

Predicting Mass Transfer Extraction with Steam Flow, Applying Boundary-Layer Concepts

Jose Antonio Rocha-Uribe^{1*}, Laura Catalina Soto-Armenta², Alfredo Raul Hernandez-Ruiz¹,
Jorge Ciro Jimenez-Ocaña³

¹Colegio de Bachilleres de Chiapas, Tuxtla Gutiérrez, Mexico

²Campus Merida, Universidad del Valle de Mexico, Mérida, Mexico

³Instituto Tecnológico de Tuxtla Gutiérrez, Tuxtla Gutiérrez, Mexico

Email: *antonio.rocha@uady.mx

How to cite this paper: Rocha-Uribe, J.A., Soto-Armenta, L.C., Hernandez-Ruiz, A.R. and Jimenez-Ocaña, J.C. (2021) Predicting Mass Transfer Extraction with Steam Flow, Applying Boundary-Layer Concepts. *Journal of Materials Science and Chemical Engineering*, 9, 46-58.

<https://doi.org/10.4236/msce.2021.96004>

Received: May 26, 2021

Accepted: June 27, 2021

Published: June 30, 2021

Copyright © 2021 by author(s) and Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY 4.0).

<http://creativecommons.org/licenses/by/4.0/>



Open Access

Abstract

Theory and concepts of boundary layer mass transfer is applied to correlate experimental data on extraction of essential oils from vegetable leaves and stems, using steam. From these theory, concepts and experimental data with seven systems, two correlations are developed to predict the Sherwood number and mass transfer coefficient as function of Reynolds and Schmidt numbers. From these equations, the molar flux, the amount of solute extracted, and the yield of extraction is predicted. A steam of higher temperature normally improves the mass transfer and the yield. A method to estimate the enhancement for temperature increase is proposed. The correlations developed are applied to a case with industrial size that was no part of the data for correlation generation. Theory may be applied for industrial applications.

Keywords

Boundary Layer, Essential Oil, Extraction, Yield, Steam Distillation, Mass Transfer Coefficient

1. Introduction

Essential oil from plants is used in food, pharmacy, and fragrance industries due to their organoleptic and biological properties associated with their natural characteristics. Leaves and stem from plants are the raw material for the extraction of the essential oil. The total extraction of essential oil from vegetal leaves is usually small than 5% and there are several methods to perform the extraction. Hydro distillation with water in contact with the plant [1], steam distillation, with steam (but not water) contacting the plant, mechanical pressure (squeezing) [2], soxh-

let extraction with organic solvents [3], extraction with supercritical solvents like CO₂, and microwave extraction [4].

The extraction of essential oil by steam distillation uses a cylindrical column filled with vegetal leaves and stems. The steam flow through the leaves and stems, first heating them and then dissolving on it the essential oil, and taking out from the column with the flowing steam. The flowing steam that leaves the column is passing to a condenser where the oil and water usually form two different liquid phases and are separated in equipment called Florentine. **Figure 1** shows a scheme of a steam distillation system and a typical diagram from experimental results taken from Cerpa's Dissertation [5].

The experimental data of yield versus time of **Figure 1(b)** is modeled, by example with Xavier *et al.* [6] approach, using the mechanistic model proposed by Cerpa, Mato and Cocero [7], or some other.

In this manuscript, the final yield is modeled by using the concepts of boundary layer that were developed first for fluid flow by Ludwig Prandtl in 1904 who develop the first differential equations to model the hydraulic phenomena. Blausius helps to solve the mathematical model. Prandtl and other researchers began to apply it to heat transfer, Chilton-Coulburn and Guilliland-Sherwood applied it to mass transfer. Latter Bird Stewart and Lightfoot developed the concept of transport phenomena. This lead to apply the boundary layer theory to experimental and industrial cases, help the field of applied chemistry to be converted on chemical engineering and get maturity as science and engineering.

Chemical engineering applies the boundary layer concepts to correlate experimental data on flow of fluids, heat transfer, and mass transfer, as function of dimensionless numbers.

For mass transfer: Reynolds $Re = \frac{U_{ef} \rho_V D_c}{\mu_V}$, Schmidt $Sc = \frac{\mu_V}{\rho_V D_{AB}}$, and Sherwood $Sh = \frac{k_C D_C}{D_{AB}}$. Basically:

$$Sh = \alpha_1 Re^{\alpha_2} Sc_V^{\alpha_3} \quad (1)$$

Several series of experimental and reported data is used to get variation on

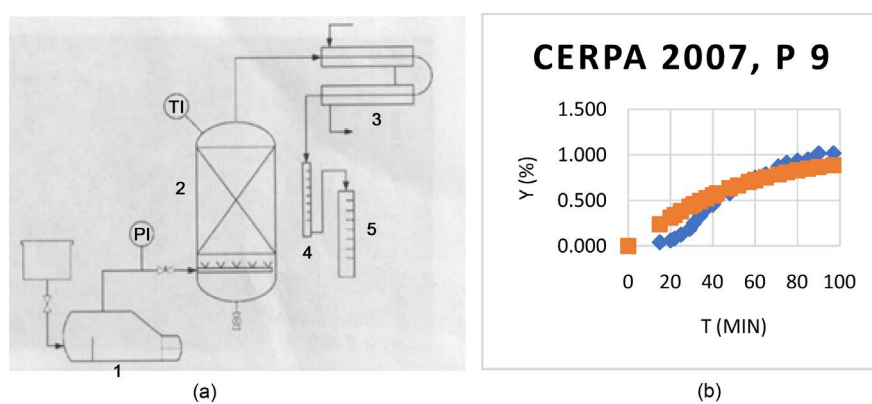


Figure 1. (a) Scheme of steam extraction system, (b) Yield of extraction versus time.

operational, physical properties, and geometrical parameters, to generate correlations to predict Sherwood number., and to calculate mass transfer, and yield of extraction.

2. Materials and Methods

2.1. Experimental Reported Data Used

Table 1 shows the systems used.

2.2. Boundary Layer Concept Applied to Mass Transfer

(Taken from [8]) A concentration gradient is formed together to the hydrodynamic and thermal one. Let C_{AO} be the concentration of the incoming flow to a plate made of a solid that is soluble in the liquid. C_{AO} will be the concentration also at core of the flow, far from the plate. When the liquid is in contact with the plate the equilibrium is reached instantaneously at the interface liquid-solid. The concentration of A at the fluid, at the plane of contact with the solid surface will be that of saturation ($C_{As} = C_{Ai}$). The mass molecular diffusion at y direction will set that the concentration gradient be growing when the liquid advance in x .

Authors or researchers from **Table 1**, report the dynamic (yield versus time). In this study only the final yield is correlated with physical properties, geometrical characteristics, and operational parameters. Defining the variable $\gamma = C_{Ai} - C_A$ (analogous to temperature in excess), the concentration gradient will be that of **Figure 2**. The dotted line is laminar underlayer.

The edge of the concentration boundary layer is then the geometric place where $\gamma_A = 0.99\gamma_{Ao}$, being $\gamma_{Ao} = C_{Ai} - C_{Ao}$ the maximum value de γ .

Table 1. Characteristics of the studied systems.

Author(s)	Journal	Plant	Solute	Dc (m)	Zc (m)	Q _v (L/h)
Cerpa <i>et al.</i> 2007, 2008 [5] [7]	Ph.D. (2007) Dissertation, AIChE J. 2008	Lavender	Linalool and linalyl acetate	0.35	0.42	0.6 - 2.10
Masango, 2005 [9]	J. of Cleaner Production	Artemisia	Camphor-L	0.09	0.34	0.15 - 1.19
Soto-Armenta <i>et al.</i> 2017 [10]	J. of Essential Oil Bearing Plants	Lippia graveolens (oregano)	Carvacrol and Thymol	0.10	0.76	1.4 - 6.98
Malekydozzadeh, 2012 [11]	Iranian J. of Chem. Eng.	Rosemary	a-pynene, 1, 8 Cineole, Camphor	0.06	0.20	240 - 420
Roautby <i>et al.</i> 2007 [12]	J. of food Engineering	Thyme	Thymol P Cymene	0.02	0.10	2678 - 4179
Romdhane and Tizaoui, 2005 [13]	J. of Chemical Technology and biotechnology	Aniseed	Anethol	0.26	0.90	7318
Ozek, 2012 [14]	Record of Natural Products	Laurel	1.8 cineole	0.68	1.36	44,143 - 88,830

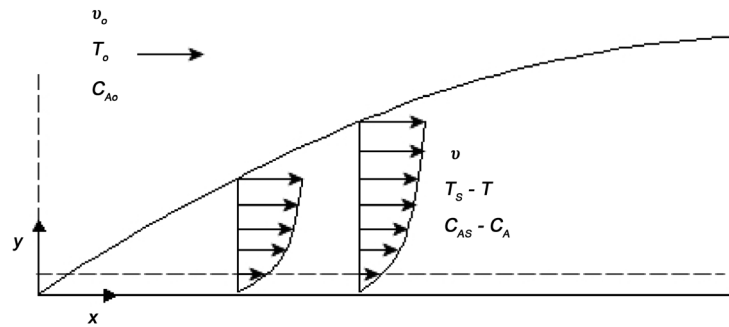


Figure 2. Gradients of velocity, temperature, and concentration at boundary layers.

The continuity equation for A , if density ρ , and diffusivity D_{AB} are constant, is:

$$v_x \frac{\partial \gamma_A}{\partial x} + v_y \frac{\partial \gamma_A}{\partial y} = D_{AB} \left(\frac{\partial^2 \gamma_A}{\partial y^2} \right) \quad (2)$$

It has as boundary conditions: $\gamma_A(x=0, y) = \gamma_{Ao}$; $\gamma_A(x, y=0) = 0$;
 $\gamma_A(x, y = \infty) = \gamma_{Ao}$

That is similar to the one Blasius solved, but now for mass transfer. The dependent variable is now $\varnothing = \frac{\gamma_A}{\gamma_{Ao}} = \frac{C_{Ai} - C_A}{C_{Ai} - C_{Ao}}$ that is function of the dimensionless variable $\eta = \frac{y}{x} \sqrt{Re_x}$.

If it is desired a mathematical expression for the flux of A at the solid surface (N_A in $\text{kmol/m}^2/\text{s}$), it is needed to use Fick's law to obtain

$$N_{A,x} = 0.332 D_{AB} (C_{Ai} - C_{Ao}) \frac{\sqrt{Re_x}}{x} \quad (3)$$

Integrating over the plate length

$$N_A = 0.664 \frac{D_{AB} (C_{Ai} - C_{Ao})}{L} \sqrt{Re_L} \quad (4)$$

By analogy to the thermal boundary layer, the Schmidt number relates the diffusivities of mass and momentum, giving:

$$Sc \equiv \frac{\nu}{D_{AB}} = \frac{\mu}{\rho D_{AB}} \quad (5)$$

Equation (4) is valid only if $Sc = 1$. For the cases with $Sc \neq 1$ it is necessary to introduce an experimental correction factor $Sc^{1/3}$

$$N_A = 0.664 \frac{D_{AB} (C_{Ai} - C_{Ao})}{L} \sqrt{Re_L} Sc^{1/3} \quad (6)$$

Equation (6) has been experimentally tested.

2.3. Mass Transfer Coefficient

Equation (6) allows the calculation of the rate of mass transfer for molecular diffusion at forced convection for laminar flow. If the flow is turbulent or the geome-

try of the system is complex, as is the case in many practical cases. For this case it is necessary to use the mass transfer coefficient, defined by Equation (7):

$$k_c \equiv \frac{N_A}{\Delta C_A} = \frac{N_A}{C_{Ai} - C_{Ao}} \quad (7)$$

Applying Equation (6) on Equation (7) we get:

$$k_c = \frac{0.664 D_{AB} \sqrt{Re_L}}{L} Sc^{1/3} \quad (8)$$

This equation may be arranged and it provide the Sherwood dimensionless number:

$$Sh = \frac{k_c L}{D_{AB}} = 0.664 \sqrt{Re_L} Sc^{1/3} \quad (9)$$

Sh is the Sherwood number, counterpart of Nusselt number in heat transfer. At turbulent flow, and for complex geometrical systems the mass transfer coefficient k_c will be empirical.

2.4. Application to Extraction with Steam Flow

From the reported data with the sources given in **Table 1**, we may calculate the amount of mass extracted with $m_{\text{extracted}} = m_o \text{ yieldx } 100$ (kg) and convert it to kmol dividing it between the molecular weight of the solute extracted. Then the flux of *A* (N_A , kmol/m²/s) will be this kmol divided between the transversal area to flow and also divided by the residence time of the flow. This last parameter may be calculated dividing the volume (m³) of extractor between the volumetric flows of steam (m³/s).

A program was developed with Excel software and applied to each series of data in **Table 1**. C_{Ai} is the concentration of solute at the surface of the vegetal leave (at $y = 0$). This may be taken as the solubility of the solute in kmol/m³. Because the steam does not contain solute: $C_{Ao} = 0$. Then using Equation (7):

$$k_c = \frac{N_A}{C_{Ai} - C_{Ao}} = \frac{\frac{\text{kmol}}{\text{m}^2 \cdot \text{s}}}{\frac{\text{kmol}}{\text{m}^3}} = \frac{\text{m}}{\text{s}} \quad (10)$$

Then with physical properties, we calculate Sherwood number ($k_c D / D_{AB}$), and

calculating Reynolds number $Re = \frac{U_e \text{den}_v D_c}{\text{visc}_v} = \frac{\frac{\text{m}}{\text{s}} \cdot \frac{\text{kg}}{\text{m}^3} \cdot \text{m}}{\frac{\text{kg}}{\text{m} \cdot \text{s}}}$ and Schmidt number

$Sc = \frac{\text{visc}}{\text{den} D_{AB}} = \frac{\frac{\text{kg}}{\text{m} \cdot \text{s}}}{\frac{\text{kg}}{\text{m}^3} \cdot \frac{\text{m}^2}{\text{s}}}$ and using a reasonable number of data points we can

correlate coefficient and exponents (α_1 , α_2 , and α_3).

2.5. Physical Properties

Table 2 shows some of the physical properties used in the Excel program.

Table 2. Physical properties of solutes that dissolves into steam.

Author(s)	Solute	Density (kg/m ³)	Viscosity (kg/m/s)	Diffusivity (m ² /s)	Molecular weight (kg/kmol)	Solubility (kmol/m ³)
Cerpa <i>et al.</i> 2007, 2008 [5] [7]	Linalool and linalyl acetate	0.555	1.32E-5	1.10E-5	175	0.080000
Masango, 2005 [9]	Camphor-L	0.555	1.32E-5	1.17E-5	152	0.080000
Soto-Armenta <i>et al.</i> 2017 [10].	Carvacrol and Thymol	0.555	1.32E-5	1.18E-5	150	0.007160
Malekydozzadeh, 2012 [11]	α -pynene, 1, 8 Cineole, Camphor	0.555	1.32E-5	1.17E-5	152	0.007600
Roautby <i>et al.</i> 2007 [12]	Thymol P Cymene	0.597 (100 °C)	1.30E-5	1.18E-5	148	0.005900
		4.515 (175 °C)	1.50E-5	1.63E-5		0.005900
		19.984 (250 °C)	1.80E-5	2.14E-5		0.005900
Romdhane and Tizaoui, 2005 [13]	Anethol	0.597	1.32E-5	9.06E-6	148	0.000750
Ozek, 2012 [14]	1.8 cineole	0.555	1.32E-5	1.16E-5	154	0.000023

Density and viscosity were taken from [8], diffusivities were predicted with the correlation of Fuller *et al.* [15]. Solubility was taken from PubChem, National Library of Medicine, Center for Biotechnology Information, that usually is expressed as mg or gr/liter. We convert it to kg and to kmol dividing between the molecular weight and converting the volume at the denominator to cubic meters.

Most of the experimental extraction with steam used atmospheric pressure and temperature of 100 °C. Only some data from Roautby *et al.* [12] and Romdhane and Tizaoui [13] were at temperature above 100 °C. These data were processed in a different Excel program, to get the effect of temperature over the yield of extraction.

In the general study, steam at 100 °C was used and the physical properties density and viscosity keep constant values. Diffusivity varies a little depending of the solute.

The exponent α_3 in Equation (1) keep a constant value of 1/3 or 0.33 for the Schmidt number in the hydrodynamic boundary layer as well as for the Prandtl thermal boundary. Then, here for mass transfer, we are going to take this exponent constant: $\alpha_3 = 0.33$.

3. Results and Discussion

3.1. Results from Excel Program for $T = 100^{\circ}\text{C}$

Table 3 shows some of the results of the Excel program applied to the data at 100°C . It is noted that the Reynolds number is less than unity for the systems of Cerpa *et al.* and Masango *et al.*, and is bigger for all other systems, reaching values above 2000 for the systems of Roautby *et al.* and Ozek.

Figure 3 shows the plot of $\text{Ln}(Sh/Sc^{1/3})$ versus $\text{Ln}(Re_{Dc})$ obtained when $\alpha_3 = (1/3)$ for all data for the several systems used. From this data, Equation (11) provides the first correlation equation.

$$Sh = \alpha_1 Re_{Dc}^{\alpha_2} Sc^{\alpha_3} = 0.2754 Re_{Dc}^{1.5338} Sc^{0.333} \quad (11)$$

If we pass the line at the intersection $Sh/Sc^{0.33} = 1.0$ to get $Re_{Dc} = 0$, we get the equation $y = 1.2964x + 1$ and from this equation we get the second correlation Equation (12). The prediction with Equation (11) and Equation (12) is shown in **Figure 4(a)** and **Figure 4(b)**. The two correlations may be considered limits for prediction.

$$Sh = \alpha_1 Re_{Dc}^{\alpha_2} Sc^{\alpha_3} = 2.7182 Re_{Dc}^{1.2964} Sc^{0.333} \quad (12)$$

3.2. Results for Temperature Increase

Rouatby *et al.* [12] studied the extraction of essential oil of thyme by superheated steam. They used steam temperatures of 100°C , 175°C , and 250°C . They found that at higher temperatures the yield of extraction increases. Because the physical

Table 3. Parameters and mass transfer coefficient and exponent, from correlated data, for $\alpha_3 = 1/3$.

Author(s)	Re_{Dc}	m_A kg	N_A kmol/m ² /s	K_c m/s	$Sh_{a1a2}\alpha_1\alpha_2$	$Sh_{a1a2}\alpha_1\alpha_2$	$Sh_{a1a2}\alpha_1\alpha_2$
Cerpa <i>et al.</i> 2007, 2008 [5] [7]	0.032/0.124	0.026/0.036	6.41E-9/ 3.09E-8	8.01E-8/ 3.86E-7	2.55E-3/ 1.23E-2	0.0801	1.0672
Masango, 2005 [9]	0.035/0.274	2.33E-4/ 7.13E-4	1.68E-8/ 4.34E-8	2.10E-7/ 5.43E-7	1.54E-3/ 3.99E-3	0.0057	0.4547
Soto-Armenta <i>et al.</i> 2017 [10]	0.288/1.440	3.92E-3/ 9.87E-3	4.69E-7/ 1.96E-6	6.54E-5/ 2.73E-4	5.55E-1/ 2.32E0	1.1763	0.6177
Malekydozzadeh, 2012 [11]	79.3/178.4	8.30E-4/ 1.55E-3	1.26E-4/ 5.63E-4	1.65E-2/ 7.41E-2	8.48E1/ 3.80E2	1.0550	1.0447
Roautby <i>et al.</i> [12]	2092.1/4525.7	0.000231/ 0.000420	5.54E-3/ 2.44E-1	1.80/ 78.6	1671.4/ 133,160.6	1.5600	1.2265
Romdhane and Tizaoui [13]	787.7/812.4	0.036/0.098	1.51E-4/ 3.51E-4	2.02E-1/ 4.69E-1	6.99E3/ 1.88E4	0.3470	1.3527
Ozek, 2012 [14]	1287.1/2590.1	0.350/1.380	2.73E-4/ 8.06E-4	12.0/35.5	7.04E5/ 2.08E6	1.201	1.8199
All prediction 1	0.032/4525.7	2.31E-4/ 1.38E0	6.41E-9/ 2.33E-1	8.01E-8/ 3.96E1	1.54E-3/ 2.08E6	0.2752	1.5338
All prediction 2	0.032/4525.7	2.31E-4/ 1.38E0	6.41E-9/ 2.33E-1	8.01E-8/ 3.96E1	1.54E-3/ 2.08E6	2.7182	1.2964

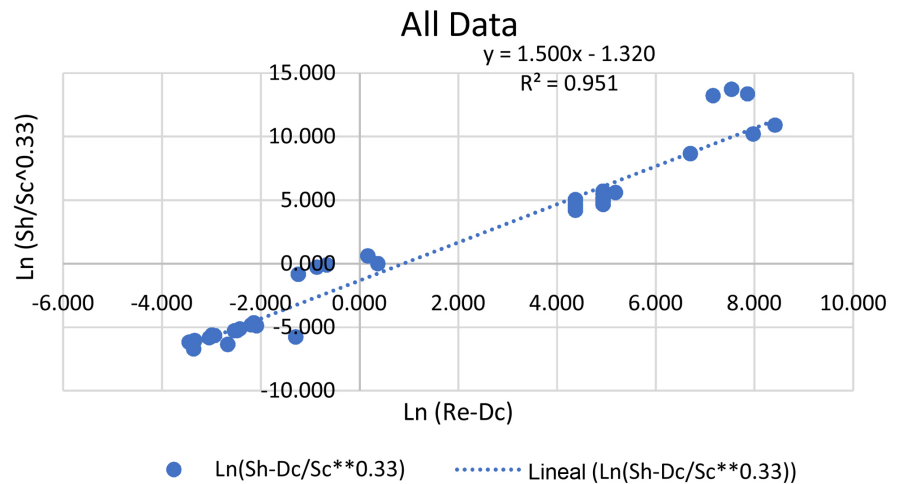


Figure 3. $\ln(Re)$ versus $\ln(Sh/Sc^{0.33})$ used to get α_1 and α_2 .

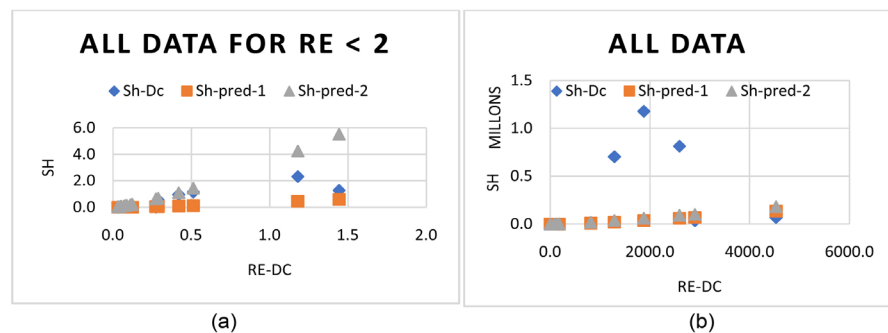


Figure 4. Prediction of Sherwood number for all data. (a) For $RE < 2$, (b) ALL DATA.

properties changed, most of the parameters changed as well. **Table 4** shows some of the values obtained.

The last two rows of **Table 4** provide the ratio of the property or parameter at $175^\circ\text{C}/100^\circ\text{C}$, and $250^\circ\text{C}/100^\circ\text{C}$. When that ratio is unity, the values are similar for the three temperatures.

When the ratio is fractional, by example the volumetric flow of steam: $\frac{Q_{175}}{Q_{100}} = 0.132$ means that the volumetric flow rate of steam at 175°C is 0.132 times the volumetric flow rate at 100°C . This happen because the density of steam at 175°C is 7.56 times higher than at 100°C .

For the flow at 250°C the ratio is $\frac{Q_{250}}{Q_{100}} = 0.030$ this means that the flow rate of steam at 250°C is about 3% of the volumetric flow rate of steam at 100°C .

When the ratio is higher than unity, by example $\frac{Y_{175}}{Y_{100}} = 1.205$ this means that the yield of extraction is 1.205 higher at 175°C than at 100°C .

Note that the superficial and effective velocities are higher at low temperatures (100°C) than at 175°C or 250°C , residence time, density, viscosity, diffusivity, and the mass extracted are higher for bigger temperatures. Reynolds, Schmidt,

Table 4. Some values for Data of Roautby *et al.* [12] for the extraction of thyme leaves.

(a)									
Roautby <i>et al.</i> [12]	min	sec	m	m	m ³ /m ³	kg	m ³ /s	%	
	t_{min}	t	D_c	Z	E	M_o	Q	Y	Y
$m = 1.6 \text{ k/h}, Q = 0.000744, 100^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.000744	3.30	
$m = 2.5, Q = 0.001163, 100^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.001161	4.20	
$m = 1.6 \text{ k/h}, Q = 0.000098, 175^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.000098	4.10	
$m = 2.5, Q = 0.000153, 175^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.000153	4.90	
$m = 1.6 \text{ k/h}, Q = 0.000022, 250^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.000022	5.00	
$m = 2.5, Q = 0.000034, 250^\circ\text{C}$	40.0	2400.00	0.020000	0.10	0.750	0.007	0.000034	6.00	
x_5/x_3	1.000	1.000	1.000	1.000	1.000	1.000	0.132	1.242	
x_7/x_3	1.000	1.000	1.000	1.000	1.000	1.000	0.030	1.515	
x_6/x_4	1.000	1.000	1.000	1.000	1.000	1.000	0.132	1.167	
x_8/x_4	1.000	1.000	1.000	1.000	1.000	1.000	0.029	1.429	
$(x_5/x_3 + x_7/x_3)/2$	1.000	1.000	1.000	1.000	1.000	1.000	0.132	1.205	
$(X_6/X_4 + X_8/X_4)/2$	1.000	1.000	1.000	1.000	1.000	1.000	0.030	1.472	

(b)									
m ²	m ³	m/s	m/s	s	kg/m ³	kg/m/s	m ² /s	kg/kmol	kmol/m ³
A	V	Us	Uef	tR	den	vis	DAB	PMA	Cai-solub
0.000314	0.000031	2.368220	3.157627	0.042	0.597	1.30E-05	1.18E-05	1.42E+02	0.003
0.000314	0.000031	3.695569	4.927426	0.027	0.597	1.30E-05	1.18E-05	1.42E+02	0.003
0.000314	0.000031	0.313216	0.417622	0.319	4.515	1.50E-05	1.63E-05	1.42E+02	0.003
0.000314	0.000031	0.487013	0.649351	0.205	4.515	1.50E-05	1.63E-05	1.42E+02	0.003
0.000314	0.000031	0.070665	0.094220	1.415	19.984	1.80E-05	2.14E-05	1.42E+02	0.003
0.000314	0.000031	0.108225	0.144300	0.924	19.984	1.80E-05	2.14E-05	1.42E+02	0.003
1.000	1.000	0.132	0.132	7.561	7.563	1.154	1.381	1.000	1.000
1.000	1.000	0.030	0.030	33.514	33.474	1.385	1.814	1.000	1.000
1.000	1.000	0.132	0.132	7.588	7.563	1.154	1.381	1.000	1.000
1.000	1.000	0.029	0.029	34.147	33.474	1.385	1.814	1.000	1.000
1.000	1.000	0.132	0.132	7.575	7.563	1.154	1.381	1.000	1.000
1.000	1.000	0.030	0.030	33.830	33.474	1.385	1.814	1.000	1.000

(c)									
U*den*Dc/vis	den*vis/DAB	kg	kmol/m ² /s	m/s	Kc*Dc/DAB	Roautby <i>et al.</i> [12]			
Re-Dc	Sc	mA	NA	Kc	Sh-Dc	Sh-Dc -p1			
2900.16	1.845	0.000231	0.123	39.56	67,047.3	21,248.9	$m = 1.6 \text{ k/h}, Q = 0.000744, 100^\circ\text{C}$		
4525.65	1.845	0.000294	0.244	78.56	133,160.6	84,452.8	$m = 2.5, Q = 0.001163, 100^\circ\text{C}$		
2514.08	0.204	0.000287	0.020	6.50	7975.7	6546.4	$m = 1.6 \text{ k/h}, Q = 0.000098, 175^\circ\text{C}$		
3909.09	0.204	0.000343	0.037	12.08	14,821.0	25,729.6	$m = 2.5, Q = 0.000153, 175^\circ\text{C}$		
2092.09	0.042	0.000350	0.006	1.79	1671.4	2188.8	$m = 1.6 \text{ k/h}, Q = 0.000022, 250^\circ\text{C}$		
3204.10	0.042	0.000420	0.010	3.29	3071.8	8208.3	$m = 2.5, Q = 0.000034, 250^\circ\text{C}$		
0.867	0.110	1.242	0.164	0.164	0.119	0.308	x_5/x_3		
0.721	0.023	1.515	0.045	0.045	0.025	0.103	x_7/x_3		
0.864	0.110	1.167	0.154	0.154	0.111	0.305	x_6/x_4		
0.708	0.023	1.429	0.042	0.042	0.023	0.097	x_8/x_4		
0.865	0.110	1.205	0.159	0.159	0.115	0.306	$(x_5/x_3 + x_7/x_3)/2$		
0.715	0.023	1.472	0.044	0.044	0.024	0.100	$(X_6/X_4 + X_8/X_4)/2$		

and Sherwood numbers, as well as the molar flux and the mass transfer coefficient are lower for the higher temperatures. For predicted Sherwood number:

$$\frac{Sh_{175}}{Sh_{100}} = 0.306 \quad (13)$$

$$\frac{Sh_{250}}{Sh_{100}} = 0.100 \quad (14)$$

Figure 5 provides a method to estimate the Sherwood number at different temperatures of steam.

4. Case of Study, Prediction of Yield

The data on the paper of Koul *et al.* [16] will be taken as example to predict the yield of experiments 3, 4, 5, 6, and 7. In this case lemon grass oil is obtained by steam distillation of lemon grass (*Cymbopogon* spp.) the main solute is citral or geranial ($C_{10}H_{16}O$), that has the same formula than camphor then ($D_{AB} = 1.17E-5$ m²/s) but the solubility is $C_{Ai} = 0.003289$ kmol/m³.

The first two experiments used $m_o = 70$ kg, and the last three used 1000 kg. These are industrial quantities. In **Table 1** the data of Ozek use the biggest equipment size (0.5 m³) and the highest quantity of vegetal leaves (24 - 38 kg). We are going to use the data of Ozek to estimate the volume of cylinder needed for Koul experiments. Ozek [14] used $V = 0.5$ m³ for 35 kg of mass. Then for Koul:

$$V_1 = 0.5 \times 100 / 35 = 1.428 \text{ m}^3 \quad \text{and} \quad V_2 = 0.5 \times 1000 / 35 = 14.286 \text{ m}^3$$

Choosing a diameter of $D_c = 2.0$ m, $A = 3.1416 \cdot D_c^2 / 4 = 3.1416$ m², and $V = A \cdot z$, then $z_1 = V_1 / A = 1.428 / 3.1416 = 0.46$ m = z_1 , and $z_2 = V_2 / A = 14.286 / 3.1416 = 4.55$ m = z_2 .

The steam flow rate Q_i in m³/s used in Koul experiments were: 15, 12, 160, 125 and 140 L/h (0.015, 0.012, 0.125, 0.140 m³/h, or 4.166E-6, 3.33 E-6, 4.44E-5, 3.472E-5, 3.88E-5 m³/s).

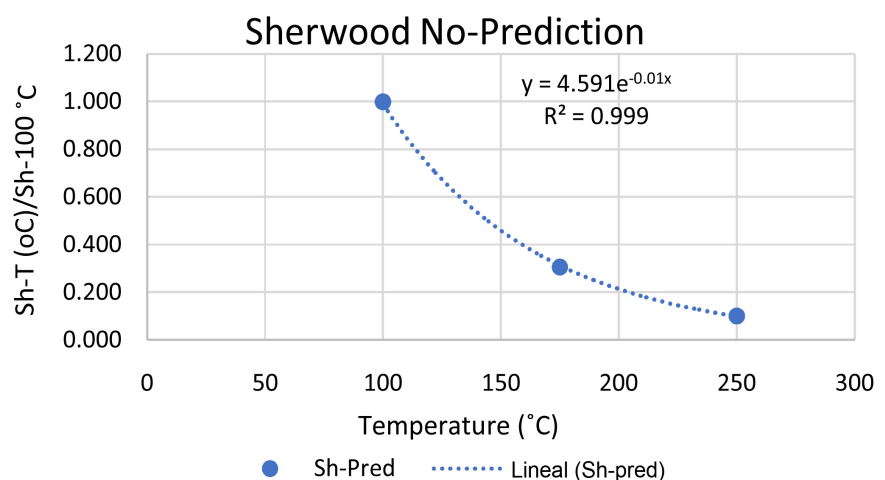


Figure 5. Prediction for temperature of steam effect on Sherwood number.

For the yield calculation, experiments 3 - 7 were: 385, 330, 5725, 5215, 5315 mL of citral oil at 5 h = 300 minutes = 18,000 seconds. With a density of citral of 0.9 gr/ml or 900 kg/m³ and the 70 kg of lemon grass for experiments 3 and 4 and 1000 kg of lemon grass for experiments 5 - 7, we get: $y_3 = 0.495$, $y_4 = 0.424$, $y_5 = 0.515$, $y_6 = 0.469$, $y_7 = 0.478$.

With the cylinder dimensions $Dc = 2$ m y $z_1 = 0.46$, and $z_2 = 4.55$ m, we get $A = \pi r^* Dc^2 / 4 = 3.1416$ m², and $V_1 = 1.44$ m³, $V_2 = 14.2$ m³. Dividing volumetric flow rate between area we get Superficial velocities, and dividing these between void fraction, we get effective velocities $U_{e\beta} = 0.0000018$, $U_{e\alpha} = 0.0000014$, $U_{e\delta} = 0.0000188$, $U_{e\epsilon} = 0.0000147$, $U_{e\zeta} = 0.0000165$ m/s.

Residence time of steam may be calculated dividing volume between steam volumetric flow rate, and we get: $t_{\beta} = 346,888.1$, $t_{\alpha} = 433,974.8$, $t_{\delta} = 321,943.2$, $t_{\epsilon} = 411,701.6$, $t_{\zeta} = 368,409.3$ seconds.

Now, we can calculate Reynolds numbers with Equation (15)

$$Re_i = \frac{U_{efi} den_{vap} Dc}{Visc_{vap}} \tag{15}$$

And Schmidt and Sherwood numbers with Equation (16) and Equation (11) or Equation (12)

$$Sc = \frac{visc_{vap}}{den_{vap} D_{AB}} \tag{16}$$

Table 5. Calculated values for Kaoul *et al.* [16] yields.

	<i>Re</i>	<i>k</i> _{C1}	<i>k</i> _{C2}	<i>N</i> _{A1}	<i>N</i> _{A2}	<i>m</i> _{A1}	<i>m</i> _{A2}	<i>y</i> _{AP-1}	<i>y</i> _{AP-2}	<i>y</i> _{A-Exp}
E-3	0.15	1.098E-07	3.545E-06	3.610E-08	5.601E-09	0.060	0.929	0.09	1.33	0.50
E-4	0.12	7.785E-08	2.652E-06	2.561E-10	4.189E-09	0.053	0.869	0.08	1.24	0.42
E-5	1.58	4.137E-06	7.619E-05	1.361E-08	1.204E-07	2.095	18.533	0.21	1.85	0.52
E-6	1.24	2.837E-06	5.539E-05	9.332E-09	8.751E-08	1.837	17.230	0.18	1.72	0.47
E-7	1.38	3.364E-06	6.397E-05	1.107E-07	1.011E-07	1.950	17.807	0.19	1.78	0.48

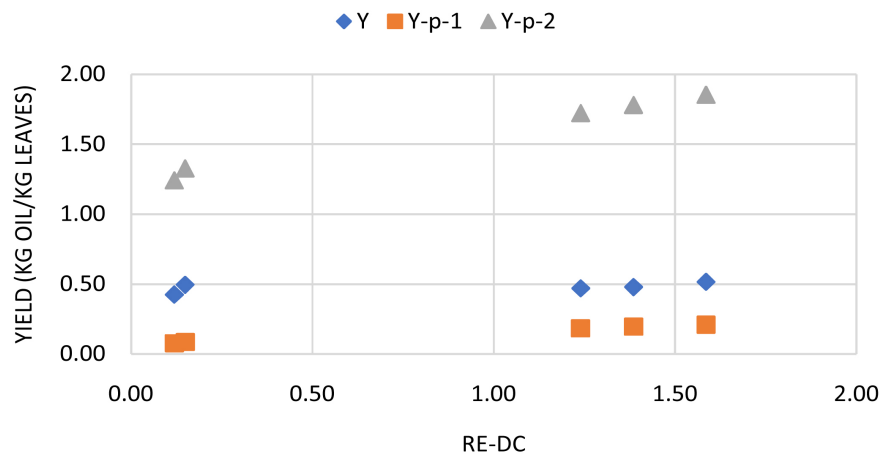


Figure 6. Prediction on Koul [16], using the present model.

With Sherwood number, we can get the mass transfer coefficient k_c and from this, the flux N_A , then, m_A , and finally the yield y_A with Equations (17)-(20). Because the steam does not have solute $C_{Ao} = 0$

$$k_c = \frac{ShD_{AB}}{D_C} \quad (17)$$

$$N_A = k_c (C_{Ai} - C_{Ao}) \quad (18)$$

$$m_A = N_A \times A \times t_R \times PM_A \quad (19)$$

$$y_{ai} = \left(\frac{m_A}{m_o} \right) \times 100 \quad (20)$$

Table 5 provides the main calculated values, and **Figure 6** provides the comparison between reported and predicted values.

On **Figure 6** it is observed that both predictions 1 and 2 follow the order of the reported data. Prediction 1 underpredicts 0.31, and prediction 2 overpredicts 3.32 the values of reported yield of extraction from Koul *et al.* [16].

5. Conclusions

The proposed Equation (11) and Equation (12) provide correlations to predict the yield of extraction, by first estimating the dimensionless numbers Reynolds, Schmidt, and Sherwood numbers, and using equations for the mass transfer involved in the extraction of solute from vegetable leaves to steam, using boundary layer concepts and definitions like molar flux and mass transfer coefficient.

The predicting Equation (11) and Equation (12) provide limits to experimental or reported yields and predict well the effect of steam flow.

Figure 5 and Equation (21) help to predict Sherwood number for superheated steam at temperatures above 100°C.

$$\frac{Sh(T^\circ\text{C})}{Sh(100^\circ\text{C})} = 4.591 \exp^{-0.015 \times T(^\circ\text{C})} \quad (21)$$

Using steam at temperatures higher than 100°C improves the extraction yield, but at temperatures above 200°C, the temperature degrades some components of the mixture of essential oil.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- [1] Husar, E., Dzieciol, M., Wodnicka, A., Orun, H., Koz, A. and Cicek, E. (2018) Influence of Hydrodistillation conditions on Yield and Composition of Coriander (*Coriandrum sativum* L.) essential Oil. *Polish Journal of Food and Nutrition Sciences*, **68**, 243-249. <https://doi.org/10.1515/pjfn-2018-0003>
- [2] Geramitcioski, T., Mitievski, V. and Mijakovski, V. (2018) Design of a Small Press for Extracting Essential Oil According VDI 2221. *IOP Conference Series: Materials*

- Science and Engineering*, **393**, Article No. 012131.
<https://doi.org/10.1088/1757-899X/393/1/012131>
- [3] Gopalasatheeskumar, K. (2018) Significant Role of Soxhlet Extraction Process in Phytochemical Research. *Mintaje Journal of Pharmaceutical & Medical Sciences*, **7**, 43-47.
- [4] Bagade, S.B. and Patil, M. (2021) Recent Advances in Microwave Assisted Extraction of Bioactive Compounds from Complex Herbal Samples: A Review. *Critical Reviews in Analytical Chemistry*, **51**, 138-149.
<https://doi.org/10.1080/10408347.2019.1686966>
- [5] Cerpa-Chavez, M.G. (2007) Hidrodestilación de aceites esenciales, Modelado y caracterización. Ph. D. Dissertation, Universidad de Valladolid, Spain.
- [6] Xavier, V.B., Vargas, R.M.F., Cassel, E., Lucas, A.M., Santos, M.A., Mondinc, C.A., Santaremc, E.R., Astarita, L.V. and Sartor, T. (2011) Mathematical Modeling for Extraction of Essential Oil from *Baccharis* spp. by Steam Distillation. *Industrial Crops and Products*, **33**, 599-604. <https://doi.org/10.1016/j.indcrop.2010.12.019>
- [7] Cerpa, M.G., Mato, R.B. and Cocero, M.J. (2008) Modeling Steam Distillation of Essential Oils: Application to Lavandin Super Oil. *AIChE Journal*, **54**, 909-917.
<https://doi.org/10.1002/aic.11438>
- [8] Donde-Castro, M., Rocha-Uribe, J. A. and Sacramento-Rivero J. C. (2013) *Transferencia de Masa, Teoría y aplicaciones en procesos químicos*, Pearson, 2013.
- [9] Masango, P. (2005) Cleaner Production of Essential Oils by Steam Distillation. *Journal of Cleaner Production*, **13**, 833-839.
<https://doi.org/10.1016/j.jclepro.2004.02.039>
- [10] Soto-Armenta, L.C., Sacramento-Rivero, J.C., Acereto-Escoffie, P.O., Peraza-Gonzalez, E.E., Reyes-Sosa, C.F. and Rocha-Uribe, J.A. (2017) Extraction Yield of essential Oil from *Lippia graveolens* Leaves by Steam Distillation at Laboratory and Pilot Scales. *Journal of Essential Oils Bearing Plants*, **20**, 610-621.
<https://doi.org/10.1080/0972060X.2017.1331756>
- [11] Malekydozzadeh, M., Khavid-Parsi, P., Rezazadeh, Sh., Abolghasemi, H., Salehi, Z. and Li, Q. (2012) Application of Multistage Steam Distillation Column for Extraction of Essential Oil of *Rosemarinuse officinalis* L. *Iranian Journal of Chemical Engineering*, **9**, 54-64.
- [12] Rouatbi, M., Duquenoy, A. and Giampaoli, P. (2007) Extraction of the Essential Oil of Thyme and Black Pepper by Superheated Steam. *Journal of Food Engineering*, **78**, 708-714. <https://doi.org/10.1016/j.jfoodeng.2005.11.010>
- [13] Romdhane, M. and Tizaoui, C. (2005) The Kinetic Modelling of a Steam Distillation Unit for the Extraction of Aniseed (*Pimpinella anisum*) Essential Oil. *Journal of Chemical Technology and Biotechnology*, **80**, 759-766.
<https://doi.org/10.1002/jctb.1221>
- [14] Özek, T. (2012) Distillation for Pilot Plant Production of *Laurus novilis* Essential Oil. *Journal of Records of Natural Products*, **6**, 135-143.
- [15] Fuller, E.N., Schettler, P.D. and Giddings, J.C. (1966) New Method for Prediction of Binary Gas-Phase Diffusion Coefficients. *Industrial & Engineering Chemistry Research*, **58**, 18-27. <https://doi.org/10.1021/ie50677a007>
- [16] Koul, V.K., Gandotra, B.M., Koul, S., Ghosh, S., Tikoo, C.L. and Gupta, A.K. (2004) Steam Distillation of Lemon Grass (*Cymbopogon* spp.). *Indian Journal of Chemical Technology*, **11**, 135-139.