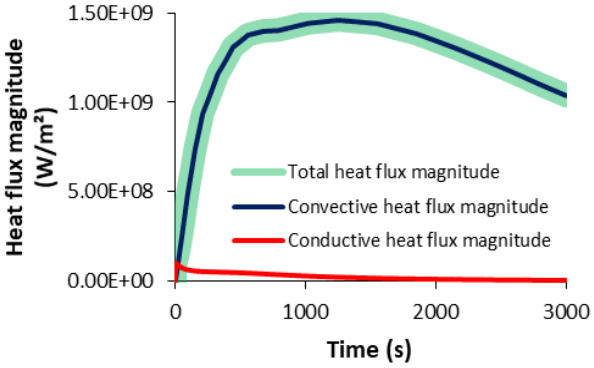


Figure 7. Heat flux magnitude calculated as convective, as conductive and as total vs time.

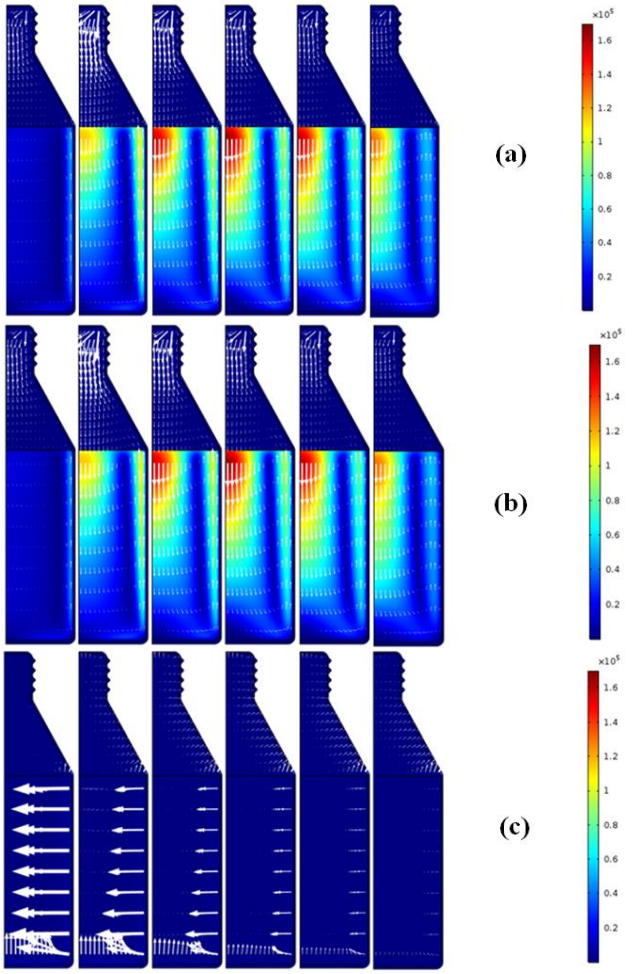


Figure 8. Heat flux magnitude (W/m^2) over axisymmetric surface calculated as total (a), as convective (b) and as conductive (c) for 100, 500 1000, 1500, 2000 and 3000 s (left to right).

Fig. 8 represents the individual convective and conductive heat flux changes as well as total heat flux. Fig. 8c represents the effect of conductive heat transfer during heating process and this creates the first temperature rise at the region close to inner side surface of glass bottle. However, that effect was suppressed by convective heat flux as a result of natural convection getting strong (Fig. 8a-b), where total heat flux was almost identical to convective heat flux diagrams.

IV. Conclusion

As conclusion, heat transfer during heating process like sterilization is crucial and it is directly affected by convective movements, in other words natural convection. Natural convection is concluded as a result of temperature dependent change in physical properties of PCA medium. Simulation results displays that conductive heat flux is negligible compared to convective one and its contribution on total heat flux remained limited. Developed model was found to have high performance to explain the temperature variation during heating process and that is important to evaluate further processes like sterilization applied for microbiological studies.

References

[1] I. Dolapçı, *Sterilizasyon ve Dezenfeksiyon*, Ankara: Ankara University Faculty of Medicine, 2015.

[2] V. Gürgün and A. Halkman, *Sterilizasyon*, in *Mikrobiyolojide Sayım Yöntemleri*, Gıda Teknolojisi Derneği, 1990.

[3] C. A. Oscroft and J. E. L. Corry, "Guidelines for the preparation, storage and handling of microbiological media," *Technical Manual: Campden and Chorleywood Food & Drink Research Association*, no. 33, 1991.

[4] MEGEP, *Besiyeri hazırlama*. Gıda Teknolojisi., Ankara: T.C. Milli Eğitim Bakanlığı, Mesleki Eğitim ve Öğretim Sistemini Güçlendirme Projesi, 2012.

[5] A. R. Lespinard and R. H. Mascheroni, "Using computational fluid-dynamics (CFD) for the evaluation of tomato puree pasteurization: Effect of orientation of bottle," in *Proc. COMSOL Conference*, Curitiba, 2014.

[6] F. Marra, *et al*., "Analysis of heat transfer during ohmic processing of a solid food," *Journal of Food Engineering*, vol. 91, no. 1, pp. 56-63, 2009.

[7] L. Wang, *et al*., "Numerical simulation of canned liquid food thermal sterilization using COMSOL multiphysics," vol. 14, pp. 76-82, 2014.

[8] Y. Jiao, J. Tang, and S. Wang, "A new strategy to improve heating uniformity of low moisture foods in radio frequency treatment for pathogen control," *Journal of Food Engineering*, vol. 141, pp. 128-138, 2014.

[9] S. Chandrasekaran, S. Ramanathan, and T. Basak, "Microwave food processing—A review," *Food Research International*, vol. 52, no. 1, pp. 243-261, 2013.

[10] V. Romano and R. Apicella, "Microwave heating of liquid foods," *Engineering*, vol. 7, no. 6, pp. 297-306, 2015.

[11] L. Wang, *et al*., "Simulation of thermal sterilization for canned tuna using COMSOL Multiphysics," vol. 15, pp. 82-88, 2015.

[12] S. K. Sastry and S. Palaniappan, "Mathematical modeling and experimental studies on ohmic heating of liquid-particle mixtures in a static heater," *Journal of Food Process Engineering*, vol. 15, no. 4, pp. 241-261, 1992.

[13] Z. Weng, *et al*., "The use of a time-temperature-integrator in conjunction with mathematical modelling for determining liquid/particle heat transfer coefficients," *Journal of Food Engineering*, vol. 16, no. 3, pp. 197-214, 1992.

[14] A. Ghani, M. M. Farid, and S. J. Zarrouk, "The effect of can rotation on sterilization of liquid food using computational fluid dynamics," *Journal of Food Engineering*, vol. 57, no. 1, pp. 9-16, 2003.

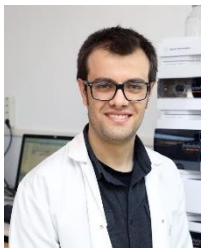
[15] D. Cacace, *et al*., "Biological validation of mathematical modeling of the thermal processing of particulate foods: The influence of heat transfer coefficient determination," *Journal of Food Engineering*, vol. 23, no. 1, pp. 51-68, 1994.

[16] Y. Choi and M. R. Okos, "Effects of temperature and composition on the thermal properties of foods," in *Food Engineering and Process Applications*, London: Elsevier Applied Science Publishers, 1986, pp. 93-101.

[17] L. Zhang, *et al*., "Rheological behavior of agar solution in relation to the making of instant edible bird's nest products," *International Journal of Food Engineering*, vol. 8, no. 3, 2012.

[18] R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2 ed., USA: John Wiley & Sons, Inc., 2002

[19] A. Kumar and I. Dilber, "Fluid flow and its modeling using computational fluid dynamics," in *Handbook of Food and Bioprocess Modeling Techniques*, S. Sablani, *et al*., Ed., CRC Press: Boca Raton, 2006.



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