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NUMERICAL ANALYSIS OF FLUID FLOW AND HEAT TRANSFER FOR BREWING PROCESS

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Abstract. *This paper presents a model for analyzing fluid flow, heat and mass transfer during the combined mashing and clarification process of barley malt. The grain bed is treated as a porous medium and a simple formulation for energy and mass transport is obtained. Temperature and concentration profiles are investigated using numerical method, providing general design parameters for recirculating mash systems commonly used in the brewing industry.*

Keywords: *brewing, heat transfer, mass transfer, porous media, numerical method*

1. INTRODUCTION

One of the main processes that take place in a brewery is the production of wort, a solution that contains a certain amount of fermentable sugars that will be converted into alcohol and carbon dioxide in a later stage called fermentation. This process is called mashing and it has continually evolved over the years as brewing processes are altered to adjust to the demands of quality, efficiency and process control required by the industry. During the last years, there has been a constant increase in the number of medium and small breweries, which have a smaller production capacity compared to large industries, in addition to generally having restrictions on the size of their facilities. The purpose of this work is to propose a mathematical model for heat and mass transfer in a recirculation system, that is, automated systems where the mash and wort filtration steps occur in parallel. These systems are characterized by the fact that they are more compact, allowing optimization of the process duration and the ability to perform more precise temperature control. These characteristics are very interesting for installations of modest dimensions found in nanobreweries, microbreweries and brewpubs.

Some of the first models developed to describe the hydrolysis of starch in mashing are Marc *et al.* (1983) and Koljonen *et al.* (1995). These models describe the kinetics of enzyme catalyzed starch hydrolysis in traditional mashing processes. The works of Quintanilha *et al.* (2015) and Zamboni *et al.* (2017), study respectively the effect of a variable temperature on the saccharification of barley malt and the effect of heat diffusion on the mash temperature profile and consequently the enzymatic reaction. The present paper seeks to investigate the heat transfer and its effects on the concentration gradients of enzymes and fermentable sugars during a recirculation mashing process.

2. PROBLEM FORMULATION

The problem investigated in this study is that of heat and mass transfer with chemical reactions in the mashing process of recirculation systems.

The aim is to study the conversion of starch into fermentable sugars, describing through a mathematical model the action of enzymes and the concentration of these carbohydrates. In this model, the transport equations of the species consider the convective term and the temperature profile is modeled by the convective transport equation in porous media, since the characteristic of the process involves the flow of wort.

Some simplifying assumptions are adopted, such as: grain bed treated as a homogeneous and isotropic porous medium, which implies constant porosity throughout the volume; flow velocity is the surface velocity according to Darcy's law and the flow is considered uniform and unidimensional; energy and mass transport occurs in transient regime, with uniform heat diffusion in the radial direction and uniform temperatures and concentrations in the direction perpendicular to the flow; insoluble starch that does not flow with the solution and only solubilized and gelatinized components participate in the chemical reactions involved.

2.1 Mass transfer

Starting from the mass balance and applying the simplifying assumptions, the convection-diffusion equation for a general species is written as:

$$\frac{\partial \rho_l}{\partial t} + \frac{\partial}{\partial z}(v_z\,\rho_l) \;=\; -\dot{\rho}_s \tag{1}$$

$$\frac{\partial}{\partial t}(\rho_l\,\omega_i) + \frac{\partial}{\partial z}(v_z\,\rho_l\,\omega_i) \;=\; \frac{\partial}{\partial z}\left(\rho_l\,\mathcal{D}_i\,\frac{\partial \omega_i}{\partial z}\right) + \rho_l\,\dot{\omega}_i \tag{2}$$

for $i = 0, \ldots, 5$, corresponding to water (ω_0), glucose (ω_1), maltose (ω_2), maltotriose (ω_3), dextrins (ω_4), and limit-dextrins (ω_5). Where ρ_l is solution density, $-\dot{\rho}_s$ is starch comsuption rate and ω_i is mass fraction of each species. The mass concentration per unit volume of each species is such that $\rho_i \;=\; \rho_l\,\omega_i$. The term v_z is seepage velocity related to intrinsic average velocity by the relationship $v_z = \varphi\,v_f$, while $\mathcal{D}_i$ is the difussion coefficient of the species in the solution.

Initial conditions are spatially uniform. For water, species and starch are written as:

$$\rho_i(z,0) = \rho_{i,0} \tag{3}$$

$$\rho_s(z,0) = \rho_{s,0} \tag{4}$$

For boundary conditions recirculation is considered. So it is imposed that the outlet ($z = 0$) condition is equal to the inlet ($z = H_b$):

$$\omega_i(H_b,t) = \omega_i(0,t), \tag{5}$$

If diffusion is taken into consideration, continuity condition of the derivative between inlet and outlet are imposed:

$$\left.\frac{\partial \omega_i}{\partial z}\right|_{z=0} = \left.\frac{\partial \omega_i}{\partial z}\right|_{z=H_b} \tag{6}$$

2.2 Enzymes

For the enzymes, the mass transport formulation considers that the enzymes are initially present in the grains ($\varepsilon_{s,j}$) and are gradually transferred to the solution (ε_j) due to the gradient of concentration

$$\frac{\partial \varepsilon_{s,j}}{\partial t} \;=\; -\frac{H_j\,M}{\mathcal{V}_g}\,(\varepsilon_{s,j} - \varepsilon_j) \tag{7}$$

$$\frac{\partial \varepsilon_j}{\partial t} \;+\; v_z\,\frac{\partial \varepsilon_j}{\partial z} \;=\; \frac{H_j\,M}{\mathcal{V}}\,(\varepsilon_{s,j} - \varepsilon_j) \;+\; \frac{\partial}{\partial z}\left(\mathcal{D}_{\varepsilon_j}\,\frac{\partial \varepsilon_j}{\partial z}\right) \;+\; \dot{\varepsilon}_j, \tag{8}$$

for $j = 1, 2$, where $j = 1$ represents α-amylase concentration and $j = 2$, β-amylase concentration. The concentrations indicated by ε are the enzymes dissolved in the wort, while ε_s represents the enzyme concentrations in the dry malt. The term $\dot{\varepsilon}_j(t)$ represents the rate of production of the enzyme dissolved in the liquid phase, which is negative because it is denatured, where H_j is the dissolution coefficient for the given enzyme and $\mathcal{D}_{\varepsilon_j}$ is the difussion coefficient of the enzyme in the solution.

Initial conditions for enzymes are written as:

$$\varepsilon_j(z,0) = 0, \tag{9}$$

These equations represent the situation where all the enzymes are initially in the grain, with nothing in solution.

Similarly to the conditions for species, boundary conditions for enzymes are given by:

$$\varepsilon_j(H_b,t) = \varepsilon_j(0,t) \tag{10}$$

$$\left.\frac{\partial \varepsilon_j}{\partial z}\right|_{z=0} = \left.\frac{\partial \varepsilon_j}{\partial z}\right|_{z=H_b} \tag{11}$$

2.3 Heat transfer

Temperature distribution is modeled by heat conduction-convection equations as:

$$(\rho\, c)_b \, \frac{\partial T}{\partial t} + (\rho\, c)_l \, v_z \, \frac{\partial T}{\partial z} \;=\; \frac{\partial T}{\partial z}\left(k_b \, \frac{\partial T}{\partial z}\right) \,+\, h_e \, S\,(T - T_{ext}) \,+\, q_b''' \tag{12}$$

where $(\rho\, c)_b$ corresponds to the porous bed thermal capacity and $(\rho\, c)_l$ corresponds to the solution thermal capacity. The penultimate term of the above equation corresponds to the heat exchange on the reactor wall, which is treated in a lumped fashion, where h_e corresponds to a convective heat transfer coefficient and S is the specific surface area. Furthermore, q_b''' is the volumetric heat generation rate in the porous medium and k_b is its thermal conductivity.

The initial condition corresponds to a uniform temperature distribution::

$$T(z, 0) \;=\; T_0, \tag{13}$$

Boundary conditions are prescribed at the inlet and outlet of the porous bed:

$$k_b \, \frac{\partial T}{\partial z} \;=\; h_{in}\,(T_{in} - T), \qquad \text{for} \quad z = H_b, \tag{14}$$

$$k_b \, \frac{\partial T}{\partial z} \;=\; h_{out}\,(T - T_{out}) \qquad \text{for} \quad z = 0, \tag{15}$$

where h_{in} and h_{out} are convective heat transfer coefficients with the portion of liquid above and below the porous bed respectively.

Additionally, in order to simulate the influence of the heater, the following expression is defined for the variation of the inlet temperature in the control volume:

$$T_{in}(t) \;=\; T_{aq} - (T_{aq} - T_0)\left(\frac{t_{\max} - t}{t_{\max}}\right) \tag{16}$$

where the inlet temperature is conditioned to reach the temperature of the heater T_{aq} at the final instant of the process $t_{\max}$ starting from the initial temperature T_0.

2.4 Saccharification

In this study, the chemical kinetics model adopted by Marc *et al.* (1983) and later by Koljonen *et al.* (1995) is considered. Enzymes are dissolved from the malt grain into the wort, and enzymatic conversions are assumed to occur only by the action of dissolved enzymes. When starch is heated in contact with water, it undergoes gelatinization, which consists of the dilation of the granules that constitute it, causing swelling, loss of crystallinity and water absorption. It is assumed that non-gelatinized starch is not hydrolyzed by the action of amylases. Gelatinized starch is converted into dextrins and maltotriose by the action of dissolved α-amylase. Dextrins are converted into sugar and limit dextrins by the action of dissolved β-amylase.

Starch is converted into maltotriose (ω_3) and dextrins (ω_4) by the action of α-amylase, so the rate of starch production is given by:

$$\dot\rho_s(t) \;=\; -\varepsilon_1\,(\gamma_3\, A_3 + A_4)\,\left(\rho_s - \rho_s^0\, u(T)\right), \tag{17}$$

where the coefficient γ_3 corresponds to the mass fraction of starch consumed ($\gamma_3 = 27/28$) as maltotriose is produced. DExtrin is converted in glucose (ρ_1), maltose (ρ_2) and limit-dextrins (ρ_5) by the action of β-amylase, thus the rate of dextrin production is given by:

$$\dot\rho_4(t) = \varepsilon_1\, A_4\,\left(\rho_s \,-\, \rho_s^0\, u(T)\right) - \varepsilon_2\,\rho_4\left(\gamma_1\, B_1 + \gamma_2\,\frac{B_2}{k_m + \rho_4} + B_5\right), \tag{18}$$

where the coefficients $\gamma_1 = 9/10$ and $\gamma_2 = 18/19$ correspond to the mass fractions of dextrin consumed as glucose and maltose are produced. The rate of water consumption ($\dot\rho_0$), as well as the production rates of glucose ($\dot\rho_1$), maltose ($\dot\rho_2$), maltotriose ($\dot\rho_3$) and limit dextrins ($rhodt_5$) are given by the following equations:

$$\dot\rho_1(t) = B_1\,\varepsilon_2\,\rho_4, \tag{19}$$

$$\dot\rho_2(t) = B_2\,\varepsilon_2\,\frac{\rho_4}{k_m + \rho_4}, \tag{20}$$

$$\dot\rho_3(t) = A_3\,\varepsilon_1\,\left(\rho_6 \,-\, \rho_6^0\, u(T)\right), \tag{21}$$

$$\dot\rho_5(t) = B_5\,\varepsilon_2\,\rho_4, \tag{22}$$

$$\dot\rho_0(t) = -\dot\rho_s(t) \,-\, \sum_{i=1}^{5}\dot\rho_i(t). \tag{23}$$

The term u represents the mass fraction of non-gelatinized starch, and is defined as:

$$u(T) = \begin{cases} 1, & T \leq T_u \\ (T_g - T)^2(3T_u - T_g - 2T)/(T_u - T_g)^3, & T_u < T < T_g \\ 0, & T \geq T_g \end{cases} \tag{24}$$

The enzymes contained in the grains are dissolved in the liquid phase, then they are denatured at a rate that depends on temperature, a process described by the following equations:

$$\dot{\varepsilon}_1(t) = -C_\alpha \, \varepsilon_1, \tag{25}$$

$$\dot{\varepsilon}_2(t) = -C_\beta \, \varepsilon_2, \tag{26}$$

where ε_1 and ε_2 represent the concentrations of enzymes dissolved in the liquid phase.

The coefficients A_i, B_i, C_α, C_β, which represent the rates of enzymatic conversions and enzymatic denaturation reaction depend on temperature according to Arrhenius and are given by:

$$A_3 = A_{3,0} \, \exp\left(-E_\alpha/(RT)\right) \tag{27}$$

$$A_4 = A_{4,0} \, \exp\left(-E_\alpha/(RT)\right) \tag{28}$$

$$B_1 = B_{1,0} \, \exp\left(-E_\beta/(RT)\right) \tag{29}$$

$$B_2 = B_{2,0} \, \exp\left(-E_\beta/(RT)\right) \tag{30}$$

$$B_5 = B_{5,0} \, \exp\left(-E_\beta/(RT)\right) \tag{31}$$

$$C_\alpha = C_{\alpha,0} \, \exp\left(-E_{\alpha,d}/(RT)\right) \tag{32}$$

$$C_\beta = C_{\beta,0} \, \exp\left(-E_{\beta,d}/(RT)\right) \tag{33}$$

where $C_{\alpha,0}$ and $C_{\beta,0}$ are the specific maximum rates of enzyme destruction for α- and β-amylase.

3. RESULTS AND DISCUSSION

Numerical values for the chemical kinetic-related parameters used in the solution are given in table 1. Data from Koljonen *et al.* (1995) are used for a malt variety called Kymppi and density, specific heat and conductivity data for generic barley grains are obtained from Mujumdar (2014).

Table 1. Parameter values for Kymppi malt and barley grain parameters.

Description	Symbol	Value	Reference
Hydrolysis frequency factor	$B_{1,0}$	1.62×10^{40} l/min/g	Koljonen *et al.* (1995)
	$B_{2,0}$	1.05×10^{42} l/min/g	Koljonen *et al.* (1995)
	$B_{5,0}$	1.09×10^{41} l/min/g	Koljonen *et al.* (1995)
	$A_{3,0}$	6.42×10^{9} l/min/g	Koljonen *et al.* (1995)
	$A_{4,0}$	3.77×10^{10} l/min/g	Koljonen *et al.* (1995)
Hydrolysis activation energy	E_α	1.03×10^{5} J/mol	Koljonen *et al.* (1995)
	E_β	2.93×10^{5} J/mol	Koljonen *et al.* (1995)
Denaturation frequency factor	$C_{\alpha,0}$	3.86×10^{34} min^{-1}	Koljonen *et al.* (1995)
	$C_{\beta,0}$	9.46×10^{67} min^{-1}	Koljonen *et al.* (1995)
Denaturation activation energy	$E_{\alpha,d}$	2.377×10^{5} J/mol	Koljonen *et al.* (1995)
	$E_{\beta,d}$	4.439×10^{5} J/mol	Koljonen *et al.* (1995)
Dissolution coefficient	H_1	9.72×10^{-5} l/min/g	Koljonen *et al.* (1995)
	H_2	7.57×10^{-5} l/min/g	Koljonen *et al.* (1995)
Michaelis constant	k_m	2.8 g/l	Koljonen *et al.* (1995)
Temperature	T_g	336.5 K	Koljonen *et al.* (1995)
	T_u	315.4 K	Koljonen *et al.* (1995)
Barley grain density	ρ_r	618 kg/m^3	Mujumdar (2014)
Barley grain thermal capacity	c_r	1245 J/kg/K	Mujumdar (2014)
Barley grain thermal conductivity	k_r	13.14 J/min/m/K	Mujumdar (2014)

Initial concentration values for Kymppi malt are given in table 2. Concentrations are given in mass per unit volume, defined as the product of mass fraction and solution density. Initial enzyme activity values are obtained from Koljonen

Table 2. Kymppi malt initial condition and parameters.

Description	Symbol	Value
Water	V	2.0×10^{-4} m^3
Malt	M	0.05 kg
Glucose	ρ_1	0.0 g/l
Maltose	ρ_2	0.0 g/l
Maltotriose	ρ_3	0.0 g/l
Dextrin	ρ_4	0.0 g/l
Limit-dextrin	ρ_5	0.0 g/l
Starch	ρ_s	175.0 g/l
α-amylase	ε_1	3.97×10^5 U/l
β-amylase	ε_2	1.21×10^6 U/l
Initial temperature	T_0	50 °C
Heater temperature	T_{aq}	75 °C
Malt-to-water ratio	r_g	4 l/kg
Flow velocity	v_z	0.015 m/min
Liquid column height	H_f	0.05m

et al. (1995). The table also shows the values of the initial temperature, heater temperature, malt-to-water ratio, flow velocity and liquid column height.

Some studies, such as Longsworth (1952) and Longsworth (1953), experimentally determined the diffusion coefficients for a series of amino acids, peptides and sugars in aqueous solution. Price *et al.* (2016) experimentally estimated the diffusion of sucrose in aqueous solution, while Bashkatov *et al.* (2003) estimated the diffusion coefficient of glucose in human tissue, providing reference values for the diffusion coefficient of glucose in water. These works were used as a reference to estimate the value of the diffusion coefficients of carbohydrates and enzymes in the model, so that the value used in the numerical solution was 10^{-8} m^{2}min^{-1} for carbohydrates and 10^{-9} m^{2}min^{-1} for enzymes, the same order of magnitude presented in the cited studies, adjusted in order to make the units compatible.

Using the finite element method, the spatial discretization of the previously presented transport equations were implemented in the Wolfram Mathematica software, using numerical values for the parameters and initial values for Kymppi malt.

The model takes into account wort recirculation and temperature ramp as boundary condition at the inlet. Inlet temperature variation is shown in figure 1.

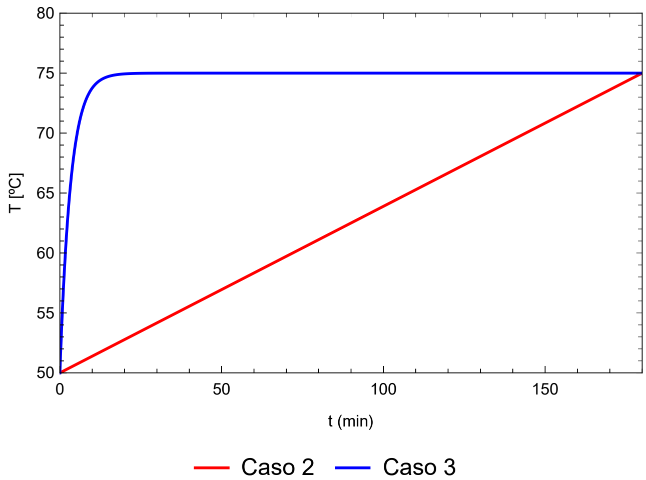

Figure 1. Inlet temperature as a function of mashing duration.

As a preliminary analysis, the convective heat transfer coefficients $\hat{h}_{out}$ and h_e are considered null in all cases, and the fraction of non-gelatinized starch $u(T)$ is also null in cases where temperature transient appear. Despite being null, the code was written including these parameters in the model. Numerical integration over time is performed using NDSolve function, to solve the coupled equation system and find the values of discrete temperatures and concentrations at each mesh node as a function of time, using default values of function option.

3.0.1 Temperature

The average temperature and temperature profile that develops at the outlet of the control volume as a function of time are shown in figure 2, where it can be seen that the inlet temperature in this case increases slowly.

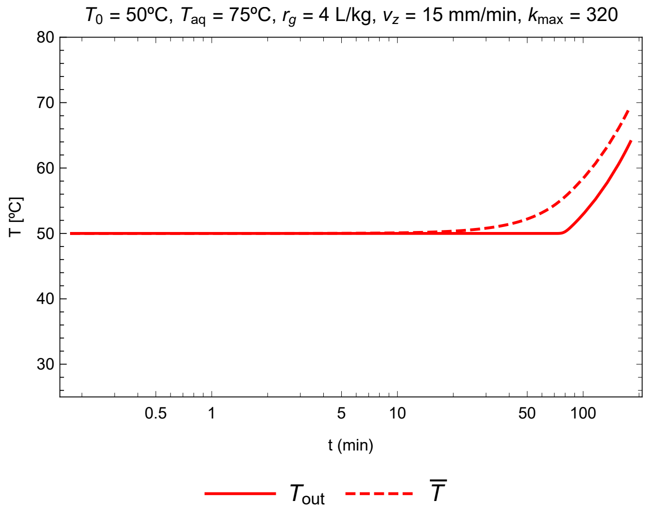

Figure 2. Outlet temperature and average temperature as function of mashing duration.

In addition to the results evaluating the average of the properties and at the outlet of the control volume, graphs were generated demonstrating the spatial variation of these quantities, allowing to follow the distribution of the variables in all points of the reactot. The figure 3 shows the temperature profile along the reactor at different times, verifying that the temperature varies linearly from the inlet.

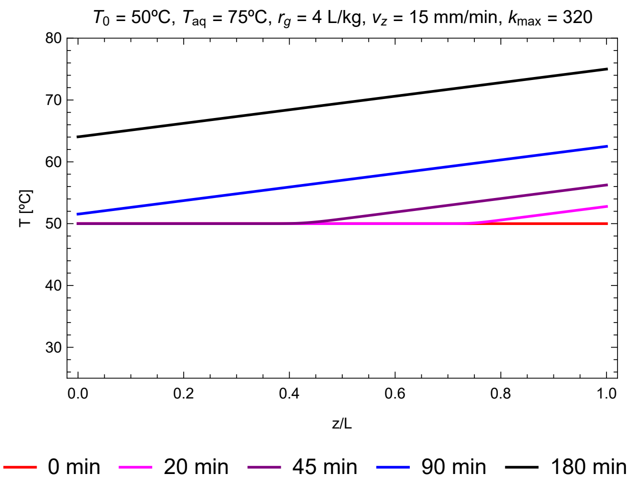

Figure 3. Spatial variation of temperature for different instants.

3.0.2 Concentrations

The figure 4 shows the average and outlet concentrations for carbohydrates as a function of mashing duration. The greatest contribution to the variation of carbohydrate concentration comes from the terms of production or consumption, the temperature gradients are initially very low, so that during a significant part of the time the control volume outlet is at the same temperature. As heat is transported and the outlet temperature reaches higher values, the effect of convective transport takes effect, but still showing low gradients. The effect of the recirculation of the species dissolved in the wort is observed, but its effect is reduced due to the low temperature gradient.

The concentration of enzymes in the solid fraction ($\varepsilon_{s,j}$) at the outlet of the mash vat decreases as the concentration of enzymes in the liquid phase increases (ε_j), according to the figure 6, due to the dissolution of the enzymes from the solid fraction to the liquid phase. It is important to note that very high temperatures will favor the denaturation of the enzymes. Activity reduction of dissolved enzymes is notably higher for β-amylase, due to the fact that β-amylase

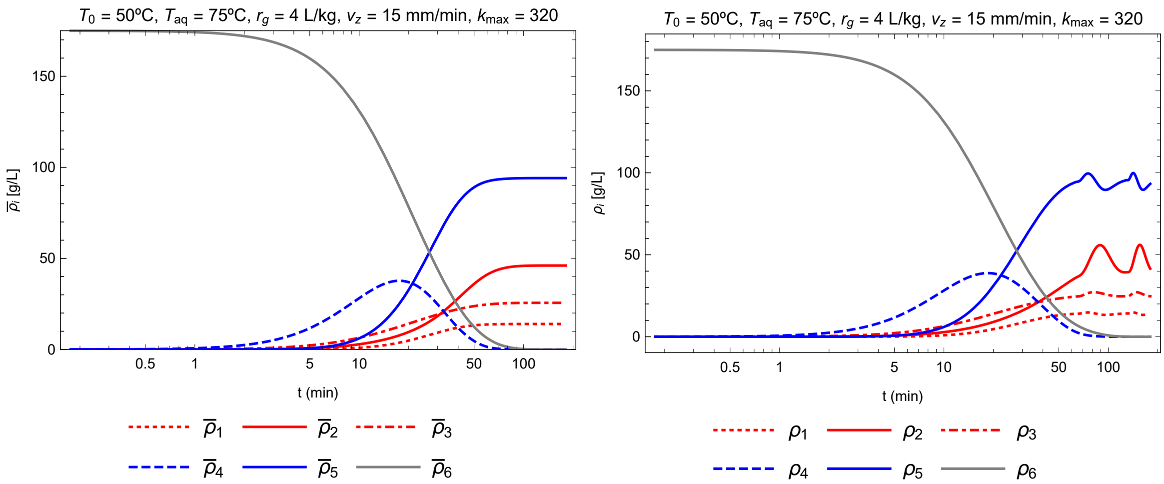

Figure 4. Average and outlet concentrations for carbohydrates as a function of mashing duration.

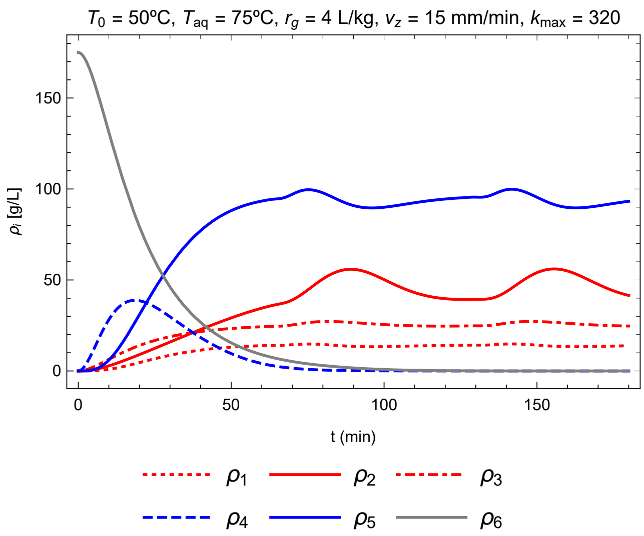

Figure 5. Outlet carbohydrate concentrations as a function of mashing duration, linear time scale.

undergoes degradation at temperatures below the denaturation temperature of α-amylase.

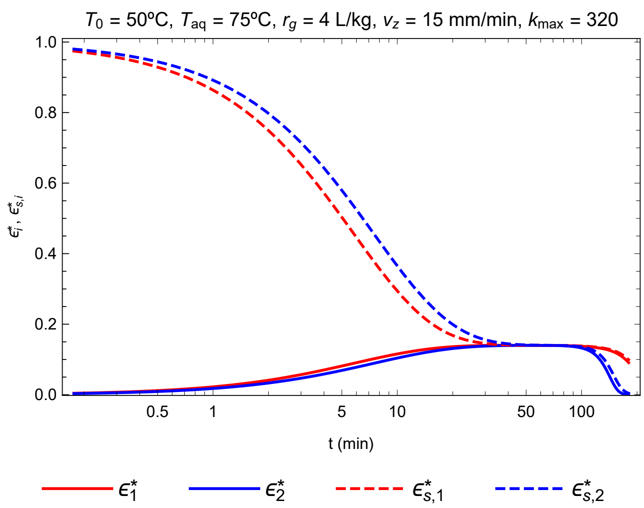

Figure 6. Outlet enzyme concentrations in solid ($\varepsilon_{s,j}$) and liquid (ε_j) fractions as a function of mashing duration.

4. SUMMARY AND CONCLUSIONS

The present study aimed to investigate the production of carbohydrates resulting from the hydrolysis of starch in mash recirculation systems. The work starts from the general conservation equations and uses chemical kinetic models from previous studies to improve the evaluation of the effect of heat and mass transfer by convection and diffusion on the concentration of starch, fermentable sugars and the enzymes that degrade these substances. It is important to note that the model was developed using data for typical recirculation systems and specific parameters for a particular type of malt. In a preliminary analysis, the results are obtained by applying the model to a system with recirculation, obtaining the temperature profile and the evolution of carbohydrate concentrations. The main objective of the model is, from this data, to assist in obtaining optimal periods and temperatures for the process that will lead to the highest possible production of extracts and, in addition, greater production of fermentable sugars to obtain better performance in later processes.

It is possible to infer from the analysis of the data that the most efficient temperature in terms of production of fermentable sugars is around 65°C, above this temperature, the production of extracts occurs more quickly, but part of this extract is composed of dextrins, which is not interesting for the subsequent fermentation process. In processes with temperatures below 65°C, incomplete gelatinization of the starch causes the production of extracts to be compromised.

In the case of recirculation processes, it is possible to understand how the temperature gradient is established, allowing the system to be dimensioned to reach a certain operating temperature range. The results of species conmcentrations allow the evaluation of the duration of the process necessary to reach the total conversion of starch in extracts, in addition to allowing the adjustment of parameters such as heater temperature, flow velocity, malt-to-water ratio, heat transfer coefficients, so that to evaluate their effect on the production of extracts. These data can be used in the design of recirculation systems, helping in their construction and operation, which can generate greater savings in both materials and energy.

5. ACKNOWLEDGEMENTS

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