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MATHEMATICAL MODELLING AND SIMULATION OF MICROALGAE BIOMASS DRYING PROCESS

Fernanda Perazzolo Disconzi
Wellington Balmant
José Viriato Coelho Vargas

Federal University of Paraná, Postgraduate Program in Mechanical Engineering (PG-Mec), Curitiba, Brazil
fernandadisconzi@gmail.com
wbalmant@gmail.com
vargasjvcv@gmail.com

Abstract. *Microalgae cultivation have been increased considerably in the last decades due to the interest in the use of biomass as a source of clean energy generation like the biofuels and in the order to feedstock like animal feed, pigments and antioxidants, applied widely in the industry. Among the steps to obtain these products, usually, the biomass drying process is necessary to extend its shelf life and to increase the lipid extraction. However, the biomass drying process has a high-energy expenditure that raises the production costs and in this way, it is necessary to improve the drying process, leading to an energy consumption reduction. The objective of this work was to develop a mathematical and computational modelling focused on the microalgae biomass drying process, considering the system defined by two phases, the solid and gas phases. In this context, the gas phase is a hot air flowing parallel over the solid phase, in which it is the wet biomass. The mass and thermal energy balance have been done for each of the phases, as well as a balance of energy in the electric resistance of the oven. The computational analyses were performed to predict the biomass drying time, focusing on the reduction of energy.*

Keywords: *mathematical modelling, drying, microalgae*

1. INTRODUCTION

The microalgae biomass is composed of lipids, consequently being a promising source of raw materials in a wide range of applications, such as feed, pigment industry, and antioxidant compounds. In addition, microalgae biomass is used biodiesel production, undergoing a multi-step process that includes cultivation, harvesting, drying, extraction of lipids and conversion from lipids to biodiesel. Drying of harvested biomass is necessary to increase the viability of biomass for lipid extraction and to extend its shelf life. The harvested biomass has 5 to 15% dry solids (Grima, et al., 2003), which put an obstruction to make the algal biodiesel commercially viable, as it requires a large quantity of energy and time to obtain the dried biomass for lipid extraction. Based on the work of Chen, *et al.* (2009), the drying of microalgae biomass could account for 30% of the total production costs. Drying methods may include natural sun drying, freeze-drying, drum drying, convection oven drying, spray drying and fluidized bed drying.

If the biomass is exposed to air at a given temperature and humidity, she either will lose or gain water until an equilibrium condition is established (Harker, Backhurst and Richardson, 2002). During the drying process, the biomass will lose water. The interactions between the heat and mass transfer phenomena that occur on the drying process can be mathematically modeled. Thus, many mathematical models have been proposed to describe the drying process, among which multiphase model has been used. This model is based on the approaches proposed by Whitaker (1977) and Hassanizadeh and Gray (1979) to porous media. All the present phases (free water, bound water, water vapor, and solid) and their possible transfer mechanisms are represented in the heat and mass transfer equations.

Von Meien and Mitchell (2002) developed a two-phase dynamic model that described heat and mass transfer in solid-state fermentation bioreactors. The model described the temperature and moisture non-equilibrium situation between the gas and solid phases. Mancini, Massarani and Biscaia (2002) mathematically modeled the corn drying in thick layer fixed bed and continuous cross-flow sliding bed dryers. The mathematical model of the process was done according to the two-phase model, one gaseous phase (dry air + water vapor) and the other solid phase (dry solid + liquid water), based on the thermodynamics of mixtures. A new correlation to the global mass transfer coefficient was proposed. According to the authors, the comparison between the experimental and simulated results allowed

concluding that the correlation satisfactorily described the mass transfer coefficient variations, since the average deviations were less than 15% in all cases. Petry, Bortoli and Khatchatourian (2006) presented a mathematical model for heat and mass transfer inside a granular medium, during the grains drying process. The set of governing equations included the mass conservation and the energy, for air and solid phases. Casciatori, *et al.* (2014) proposed a two-phase and two-dimensional model to describe heat and water transfer in a packed bed bioreactor for solid-state fermentation. Both energy and water balances were applied and individual equations were proposed for gas and solid phases. To solve the system of partial differential equations, the spatial derivatives were approximated by finite volumes and the resulting set of ordinary differential equations was simultaneously numerically integrated by a 4th order Runge-Kutta method with a variable time step size. Simo-Tagne *et al.* (2016) modeled coupled heat and mass transfer during drying of woods. The model took into account the Soret effect, mass transfer induced by a temperature gradient, and Dufour effect, heat transfer favored by a concentration gradient.

It was verified, therefore, that most of the mathematical models that evaluate the simultaneous heat and mass transfer are focused on the study of fermentation bioreactors and the drying of foods, grains or wood. However, there are no mathematical models developed exclusively for the drying of microalgae biomass. Because of this, in the present article, a two-phase model to describe heat and mass transfer between the hot air flow (gas phase) and the wet microalgae biomass (solid phase) within a convection oven was developed. The model is used to predict the drying time of the biomass and the solid and gas temperatures.

2. MATHEMATICAL MODEL AND NUMERICAL METHOD

The physical model of convection oven consists of a rectangular chamber where the wet biomass stays uniformly distributed inside a tray at the bottom of the chamber (Figure 1). At the front of the chamber, an electrical resistance generates heat that is dissipated by a fan. Thus the air heated flows parallel to the biomass. The system is set to two different phase: solid phase (wet biomass) e gas phase (hot moist air). The gas phase provides convective heat to the solid phase, increasing the temperature of the solid. At the same time, there is evaporation of the water from the biomass, raising the moisture content of the gas phase. After exchanging heat and mass with the solid phase, the hot moist air exits the system at the back of the chamber. So two variables are very important in the drying process, the temperature and moisture content of solid phase. Both energy and mass balances are done, and in both cases, separate balances are written for the gas and solid phases, as well as a balance of energy in the electric resistance of the oven, resulting in a system of partial differential equations.

The model is then discretized in space with a simple cell centered finite volume scheme, using equally sized elements. The combination of the proposed simplified physical model with the finite volume scheme for the numerical discretization of the differential equations is called a volume element model (VEM), proposed by Vargas, *et al.* (2001). From this procedure, a system of ordinary differential equations results, having time (t) as the independent variable. Each volume element (VE_i , where $1 \leq i \leq N$ and $N =$ total number of volume elements) interacts with the other adjacent elements and between the gas and solid phases.

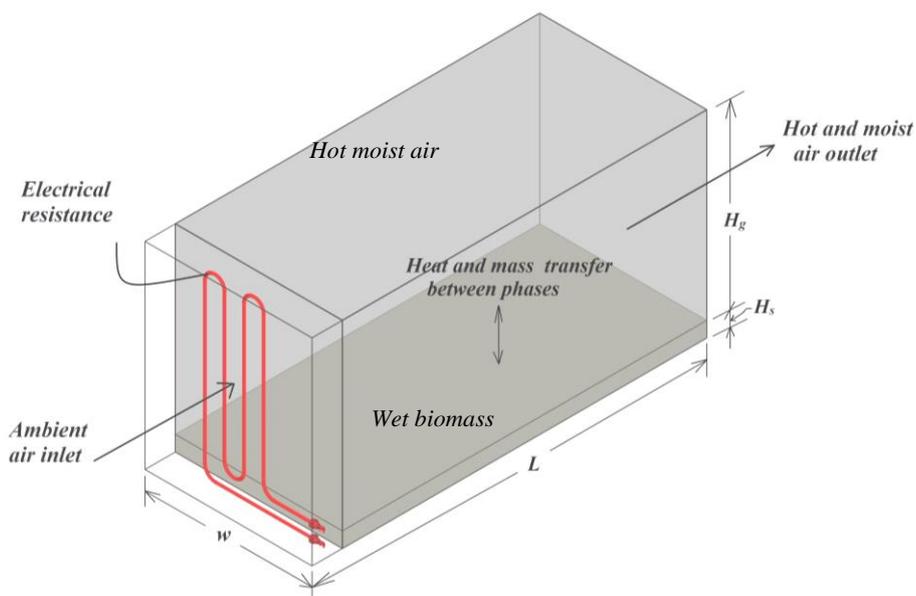


Figure 1. Physical model scheme.
Source: The Authors (2017)

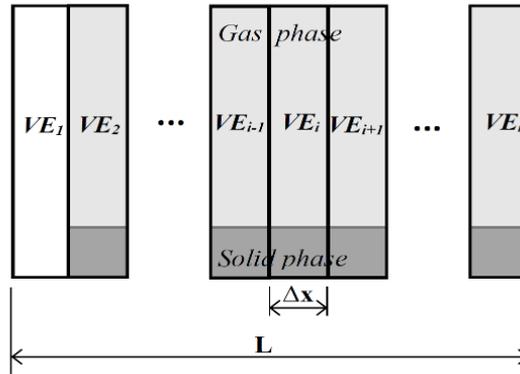


Figure 2. Volume elements (VE_i).
Source: The Authors (2017)

2.1 Hypotheses

The following assumptions are made during the development of the mathematical model:

- All water is absorbed in the solid phase in the form of bound water, i.e., the liquid phase is not considered in the model;
- The properties of dry air and dry solid are constant;
- The inlet air flow rate is constant;
- The convection oven walls are thermally insulated;
- Diffusive effects of heat and mass are disregarded in both phases;
- The shrinkage is not considered in this study;
- There is no thermal equilibrium between the phases;
- The initial moisture content and temperature are uniform along the spatial direction.

2.2 Energy balance for the electric resistance, in the first volume element (VE_1)

The energy balance gives:

$$\frac{dT_{air1}}{dt} = \frac{\left[\dot{m}_{dry_air} (T_{\infty} - T_{air1}) (U_{air\infty} C_{p_{vap}} + C_{p_{dry_air}}) + \dot{Q}_{res} \right]}{\rho_{dry_air} \forall_{elem} (U_{air\infty} C_{v_{vap}} + C_{v_{dry_air}})} \quad (1)$$

where T_{air1} is the air temperature at the center of VE_1 ; ρ_{dry_air} is the density of the dry air; \forall_{elem} is the cell volume; $C_{p_{vap}}$, $C_{v_{vap}}$ are specific heats of the water vapor at constant pressure and constant volume, respectively; $C_{p_{dry_air}}$, $C_{v_{dry_air}}$ are specific heats of the dry air at constant pressure and constant volume, respectively; \dot{m}_{dry_air} is the mass flow rate of the dry air; T_{∞} is ambient temperature; $U_{air\infty}$ is the moisture content of the ambient air; \dot{Q}_{res} is the power dissipated by electrical resistance.

In the Eq. (1), the first term of the numerator on the right-hand side is a variation of enthalpy between the inlet and outlet of VE_1 of dry air and water vapor, while the second term represents the heat supplied by an electric resistance. The denominator represents the energy accumulated in VE_1 .

2.3 Energy and mass balance for the i -th volume element (VE_i), $2 \leq i \leq N$, of the gas phase

For the energy balance over the gas phase, we have:

$$\frac{dT_{air(i)}}{dt} = \frac{\left[\dot{m}_{dry_air} (T_{air(i-1)} - T_{air(i)}) (U_{air(i)} C_{p_{vap}} + C_{p_{dry_air}}) + k_m A_{elem} \rho_{dry_sol} H_v (U_{sol(i)} - U_{eq(i)}) - h A_{elem} (T_{air(i)} - T_{sol(i)}) \right]}{\rho_{dry_air} \forall_{elem} (U_{air(i)} C_{v_{vap}} + C_{v_{dry_air}})} \quad (2)$$

The water balance of the gas phase is as follows:

$$\frac{dU_{air(i)}}{dt} = \frac{[\dot{m}_{dry_air}(U_{air(i-1)} - U_{air(i)}) + k_m A_{elem} \rho_{dry_sol}(U_{sol(i)} - U_{eq(i)})]}{\rho_{dry_air} \nabla_{elemg}} \quad (3)$$

In the Eq. (2) and Eq. (3), $T_{air(i)}$ and $T_{air(i-1)}$ are the air temperatures at the centers of VE_i and VE_{i-1} , respectively; ∇_{elemg} is the cell volume of the gas phase; $U_{air(i)}$ and $U_{air(i-1)}$ are the air moisture contents at the centers of VE_i and VE_{i-1} , respectively; k_m is global mass transfer coefficient; A_{elem} is the contact surface between the gas and solid phases; H_v is the enthalpy of evaporation of water; h is convective heat transfer coefficient; $U_{eq(i)}$ is the solid phase moisture content for equilibrium with the gas phase at $T_{air(i)}$.

In Eq. (2), the terms of the numerator on the right-hand side represent: the first is variation of enthalpy between the inlet and outlet of the VE_i for the gas phase of dry air and water vapor, the second is the heat transferred from the solid phase to the gas phase by the evaporation of the biomass water and the last term is the loss of heat by convection between the gas and solid phases. The denominator denotes the energy accumulated in VE_i gas phase.

The terms on the right-hand side of the Eq. (3) mean, respectively, the variation of air moisture between the inlet and outlet of VE_i gas phase and the transfer of moisture from the solid phase to the gas phase, per mass unit of the dry air ($\rho_{dry_air} \nabla_{elemg}$).

2.4 Energy and mass balance for the i -th volume element (VE_i), $2 \leq i \leq N$, of the solid phase

Two processes affect the energy within the solid phase, the evaporation of water to the gas phase and the heat gain due to the convection between the gas and solid phases. These are represented by the two terms of the numerator on the right-hand side of the Eq. (4):

$$\frac{dT_{sol(i)}}{dt} = \frac{[-k_m A_{elem} \rho_{dry_sol} H_v (U_{sol(i)} - U_{eq(i)}) + h A_{elem} (T_{air(i)} - T_{sol(i)})]}{\rho_{dry_sol} \nabla_{elems} (U_{sol(i)} C_{v_{dry_sol}} + C_{v_{water}})} \quad (4)$$

where $T_{sol(i)}$ is the solid temperature at the center of VE_i ; ∇_{elems} is the cell volume of the solid phase; $U_{sol(i)}$ is the solid moisture content at the center of VE_i ; $C_{v_{dry_sol}}$, $C_{v_{water}}$ are specific heats of the dry solid and liquid water at constant volume, respectively; ρ_{dry_sol} is the density of the dry solid. The denominator denotes the energy accumulated in VE_i for the solid phase.

Finally, the mass balance of the solid phase is as follows:

$$\frac{dU_{sol(i)}}{dt} = \frac{[-k_m A_{elem} \rho_{dry_sol} (U_{sol(i)} - U_{eq(i)})]}{\rho_{dry_sol} \nabla_{elems}} \quad (5)$$

The right-hand side of the Eq. (5) represents the transfer of moisture from the solid phase to the gas phase per mass unit of the dry solid ($\rho_{dry_sol} \nabla_{elems}$).

2.5 Correlations

The coefficient for convective heat transfer between the solid and gas phase is calculated as a function of the mass flow rate per surface unit (G) using an empirical equation developed for the drying (Treybal (1980); Shepherd, Hadlock and Brewer (1938)):

$$h = 14.3G^{0.8} \quad (6)$$

The dependence of the global mass transfer coefficient with gas temperature is assumed as an Arrhenius type function (Guiné, Henriques and Barroca, 2009). The correlation of Prado and Sartori (2008) was adjusted by the numerical sensitivity test to match the predicted with the experimental data:

$$k_m = 0.0011 \exp \left[-\frac{201.8}{T_{ar}} \right] \quad (7)$$

Mathematical models for the equilibrium moisture content (U_{eq}) were selected and tested to find the fit better with experimental data. The chosen model was the Oswin model (1946):

$$U_{eq} = \frac{A}{100} \left[\frac{a_w}{1 - a_w} \right]^B \quad (8)$$

where a_w is the water activity, A and B are coefficients based on experimental data and depend on the air temperature:

$$A = -13.562 \ln(T_{ar}) + 61.145 \quad (9.a)$$

$$B = 0.319 \ln(T_{ar}) - 0.918 \quad (9.b)$$

The water activity, a_w , which is equivalent to the percentage relative humidity divided by 100, is given by the actual vapor pressure of water, P_{vap} , divided by the saturation vapor pressure, P_{vap}^{sat} , at the same temperature:

$$a_w = \frac{P_{vap}}{P_{vap}^{sat}} = \frac{U_{air} P}{(U_{air} + 0.622) P_{vap}^{sat}} \quad (10)$$

where P is the total pressure of a mixture (air + water vapor).

The saturation partial pressure is derived from the Antoine equation (Poling, Prausnitz and O'Connell, 2004):

$$P_{vap}^{sat} = 10^{[a - (b / (T_{ar} + c))]} \quad (11)$$

In the Eq. (11), the unit of P_{vap}^{sat} is bar (1 bar = 101.325 kPa), and the constants for the water are: $a = 5.116$; $b = 1687.54$; $c = 230.17$.

2.6 Initial conditions, parameters and variables for computational simulation

For the system of ordinary differential equations are necessary initial conditions, parameters and variables for the simulation with the mathematical model. Table 1 presents these items with their units and sources.

2.7 Numerical method

The before equations define a system of $4N-3$ ordinary differential equations with time as the independent variable, and the initial conditions for the unknowns T_{air} , U_{air} , T_{sol} and U_{sol} . The system is integrated in time from the initial conditions explicitly, using an adaptive time step 4th/5th order Runge-Kutta-Fehlberg method (Kincaid and Cheney, 1991). The time step chosen was 0.1 s.

3. RESULTS AND DISCUSSION

The developed mathematical model was used in this section to predict results to evaluate the biomass drying time and biomass temperature. For that, a Fortran code was written based on the model and all simulations were performed in a laptop Intel (R) Core (TM) i7-7700HQ CPU @ 2.80 GHz, 16 GB RAM, 64-bit operating system.

Figure 3 shows the predicted profiles of drying rate (dU_{sol}/dt) and biomass temperature (T_{sol}). Initially, occurs the heat transfer from air to biomass, raising its temperature. Thereafter, takes place the water evaporation, i.e., the mass transfer from the solid phase to the gaseous phase. At that time, the temperature of the biomass rises slowly, because a portion of the heat supplied by the drying air is used to evaporate the water and the other portion is used to increase the temperature of the solid. The amount of water in the biomass decreases and the drying rate follows this reduction. At the end of drying, the biomass temperature rises more rapidly, because the heat supplied by the drying air is used almost

exclusively for increasing the temperature of the solid, since the amount of water in the biomass is low. The drying rate decreases rapidly until it reaches the thermodynamic equilibrium.

Table 1. Initial conditions, parameters and variables.

Parameter or variable	Description	Value	Source
t	time (independent variable)	$t = 0$ [s] (initial)	-
T_{air}	air temperature at the center of VE (dependent variable)	$T_{air} (t = 0) = T_{\infty} = 20$ [°C]	chosen
U_{air}	air moisture content at the centers of VE (dependent variable)	$U_{air} (t = 0) = U_{air\infty} = 6.5 \times 10^{-3}$ [kg-water.kg-dry-air ⁻¹]	chosen
T_{sol}	biomass temperature at the center of VE (dependent variable)	$T_{sol} (t = 0) = T_{\infty} = 20$ [°C]	chosen
U_{sol}	biomass moisture content at the centers of VE (dependent variable)	$U_{sol} (t = 0) = 2.0$ [kg-water.kg-dry-solid ⁻¹]	chosen
\dot{m}_{dry_air}	mass flow rate of the dry air	0.1 [kg-dry-air.s ⁻¹]	chosen
ρ_{dry_air}	density of the dry air	1.15 [kg-dry-air.m ⁻³]	Himmelblau (1982)
ρ_{dry_sol}	density of the dry biomass	1100 [kg-dry-solid.m ⁻³]	Zeng <i>et al.</i> (2013)
\dot{Q}_{res}	power of electrical resistance	1500, 2000, 3000 [W]	chosen
$C_{p_{dry_air}}$	specific heat of the dry air at constant pressure	1007 [J. kg-dry-air ⁻¹ .K ⁻¹]	Himmelblau (1982)
$C_{v_{dry_air}}$	specific heat of the dry air at constant volume	719.3 [J. kg-dry-air ⁻¹ .K ⁻¹]	Himmelblau (1982)
$C_{p_{vap}}$	specific heat of the water vapor at constant pressure	1875 [J. kg-water ⁻¹ .K ⁻¹]	Himmelblau (1982)
$C_{v_{vap}}$	specific heat of the water vapor at constant volume	1339.3 [J. kg-water ⁻¹ .K ⁻¹]	Himmelblau (1982)
$C_{v_{water}}$ or $C_{p_{water}}$	specific heat of the water at constant volume or constant pressure	4178 [J. kg-water ⁻¹ .K ⁻¹]	Himmelblau (1982)
$C_{v_{dry_sol}}$ or $C_{p_{dry_sol}}$	specific heat of the dry biomass at constant volume or constant pressure	1595 [J. kg-dry-solid ⁻¹ .K ⁻¹]	Zeng <i>et al.</i> (2013)
H_v	enthalpy of evaporation of water	2556×10^3 [J. kg-water ⁻¹]	Himmelblau (1982)
N	total number of VEs	5	chosen
L	length of convection oven	1.2, 0.6, 0.3 [m]	chosen
w	width of convection oven	0.1, 0.2, 0.4 [m]	chosen
H_g	height for gas phase	0.2 [m]	chosen
H_s	height for solid phase	0.01 [m]	chosen
A_{elem}	contact surface	$0.12/N$ [m ²]	-
\forall_{elem}	cell volume	$\forall_{elemg} + \forall_{elem s}$ [m ³]	-
\forall_{elemg}	cell volume of the gas phase	$0.12H_g/N$ [m ³]	-
$\forall_{elem s}$	cell volume of the solid phase	$0.12H_s/N$ [m ³]	-
h	convective heat transfer coefficient	[Wm ⁻² K ⁻¹], Eq. (6)	Treybal (1980)
k_m	global mass transfer coefficient	[ms ⁻¹], Eq. (7)	Adjusted of Prado and Sartori (2008)
U_{eq}	equilibrium moisture content	[kg-water.kg-dry-solid ⁻¹], Eq. (8)	Oswin (1946)
A and B	coefficients	dimensionless, Eq. (9.a), Eq. (9.b)	determined
a_w	water activity	dimensionless, Eq. (10)	-
P	total pressure	1.0 [bar]	-
P_{vap}^{sat}	saturation vapor pressure	[bar], Eq. (11)	Poling, Prausnitz and O'Connell (2004)

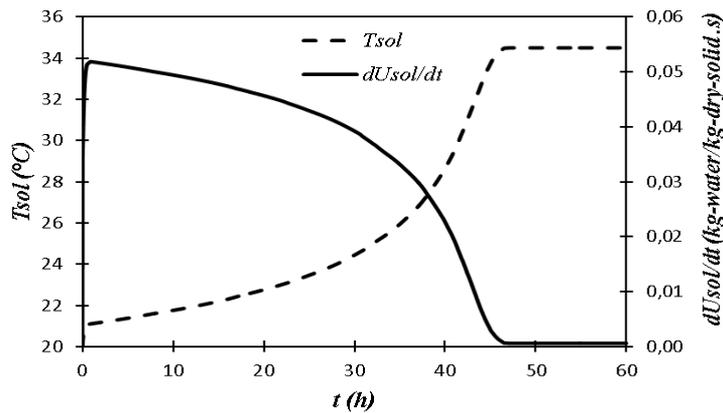


Figure 3. Predicted profiles of biomass temperature and drying rate.

In other computational simulations, different values of the power of the electric resistance (\dot{Q}_{res}) and the w/L rate (width/length) of convection oven were analyzed, remaining unchanged the other parameters.

A standard configuration with $L = 0.6$ m and $w = 0.2$ m ($w/L = 1/3$) was used to simulate different values for the electrical resistance power. The electric powers used in the simulation (Tab. 1) led to the results presented in the graph of Fig. 4 and Fig. 5. In them, it is possible to note that the higher the power, the higher the temperature that the biomass reaches and the lower the biomass drying time. For example, at a power of 3000 W, the biomass reaches a temperature of 50 °C for a drying time of approximately 24 hours. Whereas, for a power of 1500 W, the temperature reaches close to 35 °C for a drying time of 47 hours. It should also be noted that when the electric power increases, the U_{sol} values tend to fall very rapidly until reaches the moisture content of the environment ($U_{air\infty}$) and not smoothly as in lower powers.

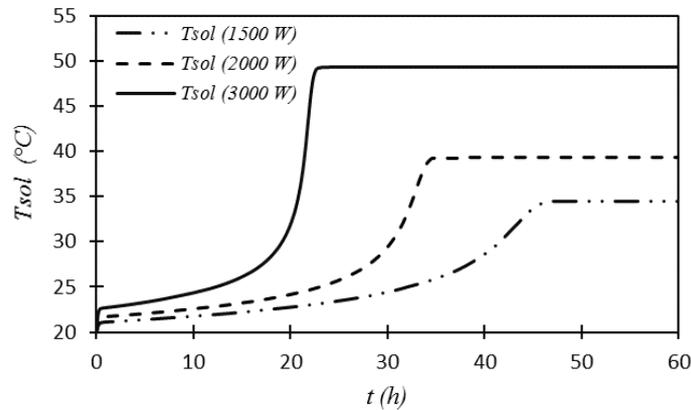


Figure 4. Predicted profiles of biomass temperature with respect to time.

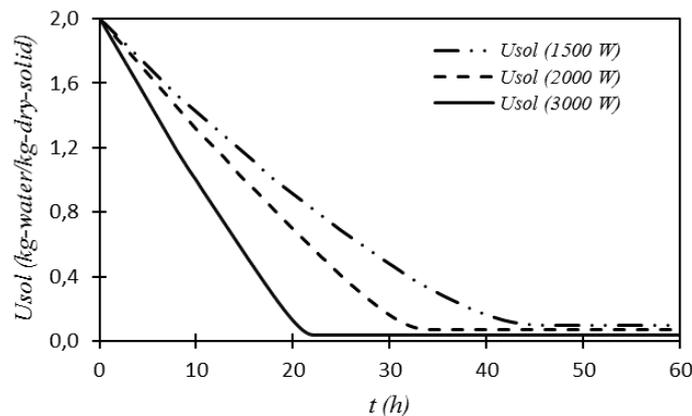


Figure 5. Predicted profiles of Biomass moisture content with respect to time.

With the values of w and L (Tab. 1), we defined w/L ratios for the simulation as: $1/12$; $1/3$ and $4/3$, for the electrical power of 1500 W . According to Fig. 6 and Fig. 7, with the ratio $w/L = 1/12$, the microalgae biomass dried in approximately 32 hours, while for the $1/3$ and $4/3$ ratios, the biomass takes about 47 and 75 hours, respectively. Therefore, it can be concluded that the smaller the width of the convection oven, keeping the same contact surface, the faster the biomass drying. This is likely because of the increase in the air flow velocity, which leads to the increase of the convective heat transfer coefficient. Thus, the heat exchange takes place more quickly and, consequently, the evaporation of the water increases.

In addition, we can note that using the highest electrical resistance power (3000 W) the drying time is similar to drying time at the $w/L = 1/12$ setting. Therefore, in order to reduce the energy expenditure, could be chosen a narrower and longer convection oven for biomass drying instead of an electric resistance with high power.

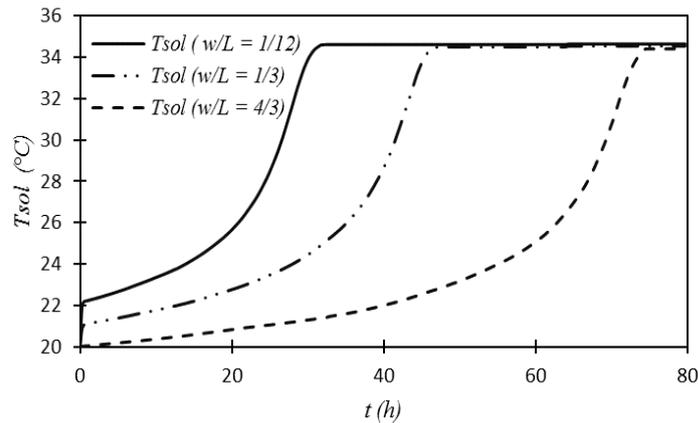


Figure 6. Predicted profile of biomass temperature with respect to time, for the w/L ratios.

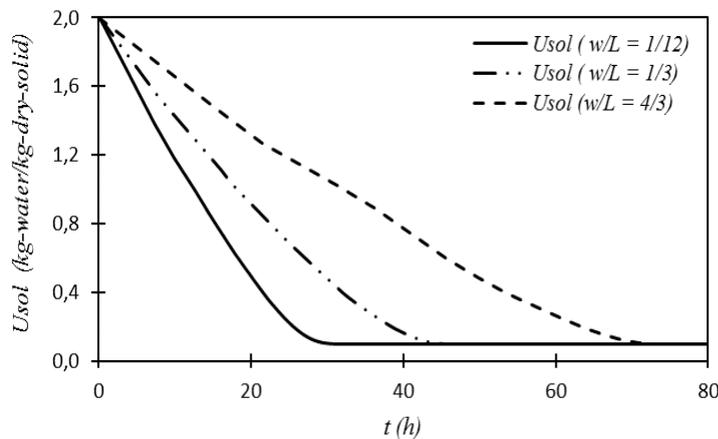


Figure 7. Predicted profile of biomass moisture content with respect to time, for the w/L ratios.

4. CONCLUSIONS

The following conclusions can be made from numerical results:

- The drying process is strongly dependent on temperature and flow velocity of the drying air, because of their influence on the heat and mass transfer coefficients;
- The higher the \dot{Q}_{res} value, the higher the air temperature and the drying of the biomass occurs faster;
- The lower the w/L ratio, keeping all other dimensions constant, the higher the flow velocity, consequently, the higher the heat transfer coefficient, which leads to a reduction in the drying time;
- For the configurations $w/L = 1/12$ ($\dot{Q}_{res} = 1500\text{ W}$) and $w/L = 1/3$ ($\dot{Q}_{res} = 3000\text{ W}$), the respective biomass drying times are low and similar, therefore, to reduce energy expenditure, it is interesting to use the first configuration;
- Experimental validation of the mathematical model and parameter adjustment are required for design and optimization of a convection oven.

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