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MODELING AND MATHEMATICAL ANALYSIS OF MASS TRANSFER IN POROUS MEDIA IN LAUTERING PROCESSES

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Abstract. *Lautering is a crucial filtration step in brewing, since it is directly related to the product quality and production efficiency. Hence, this paper proposes the development of a simplified model which describes the mass transfer analysis for different operation conditions. Under this scenario, the problem was described using the linear transient one-dimensional advection-diffusion equation with both Neumann and Dirichlet boundary conditions and a well-defined initial condition. To approximate the mathematical formulation from the physical model, the linear Freundlich isotherm was applied to represent the additional sugar extraction from the barley malts, also defined as retardation function. The governing equation was numerically solved using a traditional discretization-based procedure with central and upwind-differencing schemes for the advection term. The method of lines (MOL) was applied through computational implementations which aimed at developing a code under a Finite-Differences framework capable of performing different numerical simulations. The code was validated with the literature showing a good agreement. A mesh convergence analysis was performed and the results were computed using a non-uniform mesh, which showed a good performance to represent lautering processes for low Péclet numbers. Numerical simulations were calculated for different retardations and Péclet numbers in order to demonstrate the influence of these variables in process. The outcome shows that the technique introduced in this work is easy to apply and has a great performance for the proposed model.*

Keywords: *Advection-Diffusion Problems, Lautering, Porous Media, Method of Lines, Finite Difference Method*

NOMENCLATURE

c	solute concentration of the liquid phase	s	solid phase (grain bed) solute concentration
c_{sat}	saturation concentration of the liquid phase	K_g	partition coefficient
c^*	dimensionless concentration of the liquid phase	ρ_g	grain bed density
t	time	θ	volumetric water content
τ	dimensionless time	R_g	retardation function
v	velocity	Pe	Péclet number
x	axial coordinate	CFD	Computational Fluid Dynamics
L	domain length		
ξ	dimensionless axial coordinate		
D	diffusion coefficient		

1. INTRODUCTION

The concepts of transport phenomena have been proven to be effective in mass transfer analysis. According to Bird *et al.* (2002) the similarities in occurrence of the governing equations enable the application of very similar mathematical frameworks. This allows the understanding of connection between all transport mechanisms since they are ruled by the constitutive equations and the conservation laws. Some of these principles have already been used to describe chemical processes in membrane distillation presented by Kimura *et al.* (1987), biological systems introduced by Truskey *et al.* (2004) and the basics concepts in food engineering to simulate and design the food preservation processes as shown by Welti-Chanes *et al.* (2005).

The brewing process aims at producing a sweet liquid, also referred to as wort, through solubilization of several compounds present in grains into hot water. Lautering, also known as clarification, is a crucial step in brewing. It directly affects the production efficiency and beer quality as shown by Kühbeck *et al.* (2006); Schneider *et al.* (2005); Bühler (1996). Thus, the development of a model which might properly describe the physical phenomenon is essential to improve the results also exposed by Walsh (2013) using CFD analysis. This operation is based on a solid-liquid separation in which the wort is filtered from the residual husks through the formation of a grain bed that enables a flow in porous

media. Several physical parameters affect the porosity and wort viscosity as indicated by Webster (1981); Bühler *et al.* (1996); Schneider and Weisser (2004); Muller (2000). Another important factor refers to the fact that is a very time and energy consuming process which allows the development of different lautering systems, for example, using nitrogen bubble generator in the lauter tun presented by Tippmann *et al.* (2010).

In this paper, the lautering processes are described using the linear transient one-dimensional advection-diffusion equation. Most physical problems in mass transport are governed by advection and diffusion terms. Both fully analytical and numerical solutions can be easily found in literature Chalhub *et al.* (2011); Mojtabi and Deville (2015); Benton and Platzman (1972); Pandey *et al.* (2009) as well numerous forms to describe the mathematical formulation, each one with inherent characteristics for different types of application. Nevertheless, the implementation of traditional discretization-based numerical methods is a dare assignment for solving the advection-diffusion equation. Under this scenario, it is emphasized the relevance of Péclet number and its influence in partial differential equation form through the non-dissipative and dissipative components. For small Péclet numbers the governing equation turns into a diffusion-dominated process in parabolic or elliptic form, on the other hand, for high Péclet numbers it turns into a advection-dominated problem in hyperbolic form as shown by Huysmans and Dassargues (2004). The numerical solution of the advection-diffusion equation is still a hard task thanks to the numerical diffusion that happens when the transport process occurs on a smaller scale than the applied discretization and the numerical instability. Numerical diffusion in some cases may be higher than real diffusion generating mistaken results. While the instability involves large gradients which produce oscillatory results. Then, in order to obtain the numerical solution of the governing equation of this model, it must remain fully aware of the fact that each numerical scheme has its own limitations. In this regard, in this paper were applied the concepts of convergence, order of accuracy and numerical precision.

The literature presents several forms for solving the one-dimensional advection diffusion equation, however in this paper it was applied in order to evaluate the physical effects of the Péclet number in lautering processes. A simplified model was described considering the Freundlich isotherm as a source term in which the concentration only increase up to 20% more than the original potential extraction. Chemical reactions and temperature effects are not included in the mathematical formulation. Numerical schemes are approximated using Finite-Differences in order to obtain the same results found by Mojtabi and Deville (2015) to validate the code. The simulations aimed at demonstrating the influence of Péclet number in the production efficiency.

2. PROBLEM FORMULATION

The mass transfer in porous media in lautering processes occurs in lauter tun, a traditional vessel used for separation of wort from the milled barley malts, as represented in Figure 1. The mathematical formulation is described by a conventional equation used to linear transient advection-diffusion problems in one-dimensional form, also called Burger's equation, as given below:

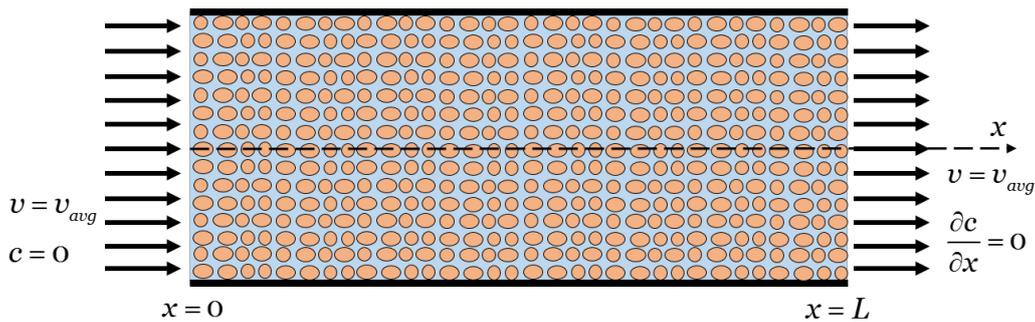


Figure 1. Lautering scheme

$$\frac{\partial c(x, t)}{\partial t} + \frac{\rho_g}{\theta} \frac{\partial s(x, t)}{\partial t} = D \frac{\partial^2 c(x, t)}{\partial x^2} - v \frac{\partial c(x, t)}{\partial x} \quad \text{for} \quad 0 \leq x \leq L \quad \text{and} \quad t \geq 0 \quad (1)$$

$$c(x, 0) = c_{sat} \quad \text{for} \quad 0 < x < L \quad (2)$$

$$c(0, t) = 0 \quad \text{for} \quad t > 0 \quad (3)$$

$$\left(\frac{\partial c}{\partial x} \right)_{x=L} = 0 \quad \text{for} \quad t > 0 \quad (4)$$

Equation (1) is used for simulating the variation of the solute concentration c in the water. The second term represents a source which symbolizes the additional extraction of residual sugars inside the barley malts during the cake washing. For this purpose, it's necessary a sorption model in order to describe correctly this increase of sugar concentration during the process. Brusseau *et al.* (1989) presented good results using the linear Freundlich equation, an important isotherm

most commonly used in groundwater contamination studies, as given below:

$$s = K_p c^N \quad (5)$$

In this work, the model is developed considering the simplest and linear form (N=1). Differentiating (5) with respect to time yields

$$\frac{\partial s}{\partial t} = K_p \frac{\partial c}{\partial t} \quad (6a)$$

Applying the following dimensionless retardation function in the original equation which according to Moltyaner and Champ (1987) is derived from column dynamic experiments:

$$R_g = \left(1 + K_p \frac{\rho_g}{\theta}\right) \quad (7a)$$

In this paper, the barley malts have an original extraction potential of approximately 80%. Thus, the term R_g represents the additional extraction that will occur during the grain bed washing, being able to increase the concentration up to 20%. The term K_p , the partition coefficient, is defined by the ratio of the sugar concentration in the mixture of two immiscible phases at equilibrium: the husks and grain bed. The grain bed density, ρ_g , depends on the degree of porous medium compaction. It is defined as the mass of many particles of the material divided by the total volume they occupy. Then, there is an inversely relation to the porosity: the more pore space in the grain bed the lower the value for bulk density. The term θ represents the quantity of water contained in the lauter tun. The volumetric water content, partition coefficient and grain bed density are defined mathematically by the following relations:

$$\rho_g = \frac{M_{\text{grains}}}{V_{\text{total}}}, \quad K_p = \frac{c_{\text{husks}}}{c_{\text{gb}}}, \quad \theta = \frac{V_{\text{water}}}{V_{\text{grains}}} \quad (8a)$$

Using the dimensionless variables and parameters as given below :

$$c^* = \frac{c}{c_{\text{sat}}}, \quad \xi = \frac{x}{L}, \quad \tau = \frac{t}{t_0}, \quad t_0 = \frac{L}{v_{\text{avg}}}, \quad \text{Pe} = \frac{v_{\text{avg}} L}{D} \quad (9a)$$

Thus, the dimensionless transformation leads to:

$$\frac{\partial c^*}{\partial \tau} = \frac{1}{R_g \text{Pe}} \frac{\partial^2 c^*}{\partial \xi^2} - \frac{1}{R_g} \frac{\partial c^*}{\partial \xi}, \quad \text{in } 0 \leq \xi \leq 1 \quad \text{for } \tau \geq 0 \quad (10)$$

Applying the following homogeneous boundary conditions in Eq. (10) as given below

$$c^*(0, \tau) = 0, \quad \text{for } \tau > 0 \quad \text{Homogeneous Dirichlet} \quad (10a)$$

$$\left. \frac{\partial c^*}{\partial \xi} \right|_{\xi=L} = 0, \quad \text{for } \tau > 0 \quad \text{Homogeneous Neumann} \quad (10b)$$

and the initial condition is given by

$$c^*(\xi, 0) = 1, \quad \text{for } 0 \leq \xi \leq 1 \quad (10c)$$

The Dirichlet boundary was applied to ensure that the interface between incoming water and wort remains with the concentration equal to zero. Low diffusion coefficients strongly contribute for the physical occurrence of this condition. Neumann boundary was defined in order to guarantee there is no aqueous flux in contour. The initial condition represents the equilibrium state in the beginning of the process when sugar concentration in solution is equal at any point in lauter tun. Over time, the addition of water through cake washing declines the concentration of sugar.

3. FINITE DIFFERENCES METHOD

The following second-order central-differencing and first-order upwind-differencing schemes were used to solve the studied problem via finite differences, the second one when applied in the advective term introduces severe numerical diffusion/dissipation in the solution where large gradients exist eliminating the Gibbs phenomenon. The adopted approximations are described below:

- For $i = 1$:
 $c(0, \tau) = 0$ Homogeneous Dirichlet Boundary Condition

- For $2 \leq i \leq i_{max-1}$:

$$\frac{\partial c_i}{\partial t} \approx \frac{1}{R_g Pe} \frac{c_{i+1}^t - 2c_i^t + c_{i-1}^t}{\Delta x^2} - \frac{1}{R_g} \frac{c_i^t - c_{i-1}^t}{\Delta x}$$

- For $i = i_{max}$:

$$\frac{\partial c_i}{\partial t} \approx \frac{2}{R_g Pe} \frac{c_{i-1}^t - c_i^t}{\Delta x^2} \quad \text{Homogeneous Neumann Boundary Condition}$$

Time step was discretized using the Mathematica **NDSolve** function.

4. RESULTS AND DISCUSSION

In order to guarantee the accuracy of the results, the code framework used in this paper was compared with another article present in literature. Despite of using the same governing equation, Mojtabi and Deville (2015) solved the linear transient one-dimensional advection–diffusion equation with Dirichlet homogeneous boundary conditions and a smooth initial sine function using separation of variables and finite element methods. Hence, these conditions were applied in the code under central-differencing schemes to evaluate the numerical results and reliability. The outcomes are shown in Tables 1, 2.

Table 1. Comparison profiles for $c(0.7 \leq x \leq 1, \tau = 1.0)$, $c(x, 0) = \sin 2\pi x$, $Pe = 40 \pi, 400, 4000$.

ξ	$Pe = 40 \pi, R_g = 2$		$Pe = 400, R_g = 2$		$Pe = 4000, R_g = 2$	
	Numerical	Mojtabi	Numerical	Mojtabi	Numerical	Mojtabi
0.70	0.81506	0.81507	0.90526	0.90527	0.94637	0.94637
0.75	0.85502	0.85503	0.95185	0.95185	0.99507	0.99508
0.80	0.81285	0.81286	0.90526	0.90526	0.94637	0.94637
0.85	0.69142	0.69142	0.77006	0.77006	0.80503	0.80503
0.90	0.50234	0.5023	0.55948	0.55948	0.58489	0.58489
0.95	0.26459	0.26459	0.29413	0.29414	0.30749	0.30750
0.97	0.16383	0.16383	0.17836	0.17836	0.18645	0.18646
0.99	0.06893	0.06894	0.06086	0.06086	0.06248	0.06248
0.995	0.04116	0.04117	0.03394	0.03394	0.03125	0.03126
0.9995	0.00520	0.00521	0.00543	0.00544	0.00353	0.00355

It can easily be seen that the results found were very close, proving the framework is capable of performing this type of problem. The solution domain is $\{(x,t) : x \in [-1,1], t \in]0,T]\}$, in other words, the space is twice the one used in this paper. Then, to obtain the expected results the velocity was reduced by half. Mojtabi and Deville (2015) have solved the advection-diffusion in both analytical and numerical forms without sorption effects and considering the Reynolds number as main dimensionless parameter. Some implementations were carried out to adopt these conditions in the evaluated code of this paper.

Table 2. Comparison profiles for $c(0.95 \leq x \leq 1, \tau = 1.6)$, $Pe = 40 \pi, 400, 4000$.

ξ	$Pe = 40\pi, R_g = 2$		$Pe = 400, R_g = 2$		$Pe = 4000, R_g = 2$	
	Numerical	Mojtabi	Numerical	Mojtabi	Numerical	Mojtabi
0.95	0.65541	0.62300	0.74874	0.74874	0.80265	0.80265
0.97	0.68241	0.68241	0.81019	0.81004	0.86941	0.86941
0.98	0.65664	0.65665	0.83608	0.83652	0.89771	0.89771
0.99	0.51887	0.51887	0.84295	0.81925	0.92246	0.92246
0.995	0.33970	0.33970	0.74949	0.68929	0.93348	0.93348
0.9995	0.04440	0.04440	0.15772	0.22293	0.82012	0.81478

The mesh convergence was performed in two different operation conditions. The first one, shown in Table 3, evaluates the rate of convergence considering $Pe = 10$ and the second one, according to Table 4, shows the rate considering $Pe = 50000$. The presentation of these two different results in a comparative way aims at establishing the influence of Péclet number in rate of convergence in studied mesh. Since the primary objective of this paper is recognize the physical influence of Péclet number in lautering processes, several simulations were performed to ensure the best outcomes for properly precision. Firstly, cases were carried out for low Péclet numbers. This can be physically described as a process with high diffusion coefficient and/or low flow velocity. As both advective and diffusive terms act in the governing

equation, the concentration gradients along domain are smooth. In Table 3, since there are low concentration gradients, the method presented great performance in mesh convergence analysis and consequently it is indicated to describe the sugar profiles in studied domain.

Table 3. Mesh Convergence Analysis - Case 1

N	Pe = 10, $R_g = 1.09$, $\tau = 1$, ξ								
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
1001	0.004401	0.013561	0.029990	0.056473	0.095564	0.14883	0.215585	0.291019	0.362168
2001	0.004369	0.013478	0.029852	0.056295	0.095380	0.148668	0.215499	0.291085	0.362435
3001	0.004358	0.013451	0.029806	0.056236	0.095318	0.148613	0.21547	0.291107	0.362524
4001	0.004353	0.013437	0.029783	0.056206	0.095287	0.148586	0.215455	0.291118	0.362569
5001	0.004350	0.013429	0.029769	0.056188	0.095269	0.14857	0.215447	0.291125	0.362596
6001	0.004348	0.013423	0.029760	0.056176	0.095257	0.148559	0.215441	0.291129	0.362614
7001	0.004346	0.013419	0.029753	0.056168	0.095248	0.148551	0.215437	0.291133	0.362627
8001	0.004345	0.013416	0.029748	0.056162	0.095241	0.148545	0.215434	0.291135	0.362637
9001	0.004344	0.013414	0.029745	0.056157	0.095236	0.148541	0.215431	0.291137	0.362644
10001	0.004343	0.013412	0.029742	0.056153	0.095232	0.148537	0.215429	0.291138	0.36265
11001	0.004343	0.013411	0.029739	0.056149	0.095228	0.148534	0.215428	0.291139	0.362655
12001	0.004342	0.013409	0.029737	0.056147	0.095226	0.148532	0.215426	0.291140	0.362659
13001	0.004342	0.013408	0.297356	0.056144	0.095223	0.148529	0.215425	0.291141	0.362662
14001	0.004341	0.013408	0.029734	0.056142	0.095221	0.148528	0.215424	0.291142	0.362665
15001	0.004341	0.013407	0.029732	0.056141	0.095219	0.148526	0.215423	0.291143	0.362668

Retardation and Péclet numbers belong to the real range of the physical problem. At the industry level, higher Péclet numbers are most frequently used in modeling. Therefore, this range must be carefully evaluated to avoid financial losses. In this regard, the model was simulated using $Pe = 50000$ and $R_g = 1.006$ to guarantee a maximum additional extraction up to 20%. However, for higher Péclet numbers, the governing equation turns into a advection-dominated process. As a consequence, without adding the numerical diffusion, the results produce oscillations also called as Gibbs phenomenon. Then, in this paper the advection term was discretized via first-order upwind scheme to introduce a dissipation effect and reduce the Gibbs phenomenon. Under this scenario, the first order method required more points to carry out the mesh convergence analysis. In addition, for higher Péclet numbers the concentration gradients around the center of domain increase relevantly. Thus, to obtain better results a non-uniform mesh was applied.

Mesh convergence for square wave equation requires high order accurate weighted essentially non-oscillatory (WENO) schemes. The numerical diffusion term reduces the method for first order, and consequently, more points are needed to converge. On the other hand, increasing the mesh refinement greatly increases the CPU(s) time. Although not obtained the convergence for $Pe = 50000$, the simulations presented good results for other cases, as shown in Table 3 in which the concentration gradient along the domain changes more smoothly.

Table 4. Mesh Convergence Analysis - Case 2

N	Pe = 50000, $R_g = 1.006$, $\tau = 1$, ξ								
	0.91	0.92	0.93	0.94	0.95	0.96	0.97	0.98	0.99
501	0.051020	0.074680	0.105796	0.145233	0.193427	0.250243	0.31488	0.385867	0.461137
1001	0.011274	0.022220	0.040957	0.070761	0.114865	0.175628	0.253611	0.346881	0.450849
1501	0.002824	0.007384	0.017447	0.037381	0.072864	0.129686	0.211610	0.318004	0.442463
2001	0.000764	0.002621	0.007861	0.020690	0.047986	0.098537	0.180094	0.294779	0.435340
2501	0.000219	0.000977	0.003690	0.011840	0.032446	0.076363	0.155353	0.275309	0.429107
3001	0.000065	0.000379	0.001790	0.006957	0.022392	0.060081	0.135383	0.258571	0.423546
3501	0.000020	0.000152	0.000893	0.004179	0.015718	0.047850	0.118948	0.243930	0.418515
4001	6.786E-6	0.000063	0.000457	0.002560	0.011196	0.038519	0.105222	0.230957	0.413914
4501	2.298E-6	0.000027	0.000239	0.001595	0.008079	0.031288	0.093628	0.219352	0.409671
5001	8.003E-7	0.000011	0.000127	0.001010	0.005898	0.025622	0.083742	0.208887	0.405735

From a physical point of view, the process is defined as sugar solute diluted in water until the concentration reaches to zero. However, several effects may influence this process. Then, in order to obtain the best results a mathematical model and formulation are necessary to evaluate the impact of different terms in the governing equation. Under this scenario, the one-dimensional advection-diffusion equation was used to demonstrate the importance of the Péclet number on lautering. Furthermore, the preferential washing of certain positions in vessel contributes to the extraction of tannins

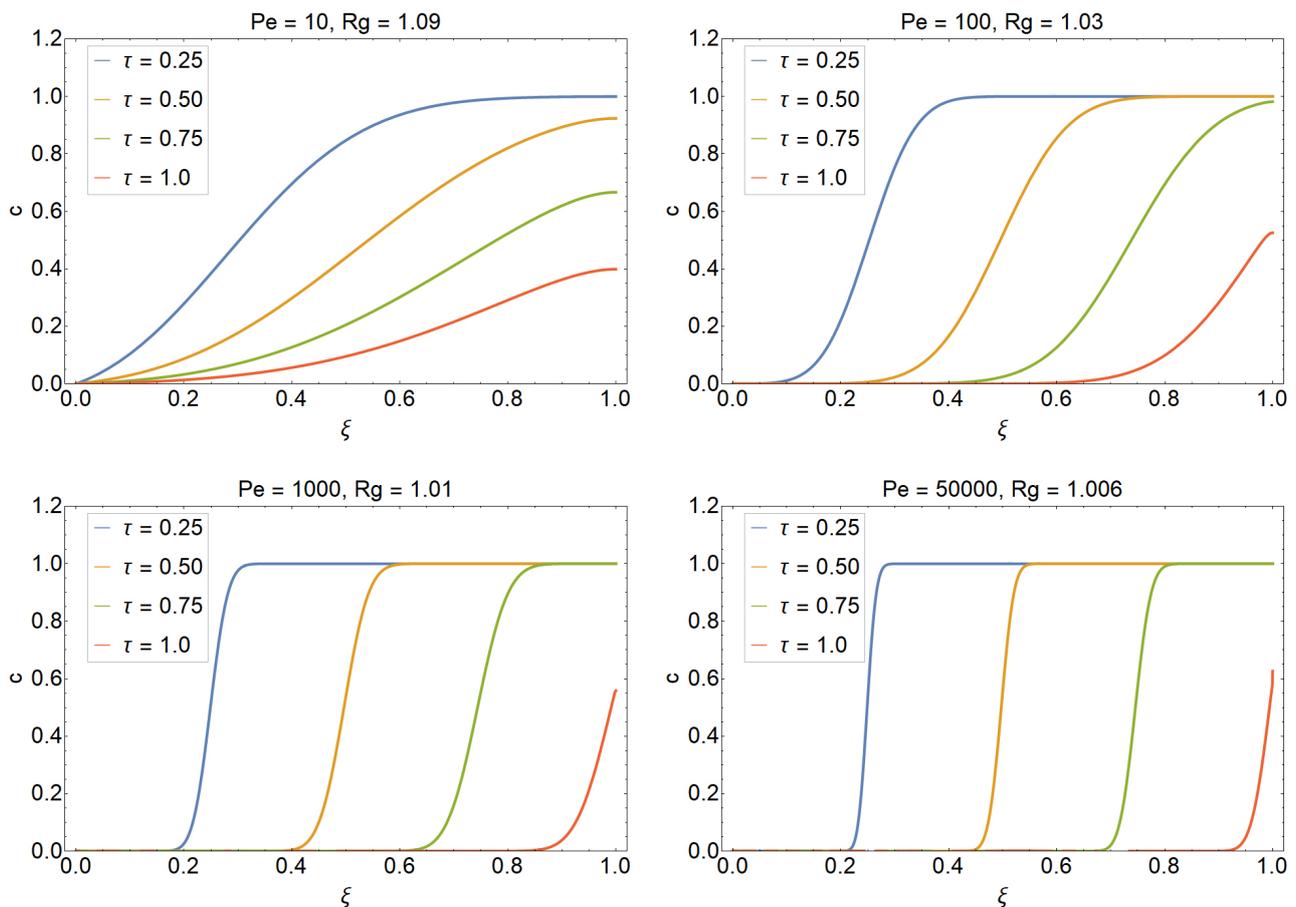


Figure 2. Sugar Profiles

from the grains, which cause astringency to the final product, so the application of this study in brewing brings significant results. Analyzing the values of the diffusion coefficients, it is perceived that they are directly related to the temperature in which the process occurs. Thus, adequate temperature control of the procedure should be adopted not only to ensure the correct extraction of the residual sugars from the interior of the grain shells, but also to certify the diffusion coefficient will have the highest possible value, remitting lower Péclet numbers.

5. CONCLUSIONS

This paper provided a numerical scheme to solve the linear transient one-dimensional advection-diffusion equation using the method of lines. It was proposed to model the mass transport problem on lautering systems through a well-know adsorption isotherm as source term which represented the additional sugar extraction from barley malts. In order to perform a fair comparison with methodology, computational implementations were applied changing the boundary and initial conditions to approach the numerical results with those ones present in literature. The profiles demonstrated good agreement between themselves. After this, an order and mesh verification were performed to ensure consistent outcomes which illustrate the concentration profiles for different operating conditions. In this regard, it was evaluated the physical effect of Péclet number in lautering efficiency. It was analyzed that for low Péclet numbers, the modeling process reduces smoothly over time and may be properly described using central and upwind-differencing schemes with a non-uniform mesh. On the other hand, high Péclet cause sharp variation among space domain and a huge reduction in the sugar concentration at the end of procedure, beyond requires high order accurate weighted essentially non-oscillatory schemes. This leads to negative consequences on lautering, since high gravity beer styles depends directly on this extraction levels. Therefore, by a proper control of process temperature and flow rate, a higher efficiency and a shorter procedure time are obtained. However, these results are preliminary and further studies must be carried out.

6. ACKNOWLEDGEMENTS

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