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MODELING MASS TRANSFER THROUGH A POROUS MEDIUM OF A RECIRCULATING MASH SYSTEM

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Abstract. *This paper presents a model for analyzing mass transfer in the saccharification kinetics during the mashing of barley malt in a recirculating mash system. A cylindrical pipe is used to model the internal flow of wort through the grain bed, which is treated as a porous medium. A simple formulation for plug flow and advection in the axial direction are considered and tube wall is supposed to be adiabatic and impermeable. The model was adapted from a previous study to include the effect of convection mass transfer and involves mass balances for starch, dextrins, maltotriose, maltose and glucose, and also for $\alpha-$ and $\beta-$ amylase activities, which are responsible for starch hydrolysis. The model is solved by a technical computing tool in order to evaluate the performance of recirculating mash systems.*

Keywords: *brewing, mashing, convection, porous media*

NOMENCLATURE

Symbol	Definition
A_i	kinetic constants of the production of species i from starch by α-amylase , [l/min.g]
$A_{i,0}$	frequency factors for the conversion of starch into species i, [l/min.g]
B_i	kinetic constants of the production of species i by β-amylase, [l/min.g]
$B_{i,0}$	frequency factors for the conversion of dextrins into species i, [l/min.g]
$\mathcal{D}$	mass diffusivity, [m^2s^{-1}]
E_α	activation energy for α-amylase, [J/mol]
E_β	activation energy for β-amylase, [J/mol]
$E_{\alpha,d}$	denaturation energy for α-amylase, [J/mol]
$E_{\beta,d}$	denaturation energy for β-amylase, [J/mol]
$\dot{g}'''$	heat production per unit volume, [J/l.min]
H_α	dissolution coefficient corresponding to α-amylase, [l/g.min]
H_β	dissolution coefficient corresponding to β-amylase, [l/g.min]
k	thermal conductivity, [W/m.K]
k_m	Michaelis constant for production of maltose from dextrins, [g/l]
k_α	kinetic constant of denaturation of α-amylase, [min^{-1}]
k_β	kinetic constant of denaturation of β-amylase, [min^{-1}]
$k_{\alpha,0}$	frequency factor for the denaturation of α-amylase, [min^{-1}]
$k_{\beta,0}$	frequency factor for the denaturation of β-amylase, [min^{-1}]
M	initial amount of malt, [g]
R	gas constant, [8.3143 J/mol.K]
t	time, [min]
T	temperature, [K]
u	mass fraction of ungelatinized starch
V	volume of the liquid phase of the mash, [l]
V_g	volume of the wet mash, [l]
$\mathbf{V}_{avg}$	intrinsic average velocity, [m/min]

v	seepage velocity, [m/min]
x_i	mass concentration of species i, [g/l]
$\dot{x}_i$	rate of production of species i
α	α-amylase activity, [U/l]
$\dot{\alpha}$	rate of production of α-amylase
β	β-amylase activity, [U/l]
$\dot{\beta}$	rate of production of β-amylase
φ	porosity of porous medium
Subscripts	**Definition**
b	porous bed
f	fluid
g	in grain
l	in liquid solution
s	solid portion of porous medium

1. INTRODUCTION

Brewing consists basically of the following stages: grain milling, mashing, lautering (or clarification), boiling, whirlpool, cooling, fermentation and conditioning, filtration and packaging. In the mashing phase, the milled barley malt added to a vessel (the mash tun) with water at a sufficiently high temperature, which results in the activation of the malt enzymes, thus promoting the conversion of starch into fermentable sugars. This phase is followed by a lautering phase, in which the wort produced in mashing is separated from grains and any suspended material. This is usually performed on a separate vessel (the lauter tun), in which the porous bed formed by the remaining solid material (mostly grain peels) acts as a filtering medium through which the wort is made to flow. In more compact systems, which can be common in smaller micro-breweries, these two processes are done in the same vessel, and in many time in parallel. This configuration is commonly called a recirculating mash system: an automated system in which the wort is constantly recirculated through the grain bed, and temperature control is usually done on the wort leaving the porous bed prior to being recirculated. There are two main ways to heat the wort, both using a pump for recirculating: there is the Recirculation Infusion Mash System (RIMS), that recirculates the wort over an electric heating element and there is the Heat Exchange Recirculating Mash System (HERMS),that recirculates the wort through a heat exchanger, usually in the form of a coiled metal tube inside a vessel of hot water. The main benefits of using a recirculating system are precise control of the mash temperature instead of relying on the mash tun's insulation, which leads to improved repeatability in the process and the possibility to perform complex mash schedules. Because these systems are increasingly being used in smaller commercial breweries and home brewers, it is important to know how the enzymatic reactions will occur in this type of system.

When a simple mash system (with no flow through the porous bed), a few models are seen in the literature. Koljonen *et al.* (1995), developed a model describing the hydrolysis of starch in mashing, where mass balance for enzymes that degrade starch (α and β amylases), and mass balances for carbohydrates (starch, dextrins, glucose, maltose, and maltotriose) are presented. Quintanilha *et al.* (2015) adapted the (Koljonen *et al.*, 1995) model to study the effect of a variable temperature on the saccharification of barley malt and performed a parametric analysis to demonstrate the evolution of different species concentrations for different temperature and mashing times. Later on, Zamboni *et al.* (2017) presented a simple heat conduction analysis during the production of wort in a cylindrical vessel, adapting study (Quintanilha *et al.*, 2015) to include the effect of heat diffusion and investigate how different vapor jacket temperatures affect the mash temperature profile and consequently the enzymatic reaction, starch breakdown, and fermentable sugars concentrations. This paper presents an extension of the model used by Koljonen *et al.* (1995) to include the effects of wort flowing through the porous grain bed during mashing.

2. PROBLEM FORMULATION

The problem considered in this study is that of mass transfer in a reacting system flowing through a porous bed, as depicted in figure 1. Among the simplifying assumptions adopted to elaborate the model are: symmetry around the z-axis; isothermal operation; adiabatic outer walls; one-dimensional uniform flow over the cross section of the vessel; negligible mass diffusion; homogeneous and isotropic porous medium; Dupuit-Forchheimer relationship between seepage velocity and intrinsic average velocity.

2.1 Chemical kinetics

The chemical kinetic model developed by Koljonen *et al.* (1995) is considered in this study, to model starch degradation, as illustrated in figure 2. The enzymes dissolve from grist to wort and the enzymatic conversions take place by the action of dissolved enzymes. Starch when heated in contact with water undergoes gelatinization, which consists of the

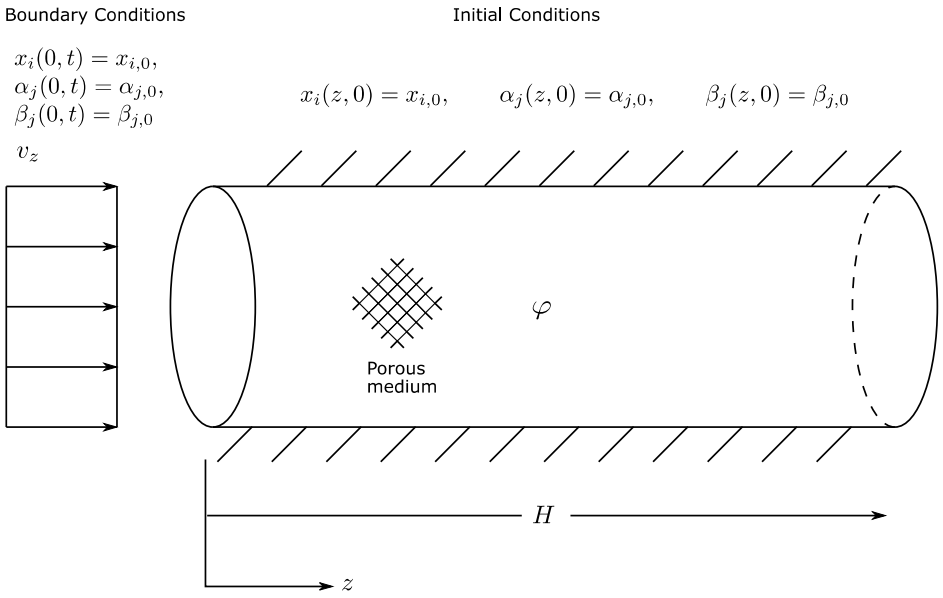

Figure 1. Problem Diagram.

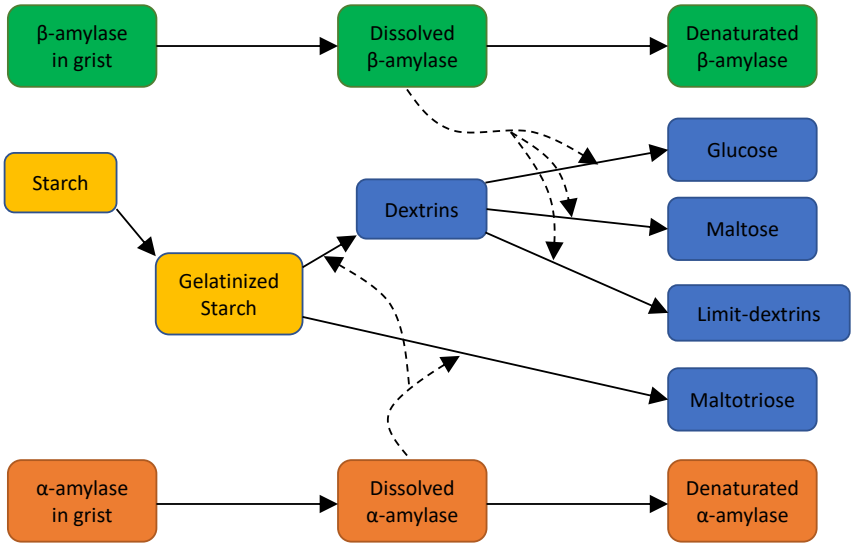

Figure 2. Schematic representation of the reactions included in the model. Solid lines represent mass flow, dashed lines represent the actions of enzymes.

expansion of the granules that constitute it, causing swelling of the granules, 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 to sugars and limit-dextrins by the action of dissolved β-amylase.

Starch is converted to maltotriose (x_5) and dextrins (x_2) by the action of α-amylase, thus the rate of production of starch is given by:

$$\dot{x}_1(t) = -\alpha_l\,(\gamma_5\,A_5 + A_2)(x_1 - x_1^0\,u(T)), \tag{1}$$

where the coefficient γ_5 corresponds to the mass fraction of starch consumed ($\gamma_5 = 27/28$) per mass of maltotriose produced. Dextrin is converted to glucose (x_3), maltose (x_4) and limit-dextrins (x_6) by β-amylase enzyme, thus the rate of production of dextrins is written as:

$$\dot{x}_2(t) = \alpha_l\,A_2\,(x_1 - x_1^0\,u(T)) - \beta_l\,x_2\,(\gamma_3\,B_3 + \gamma_4\,\frac{B_4}{k_m + x_2} + B_6), \tag{2}$$

where the coefficients $\gamma_3 = 9/10$ and $\gamma_4 = 18/19$ corresponds to the mass fractions of dextrin consumed as glucose and maltose are produced. The rate of production of glucose glucose (x_3), maltose (x_4), maltotriose (x_5) and limit-dextrins (x_6) are written as:

$$\dot{x}_3(t) = B_3\,\beta_l\,x_2, \tag{3}$$
$$\dot{x}_4(t) = B_4\,\beta_l\,\frac{x_2}{k_m + x_2}, \tag{4}$$
$$\dot{x}_5(t) = A_5\,\alpha_l\,(x_1 - x_1^0\,u(T)), \tag{5}$$
$$\dot{x}_6(t) = B_6\,\beta_l\,x_2. \tag{6}$$

The fact that starch needs to be gelatinized prior to its breakdown is included in the equations by introducing the quantity u, which represents the mass fraction of ungelatinized starch. This function is defined as:

$$u(T) = \begin{cases} 1, & T \le T_u \\ (T_g - T)^2(3T_u - T_g - 2T)/(T_u - T_g)^3, & T_u < T < T_g \\ 0, & T \ge T_g \end{cases} \tag{7}$$

In the model, starch is assumed to be gelatinized gradually so that at lower temperatures than T_u, all starch is ungelatinized, between T_u and T_g the proportion of gelatinized starch increases linearly until, at temperatures higher than T_g, all the starch is assumed to be gelatinized.

The enzymes contained in the grains are dissolved in the liquid phase, where they are denatured at a rate that depends on temperature. In this process, the rates of production of each enzyme in the liquid phase is given by:

$$\dot{\alpha}_l(t) = -\frac{k_\alpha}{V}\,\alpha_l, \tag{8}$$
$$\dot{\beta}_l(t) = -\frac{k_\beta}{V}\,\beta_l, \tag{9}$$

where α_l and β_l are enzyme concentrations dissolved in the liquid phase, which are given in terms of activity (U/s).

The coefficients k_α, k_β, A_i and B_i which represent the maximum specific rates of enzyme destruction and enzymatic conversions respectively are given by:

$$A_2 = A_{2,0}\,\exp\left(-E_\alpha/(RT)\right) \tag{10}$$
$$A_5 = A_{5,0}\,\exp\left(-E_\alpha/(RT)\right) \tag{11}$$
$$B_3 = B_{3,0}\,\exp\left(-E_\beta/(RT)\right) \tag{12}$$
$$B_4 = B_{4,0}\,\exp\left(-E_\beta/(RT)\right) \tag{13}$$
$$B_6 = B_{6,0}\,\exp\left(-E_\beta/(RT)\right) \tag{14}$$
$$k_\alpha = k_{\alpha,0}\,\exp\left(-E_{\alpha,d}/(RT)\right) \tag{15}$$
$$k_\beta = k_{\beta,0}\,\exp\left(-E_{\beta,d}/(RT)\right) \tag{16}$$

2.2 Mass transfer

Considering an isotropic medium, mass transport in the porous medium is written as a convection-diffusion equation for a general species i:

$$\frac{\partial x_i}{\partial t} + v_z\,\frac{\partial x_i}{\partial z} = \mathcal{D}_i\,\frac{\partial^2 x_i}{\partial z^2} + \dot{x}_i, \tag{17}$$

for $i = 1, \ldots, 5$. For the enzymes the mass transport equations are given by:

$$\frac{\partial \alpha_g}{\partial t} + v_z\,\frac{\partial \alpha_g}{\partial z} = -\frac{H_\alpha\,M}{V_g}\,(\alpha_g - \alpha_l) + \mathcal{D}_{\alpha_g}\,\frac{\partial^2 \alpha_g}{\partial z^2}, \tag{18}$$
$$\frac{\partial \beta_g}{\partial t} + v_z\,\frac{\partial \beta_g}{\partial z} = -\frac{H_\beta\,M}{V_g}\,(\beta_g - \beta_l) + \mathcal{D}_{\beta_g}\,\frac{\partial^2 \beta_g}{\partial z^2}, \tag{19}$$
$$\frac{\partial \alpha_l}{\partial t} + v_z\,\frac{\partial \alpha_l}{\partial z} = \frac{H_\alpha\,M}{V}\,(\alpha_g - \alpha_l) + \mathcal{D}_{\alpha_l}\,\frac{\partial^2 \alpha_l}{\partial z^2} + \dot{\alpha}_l(t), \tag{20}$$
$$\frac{\partial \beta_l}{\partial t} + v_z\,\frac{\partial \beta_l}{\partial z} = \frac{H_\beta\,M}{V}\,(\beta_g - \beta_l) + \mathcal{D}_{\beta_l}\,\frac{\partial^2 \beta_l}{\partial z^2} + \dot{\beta}_l(t), \tag{21}$$

where α_g and β_g are enzyme concentrations in the wet malt, also given in terms of activity (U/s). Although diffusion is included in the previous equations, for this investigation it is considered negligible. The boundary and initial conditions are given by:

$$x_i(0,t) = x_{i,0}, \qquad \alpha_j(0,t) = \alpha_{j,0}, \qquad \beta_j(0,t) = \beta_{j,0}, \tag{22}$$

$$x_i(z,0) = x_{i,0}, \qquad \alpha_j(z,0) = \alpha_{j,0}, \qquad \beta_j(z,0) = \beta_{j,0}, \tag{23}$$

for $i = 1, \ldots, 5$ and $j = l, g$. The initial condition assume that the all carbohydrates concentrations are uniform, as given by $x_{i,0}$, as are the enzymes' concentrations, as given by $\alpha_{j,0}$ and $\beta_{j,0}$. The term v_z is seepage velocity, related to v_{avg} (intrinsic average velocity) by the Dupuit-Forchheimer relationship $v_z = \varphi\, v_{avg}$.

3. RESULTS AND DISCUSSION

The the presented equations are then solved using the Wolfram Mathematica function NDSolve for solving non-linear coupled PDE systems. The adopted solution options employed mostly automatic settings, and modifying two solution parameters: MaxStepFraction is set to 1/100, and MaxStepSize is set to 1/10. The numerical values for the parameters and initial values for Kymppi malt employed in the solution are given in table 1.

Table 1. Parameters values used in simulations.

$x_{1,0}$	112.1 g/l	$x_{2,0}$	20.6 g/l	$x_{3,0}$	5.1 g/l
$x_{4,0}$	10.3 g/l	$x_{5,0}$	0.0 g/l	$x_{6,0}$	0.0 g/l
V	0.2 l	M	50 g	k_m	2.8 g/l
$A_{2,0}$	3.77×10^{10} l/min/g	$A_{5,0}$	6.42×10^{10} l/min/g	$B_{3,0}$	1.62×10^{40} l/min/g
$B_{4,0}$	1.05×10^{42} l/min/g	$B_{6,0}$	1.09×10^{41} l/min/g		
$\alpha_{g,0}$	3.97×10^{5} U/l	$\beta_{g,0}$	1.21×10^{6} U/l		
E_α	1.03×10^{5} J/mol	E_β	2.93×10^{5} J/mol		
$E_{\alpha,d}$	2.377×10^{5} J/mol	$E_{\beta,d}$	4.439×10^{5} J/mol		
$k_{\alpha,0}$	3.86×10^{34} min^{-1}	$k_{\beta,0}$	9.46×10^{67} min^{-1}		
H_α	9.72×10^{-5} l/g/min	H_β	7.57×10^{-5} l/g/min		
T_g	336.5 K	T_u	315.4 K		

Figure 3 presents the concentration distribution in the mash vessel for different mash times. As can be seen, in initial mash times the concentration of starch decreases almost uniformly throughout the vessel, as the production of carbohydrates resulting from the conversion of starch increases. However, near the vessel inlet the concentration profile along the length is different from the rest, due to unconverted wort being injected at $z = 0$. The decrease in starch concentration and increase in carbohydrate concentration that occurs almost uniformly in this initial period is due to the rate of production species component (term $\dot{x}_i$). When examining the temporal evolution of the concentration, one can note that, as expected, most of the starch is converted into extracts. However, the effect of the advection component in equation (17), becomes is evident in the figures, as the uniformly concentrated zone progresses towards the vessel outlet. At the same time that starch is transported by advection, it is consumed by the action of enzymes and converted. The process that occurs with carbohydrates is analogous to advection (mass transport in the z direction, verified by unevenly decrease in the concentration) but different from starch, the concentration outside the influence zone of advective transport increases, because the starch is just being converted into carbohydrates.

Next, figure 4 displays outlet concentrations for different mash times. As one can observe, for shorter vessel lengths, although initially the concentration of fermentable sugars increases as the conversion of starch occurs, the effect of advective transport is felt earlier soon at the outlet of the vessel, and the concentration of species becomes constant over time. It is evident from this data that for longer vessels, advective transport takes longer to have an effect on the vessel outlet, allowing higher conversion rate by the action of the enzymes. This effect would also be achieved in a shorter vessel if the flow velocity were to be increased.

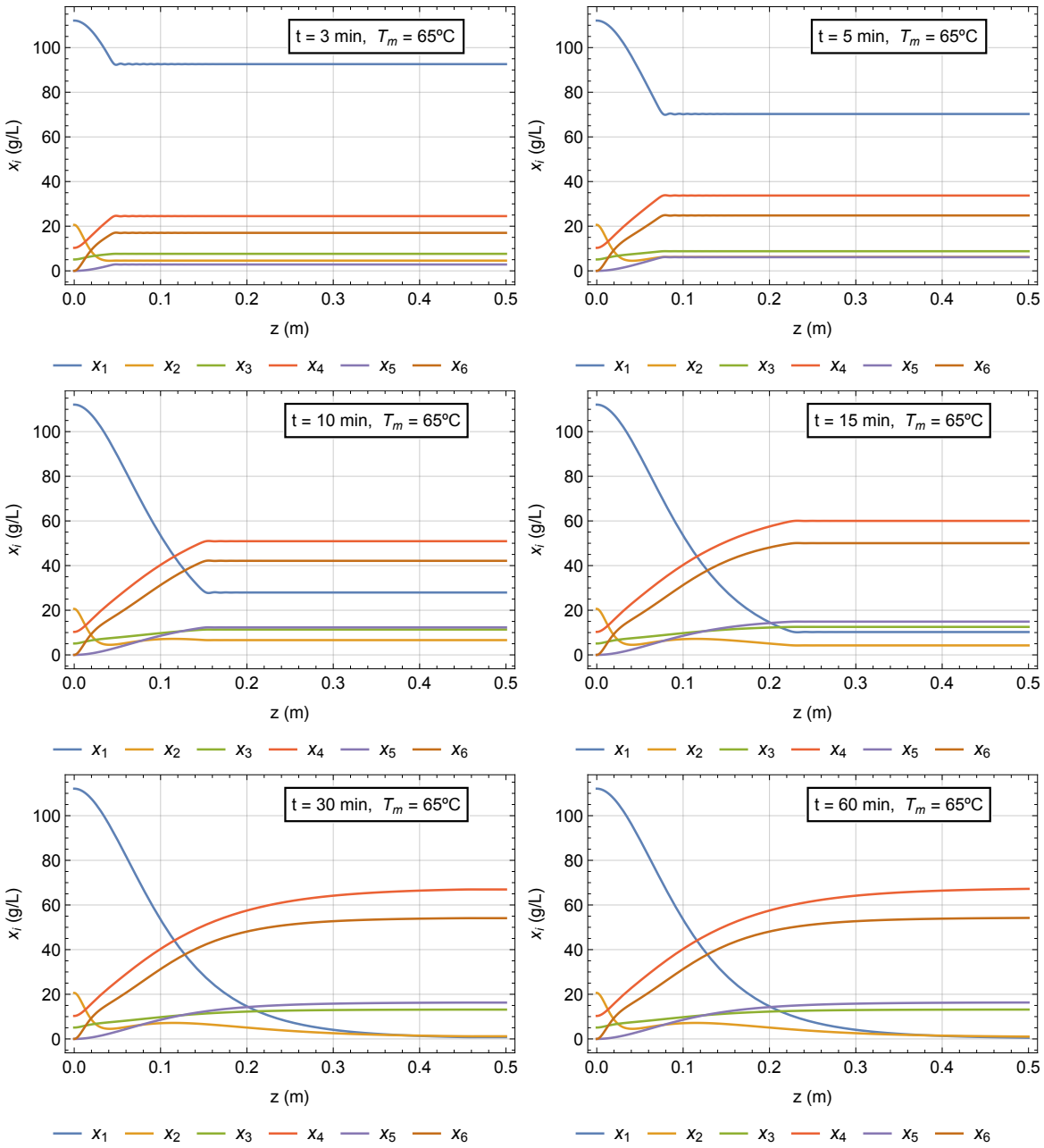

Figure 3. Concentration distribution in mashing vessel for different mash times

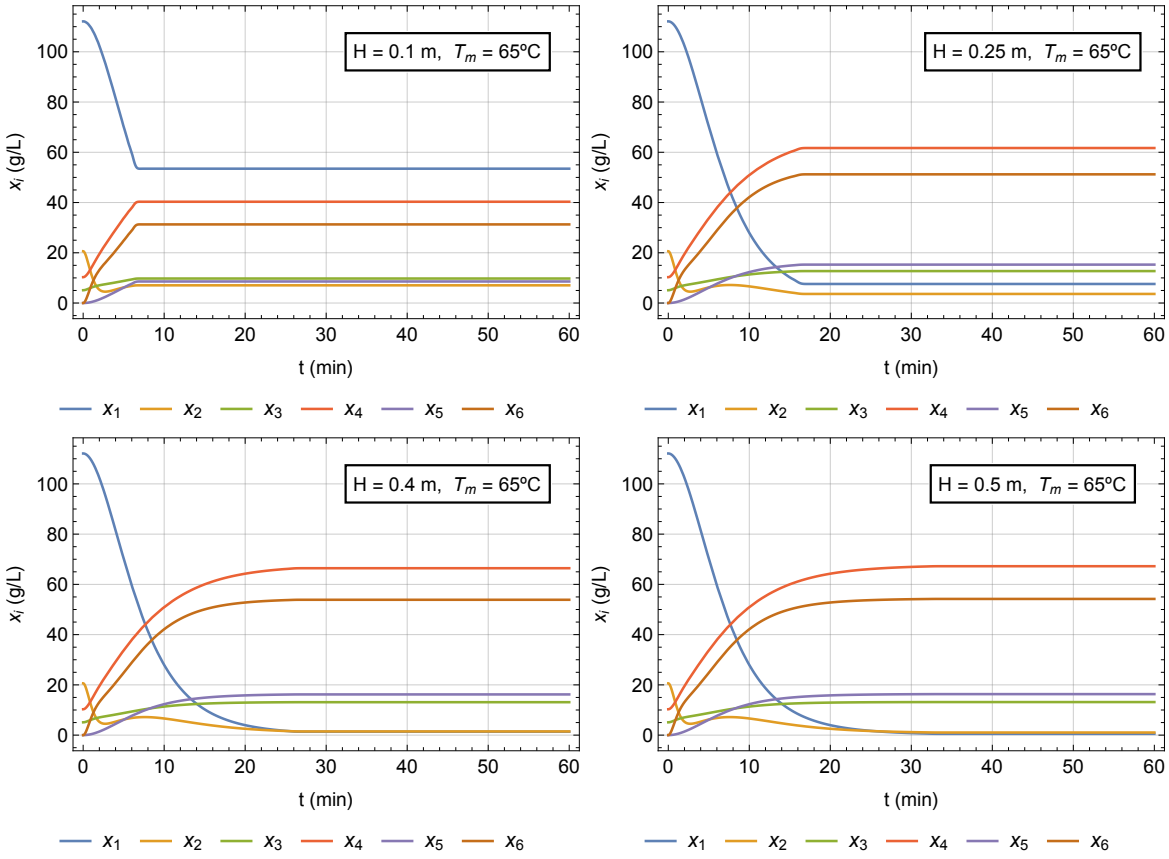

Figure 4. Outlet concentration for different mash vessel length (H)

4. SUMMARY AND CONCLUSIONS

This paper presented a study of mass transfer in a recirculating mash system. The model was adapted from a previous study to include the effect of advective mass transfer in the species concentration (starch, fermentable sugars and the enzymes that degrade these substances). Temperature is considered constant through the mash and the grain bed is treated as porous medium. The set of transport equations numerically solved using model parameters experimentally estimated in a previous study for a given malt variety. First, the concentration profile is analyzed for different mash times, where it was possible to notice the effect of the advective portion on mass transfer along the vessel length. With these results it is possible to predict optimal duration of a mashing process, avoiding short periods of mashing, which could lead to incomplete starch conversion and inefficient wort production. Finally, the species concentration is investigated at the outlet of the vessel for different lengths. This result allows the selection of optimal vessel lengths and/or wort flow-rate, which naturally influences the effect of the advective mass transfer.

5. ACKNOWLEDGEMENTS

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