Numerical optimization of guaco leaves extraction based on pre-heat treatment

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Authors' contributions

Marina Roberto Martins: investigation, data curation.

Gracielle Johann: formal analysis, writing, review and editing.

Fernando Palú: conceptualization, methodology, supervision.

Edson Antonio da Silva: methodology, supervision, writing, review and editing.

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Data availability statement

The datasets generated during the current study are available from the corresponding author on reasonable request.

Title Page

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Abstract

The mass yield of the extraction is influenced directly by the pre-treatment conditions of the raw material. In the case of leaves, drying is required to ensure their biological stability and is a pre-processing step that demands large amounts of thermal energy. In the present study, the oil extraction process was numerically optimized, considering the influence of the pre-heat treatment of the guaco leaves. An operating range between 30 and 70 ºC, 1.0 and 5.0 m/s, and recirculation between 0 and 1 was evaluated. The minimum ratio of energy consumption of drying by the amount of oil obtained after extraction (4.05×10^5 kWh/kg) was obtained under the optimal conditions of 30.02 ºC, 1.0 m/s, and 0.129 of air recycling flow rate. With our results, it is possible to guarantee safety in the storage of guaco leaves, in addition to optimizing the extraction process, maximizing the obtaining of the oil mass, and reducing energy consumption in the drying step.

Keywords: drying, energy consumption, mass yield.

Nomenclature

a	Specific area	(m^{-1})
A	Cross-sectional area to the air flow	(m^2)
cp_G	Specific heat of the drying air	(kJ/kg °C)
$d.b.$	Dry basis	(kg/kg)
D_{eff}	Coefficient of effective mass diffusivity	(m^2/min)
E_{Fan}	Total energy consumed to move the drying air	(kJ/min)
E_{Heat}	Total energy consumed to heat the drying air	(kJ/min)
h_c	Volumetric coefficient of the heat transfer	(kJ/min m^3 °C)
H_G	Enthalpy of the drying air	(kJ/kg)
H_S	Enthalpy of leaves	(kJ/kg)
k_F	External mass transfer coefficient	(kg/m^2 min)
k_S	Internal mass transfer coefficient	(min^{-1})
L	Bed height	(m)
m_{DS}	Dry mass of leaves	(kg)
m_{oil}	Extracted oil mass	(g)
$\dot{m}_E$	Output mass flow rate of the drying air	(kg/min)
$\dot{m}_M$	Mixture mass flow rate of the drying air	(kg/min)
$\dot{m}_R$	Recycling mass flow rate of the drying air	(kg/min)
Nu	Nusselt number	
OF	Objective function	
Pr	Prandlt number	
Re	Reynolds number	
t_D	Total drying time	(min)
T_G	Drying air temperature	(°C)
T_{G_0}	Room temperature	(°C)
$T_{G_{feed}}$	Drying air supply temperature	(°C)
T_S	Leaves temperature	(°C)
U_G	Internal energy of the drying air	(kJ/kg)
v	Air speed	(m/s)
V	Bed volume	(m^3)

V_G	Air volume	(m^3)
$\bar{X}$	Average moisture content of the leaves	(d.b.)
X^*	Equilibrium moisture content of the leaves	(d.b.)
Y	Moisture content of the drying air	(d.b.)
Y^*	Equilibrium moisture content of the drying air	(d.b.)
z	Spatial coordinate, parallel to the air flow	(m)
$\propto$	Parameter of Eq. (8)	
ΔP	Pressure drop	(Pa)
ε	Bed porosity	(m)
ℓ	A half of leaves thickness	(m)
λ	Heat of vaporization of pure water	(kJ/kg)
η	Fan efficiency	
ρ_G	Specific mass of the drying air	(kg/m^3)
ρ_S	Specific mass of the leaves	(kg/m^3)
Ψ	Drying rate	(kg/min^1)

Introduction

Tea, the second most consumed beverage in the world, after water only (FAO, 2016), is the result of solid-liquid extraction, in which the liquor is leached in hot water from fresh or dried leaves. The liquid extraction is between the unit operations that extract the functional properties of plants (Javed et al., 2022). The properties of the infusion obtained depend both on the leaves used and on the pre-treatment to which they were submitted. These properties can be calming, invigorating, therapeutic, or refreshing, and are directly related to the presence of essential oil in the plant matrix. Among the leaves most used to obtain therapeutic teas is guaco, or *Mikania glomerata* Sprengel, whose leachate has expectorant and bronchodilator properties.

In the literature, some studies have evaluated the influence of different heat treatments on the yield and composition of the extract obtained from guaco leaves. In terms of coumarin concentration, obtained after hydroalcoholic extraction of guaco leaves, it was reported that lyophilization results in a higher coumarin content, 17.7 mg/g, than that obtained after pre-treatment with spray dryer, 8.0 mg/g (E Silva et al., 2012). Furthermore, the coumarin contents obtained after drying in an oven at 40 °C are higher than those obtained from leaves dried in the shade (Borghi et al., 2019). For pre-drying at 50 and 60 °C, the temperature harmed the concentration of coumarin in the extract (Silva et al., 2018).

In general, the aforementioned research reports that temperature, which is the most relevant operational parameter in drying (Taskin et al., 2021), favors enzymatic and microbial action when reduced. This is due to the maintenance of water activity longer in the leaves. Higher temperatures can cause damage to the cellular matrix, that is, the temperature is directly related to the change in the chemical composition and structure of the plant tissue. Since many agricultural products, such as medicinal herbs, have a short supply period (Minaei et al., 2014), even interfering negatively in the extraction result, drying is essential to ensure biological stability and increase shelf life of these products (Tagnamas et al., 2021). Thus, for the drying operation to be successful, it must remove free water, preserve leaf quality, and minimize energy consumption (Tarhan et al., 2011). However, although it is known that the pre-heat treatment directly interferes with the composition and oil content obtained from leaves of *Mikania glomerata* Sprengel, the technical literature does not report studies that numerically optimized the extraction process considering the pre-heat treatment.

Drying, when compared to the other stages of production and commercialization, is the phase in which the highest energy consumption occurs, reaching 15% of the industrial demand (Majumder et al., 2021). In this context, during classical heated air drying, the air is blown through a heater to the drying unit, where it transfers heat to the leaves and takes the released water with it. So, the air leaving the equipment is at high temperature, but not saturated, which means a clear inefficiency in energy use (Pelegrina et al., 1999). One way to reduce waste heat is to recycle the air until it becomes saturated. However, this means an increase in drying time, as the driving force of mass transfer decreases.

Thus, the present study aimed to model and simulate the process of drying guaco leaves in a deep bed, to validate the lumped parameters model using estimated parameters in thin layer modeling and with distributed parameters; and, finally, to optimize the drying operation conditions with exhaust air recirculation, to minimize the ratio of energy consumption of drying by the amount of oil obtained after extraction.

Materials and methods

Guaco leaves were collected in Santa Terezinha de Itaipu-PR, between April and December 2018. After selection, the leaves were cut with an area of approximately 1 cm^2. The physical properties were mean thickness of 0.08 mm, bed porosity of 0.5383, and specific mass of 0.1847 kg/m^3. Moisture was determined in triplicate, using 2 g of samples, kept in an air circulation oven (SPLABOR, SP 100), with temperature control, at 105 ºC ± 3 ºC for 24 hours. The mass was obtained on a digital balance (Shimadzu, AXU220, with a precision of 0.0001 g).

Drying kinetics

The drying kinetics of the leaves in a deep bed was carried out in an experimental module constructed from a galvanized tube, 4260 mm long and 110 mm in diameter, an air fan, and two electrical resistances of 2000 W. The sheets formed a bed 75 mm height, supported by a cylindrical structure, 87 mm in diameter.

The experimental conditions of drying air were 40 and 70 ºC, and 2.2 and 4.4 m/s, in addition to the central point, 55 ºC, and 3.3 m/s. Every five minutes, the samples were weighed on an analytical balance (KERN, PCB 3500-2 with a precision of 0.01 g), being placed back in the dryer immediately after each weighing. The process was repeated until constant mass.

Mathematical modeling

As in modeling and simulation, it is always interesting to use the simplest model, if it adequately describes the process, in the present work, we chose to use a phenomenological mathematical model of lumped parameters. For this, we evaluated the parameters external mass transfer coefficient, k_F, and effective mass diffusivity coefficient, D_{eff}, adjusted in a previous paper (Martins et al., 2021). These data were obtained for the drying of guaco leaves, in the solution of a distributed and thin layer parameter model.

For the mathematical model formulation, the double resistance to mass transfer model was considered (which considers both the diffusion resistance and the external resistance to mass transfer), and the LDF (Linear Driving Force) model:

$$\Psi = \Psi_S = \Psi_F \tag{1}$$

$$\Psi_S = k_S[\bar{X}(z,t) - X^*(z,t)]m_{DS} \tag{2}$$

$$\Psi_F = k_F a V_G[Y^*(z,t) - Y(z,t)] \tag{3}$$

In which Ψ is the drying rate (kg/min), k_S is the internal mass transfer coefficient (min^{-1}), $\bar{X}$ is the average moisture content of the leaves in dry basis (d.b.), X^* is the equilibrium moisture content of the leaves (d.b.), m_{DS} is the dry mass of leaves (kg), ε is the bed porosity, k_F is the external mass transfer coefficient (kg/m^2 min), a is the specific area (m^{-1}), V_G is the air volume (m^3), Y^* is the moisture content of the drying air (d.b.), and Y is the moisture content of the drying air (d.b.).

The modeling of the drying process also considered that the leaves formed a fixed bed with homogeneous distribution; heat losses through the dryer walls were negligible; initial bed moisture content and temperature were uniforms; there was one-dimensional transport of heat and mass in the bed; there was a uniform distribution of temperature, moisture content and air velocity at the entrance of the dryer; and that the drying air behaved like an ideal gas.

The final model obtained was:

$$\rho_S(1-\varepsilon)V\frac{\partial X}{\partial t} = \Psi \tag{4}$$

$$\frac{\partial}{\partial t}[Y(z,t)\rho_G(z,t)]\varepsilon = -v\varepsilon\frac{\partial}{\partial z}[Y(z,t)\rho_G(z,t)] - \rho_S\frac{\partial X(z,t)}{\partial t}(1-\varepsilon) \tag{5}$$

$$\rho_S\frac{\partial H_S(z,t)}{\partial t}(1-\varepsilon) = \lambda\rho_S\frac{\partial X(z,t)}{\partial t}(1-\varepsilon) + h_c[T_G(z,t) - T_S(z,t)] \tag{6}$$

$$\frac{\partial}{\partial t}[\rho_G(z,t)U_G(z,t)]\varepsilon = \\ -\lambda\rho_S\frac{\partial X(z,t)}{\partial t}(1-\varepsilon) + h_c[T_S(z,t) - T_G(z,t)] - v\varepsilon\frac{\partial}{\partial z}[\rho_G(z,t)H_G(z,t)] \tag{7}$$

In which ρ_S is the specific mass of the leaves (kg/m), ε is the bed porosity, V is the bed volume (m^3), ρ_G is the specific mass of the drying air (kg/m^3), v is the air speed (m/s^1), z is the spatial coordinate, parallel to the air flow (m), h_c is the volumetric coefficient of the heat transfer (kJ/min^1 m^3 °C^1), H_S is the enthalpy of the leaves (kJ/kg), λ is the heat of vaporization of pure water (kJ/kg), T_G is the drying air temperature (°C), T_S *i*s the leaves temperature (°C), U_G is the internal energy of the drying air (kJ/kg), and H_G is the enthalpy of the drying air (kJ/kg).

The relation used for the internal mass transfer coefficient parameter, k_S, and the effective mass diffusivity coefficient parameter, D_{eff}, for flat plates, necessary for the resolution of the model, was (Mosca et al., 2010):

$$k_S = \propto \frac{D_{eff}}{\ell^2} \tag{8}$$

In which $\propto$ is equivalent to 3 for flat plates, D_{eff} is the coefficient of effective mass diffusivity (m^2/min), and ℓ is a half of leaves thickness (m).

To calculate the heat transfer coefficient, h_c, the equation valid for fixed bed was used (Whitaker, 1972):

$$Nu = \left(0.5Re^{1/2} + 0.2Re^{2/3}\right)Pr^{1/3} \quad (9)$$

In which *Nu*, *Re*, and *Pr* are the Nusselt, Reynolds, and Prandlt numbers.

To solve the differential equations system, Eq. (4) to (7), together with Eq. (2) and (3), the entire simulation was conducted in Maple 13® software. First, 10 spatial discretization elements were used, followed using the Rosenbrock numerical method, through the *dsolve* routine to solve the algebraic differential system obtained.

The parameter $\propto$ from Eq. (8) was adjusted using the Nonlinear Simplex optimization method, in the *NLPSolve* routine. The parameters were determined after minimizing the quadratic deviation of leaf moisture content (calculated value and experimental value).

Optimization

The optimized drying process was simulated based on Figure 1, consisting of an air fan, followed by a heater, a bed of guaco leaves, and a pipe that divides the flow of exhaust and recirculation air.

Fig 1 Deep bed drying process with recirculation

At first, fresh air enters the circuit, filling the pipe, and then being moved by the fan and heated by the heater. After passing through the bed of guaco leaves, part of the exhaust air is discarded into the environment and another part is recirculated and mixed with a portion of ambient air.

The energy required to move the drying air was calculated by:

$$E_{Fan} = \eta \Delta P v \quad (10)$$

In which E_{Fan} is the total energy required to move the drying air (kJ/min), η is the fan efficiency, and ΔP is the drop pressure (Pa).

For optimization, the efficiency of the axial fan was considered 80% (ASHRAE, 1985). As for the pressure drop, only the head loss due to the bed itself was considered. To this end, the empirical equation obtained for a bed of alfalfa leaves was applied (ASABE, 2011):

$$\Delta P = \frac{6.4 \times 10^4 vL}{log(3.99v + 1)} \quad (11)$$

In which L is the bed height (m).

The energy required to heat the drying air from room temperature to the dryer operating temperature was calculated by:

$$E_{Heat} = t_D v A \varepsilon \int_{T_{G_0}}^{T_{G_{feed}}} \rho_G H_G dT_G \quad (12)$$

In which E_{Heat} is the total energy consumed to heat the drying air (kJ/min), t_D is the total drying time(min), A is the cross-sectional area to the air flow (m^2), T_{G_0} is the room temperature (°C), $T_{G_{feed}}$ is the drying air supply temperature (°C), and cp_G is the specific heat of the drying air (kJ/kg °C).

The recirculation ratio was defined as:

$$q = \frac{\dot{m}_R - \dot{m}_E}{\dot{m}_M} \quad (13)$$

In which $\dot{m}_R$ is the recycling mass flow rate of the drying air (kg/min), $\dot{m}_E$ is the exhaust mass flow rate of the drying air (kg/min), and $\dot{m}_M$ is the mixture mass flow rate of the drying air (k/min).

In the simulations for the optimization, the minimization of the energy consumption ratio to heat and move the drying air, by the mass of oil obtained after extraction, was used as an objective function:

$$OF = min \frac{E_T}{m_{oil}} \tag{14}$$

In which OF is the objective function, E_T is the sum of Eq. (10) and (12), and m_{oil} is the extracted oil mass (g).

The oil extracted mass as a function of drying temperature was estimated from experimental data from the literature (Coradi et al., 2018). These authors, in drying and extracting oil from guaco leaves, observed that higher drying temperatures reduced the yield of essential oil obtained.

The speed and temperature of the drying air, as well as the recirculation rate, were considered manipulable variables. Thus, the objective function, Eq. (14), was subject to the restrictions:

$$30\ °\mathrm{C} \leq T_{G_{feed}} \leq 70\ °\mathrm{C} \tag{15}$$

$$1\ \mathrm{m\ s^{-1}} \leq v \leq 5\ \mathrm{m\ s^{-1}} \tag{16}$$

$$0\% \geq q \leq 100\% \tag{17}$$

The simulations were carried out until the average leaf bed moisture content of 10% was reached, considered adequate for the storage of herbal medicines. The conditions evaluated were 25 ºC for the ambient temperature, 0.6096 m for the bed height, and 0.1090 m^2 for the cross-sectional area of the airflow (Brooker et al., 1974), initial moisture content of 4 d.b. for the leaf bed, and ambient relative moisture content of 60%.

Results and Discussion

Drying kinetics

Table 1 presents the estimated values for the coefficient $\propto$ of Eq. (8), which relates the internal mass transfer coefficient and the effective mass diffusivity for flat plates. Also, the statistical results of the comparison between the experimental values and those calculated by the model for the average moisture content of the bed of guaco leaves are presented.

Table 1 Estimated parameters and statistical results

$T_{G_{feed}}$(ºC)	Speed (m/s)	$\propto$	R^2
40	2.2	3.08	0.92
	4.2		0.99
55	3.2	3.24	0.99
70	2.2	3.25	0.97
	4.2		0.99

In turn, Figure 2 shows the experimental and calculated drying kinetics for the average bed moisture.

Fig 2 Drying kinetics of the bed of guaco leaves. (a) 40 ºC, (b) 55 ºC, (c) 70 ºC. The continuous line represents predicted values, and individual points are measured values (□ 2.2 m/s, △ 3.2 m/s, and ○ 4.2 m/s)

As observed in Table 1 and Figure 2, it is observed that the higher the drying temperature, the faster the mass transfer process between the leaves and the air. The drying times varied between 500, 250, and 120 min, for 40, 55, and 70 ºC. This increase in the mass transfer rate is directly related to the effective mass diffusivity values, which are an Arrhenius function of temperature. In practice, the higher the temperature, the greater the excitation of the molecules and the lower the viscosity of moisture, thus facilitating mass transfer by diffusion. Similar results are reported in literature for others leaves with medicinal properties as jatilao (Mondal et al., 2021), papaya (Yap et al., 2020), and mint (Moradi et al., 2020).

The estimated values for the coefficient $\propto$, which in theory for flat plates would be equal to three, varied between 3.08 and 3.25, for temperatures of 40 and 70 ºC. These values indicate that the relationship of Eq. (8) for the internal mass transfer coefficient and the effective mass diffusivity can be used. This statement is supported by the statistical results in Table 1, which indicate that all values of the correlation coefficient, R^2, were equal to or greater than 92%.

Optimization

After the validation of the mathematical model of lumped parameters in the deep bed, and the technique of using the mass transfer coefficients obtained for the model of parameters distributed in the thin layer, the optimization of the objective function was carried out, which relates the energy consumption and the mass of oil obtained after extraction, Eq. (14).

The optimal conditions found after solving the model concomitantly with the optimization process of Eq. (14), submitted to the restrictions of Eq. (15) to (17) were temperature of 30.02 ºC, speed of 1.0 m/s, and recirculation rate of 0.129. These operating conditions (considering the process presented in Figure 1) resulted in 4.05×10^5 kWh per kg of extracted oil, which was the lowest ratio obtained numerically during the proposed optimization.

In Figure 3 the graphic results of the optimization are presented, relating temperature, $T_{G_{feed}}$, and drying airspeed, v, with the ratio energy consumption and the oil mass extracted from guaco leaves, OF, for the optimal recirculation rate, $q = 0.129$.

Fig 3 Energy consumption per mass of oil extracted as a function of drying air conditions

From Figure 3, maintaining the exhaust air recirculation rate, lower drying airspeeds, v, and temperatures, $T_{G_{feed}}$, resulted in lower kWh ratios per kg of extracted oil, $\frac{E_T}{m_{oil}}$. This behavior was expected, since, according to Eq. (10) and (12), higher drying airspeeds and temperatures require higher amounts of energy. And, according to the experimental data in the literature, higher pre-treatment temperatures by drying can cause damage to the plant matrix, destroying it, which can inhibit the easy exit of the oil and decompose it thermally.

Figure 4 shows the relationship between the recirculation ratios, q, and drying temperature, $T_{G_{feed}}$, with energy consumption, E_T, obtained by the sum of Eqs. (10) and (12), at fixed airspeed of 1.0 m/s.

Fig 4 Energy consumption as a function of recirculation rate and drying temperature

From Figure 4 under a fixed operating temperature of the dryer, the increase in the recirculation ratio, q, decreases the energy consumption of the process. This recirculation ratio increases the mixing temperature of the air entering the system, reducing the energy required by the heater to raise the temperature to the dryer's operating condition, E_{Heat}, due to the reduction of the thermal gradient. These results are opposite to those recently presented for rice drying using exhaust air recirculation (Wang et al., 2022). This is because the process energy consumption is affected by the initial moisture content of the deep bed. Depending on this, the recirculation rate could transport the water by the exhaust air, reducing the driving force for the mass transfer between the air and the solid. Thus, the drying time could increase, which causes greater energy consumption. These results ratify the importance of evaluating energy parameters in processes that involve drying operations, making the selection of operating conditions more accurate from an economic point of view.

In Figure 5 are shown, respectively, the response surfaces for the drying time, t_D, and in Figure 6 are shown the extracted mass oil, m_{oil}, as a function of drying speed, v, and air temperature, $T_{G_{feed}}$, for the optimal recirculation ratio. (0.129).

Fig 5 Drying time as a function of drying air speed and temperature

Fig 6 Extracted mass oil as a function of drying air speed and temperature

As expected from Figures 5 and 6, it is observed that lower pre-heat treatment temperatures of the guaco leaves resulted in longer drying times and higher oil mass extracted. On the other hand, the drying air velocity did not influence the drying time and the oil mass obtained after extraction.

Conclusion

A technique was tested to describe the drying kinetics of guaco leaves, applying the mass transfer coefficients from a thin layer model and distributed parameters in a deep bed model and lumped parameters. After validating the model, it was used to optimize the process of extracting oil from the leaves based on their pre-heat treatment. The optimization consisted of the numerical minimization of the relation between the energy required to heat and move the drying air and the mass of oil subsequently extracted in a dryer that operates with recirculation of exhaust air.

Considering an operating range between 30 and 70 ºC, 1.0 and 5.0 m/s, and recirculation between 0 and 1, the optimal conditions obtained were 30.02 ºC, 1.0 m/s, and a recirculation ratio of 0.129. Under these conditions, the minimum objective function ratio, 4.05×10^5 kWh/kg, was obtained. These results indicate that operating the dryer with recycling at lower temperatures and drying airspeeds leads to lower energy costs and higher levels of oil later extracted. Exhaust air recirculation is essential to reduce energy consumption, however, due to the high initial humidity of fresh guaco leaves, high recycle ratios are not indicated as they reduce the driving force of mass transfer.

Conflicts of interest/Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Figures

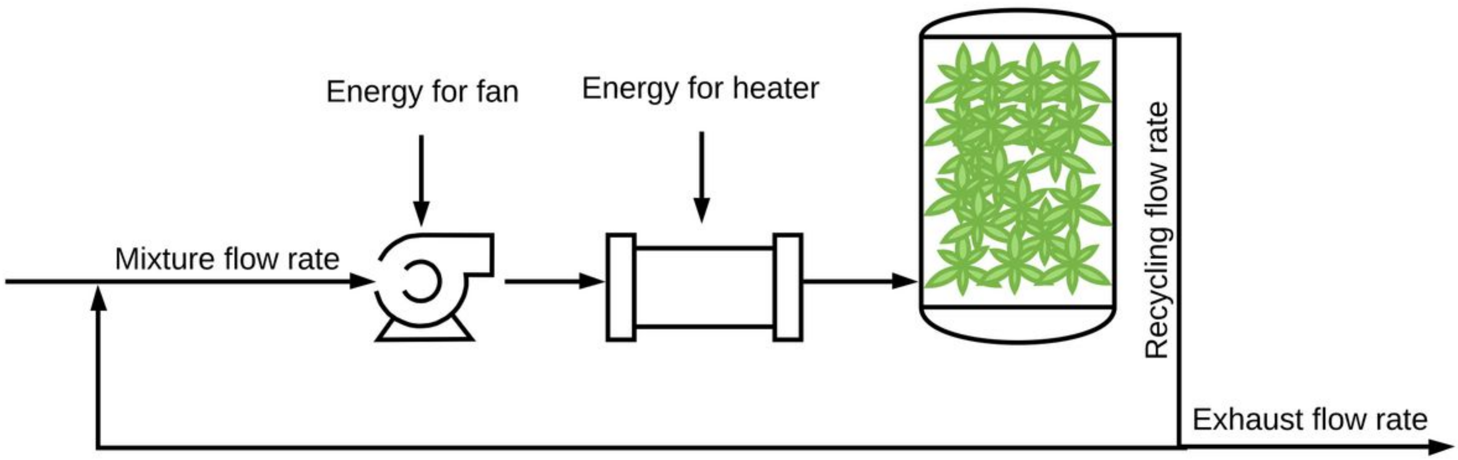

Figure 1

Deep bed drying process with recirculation

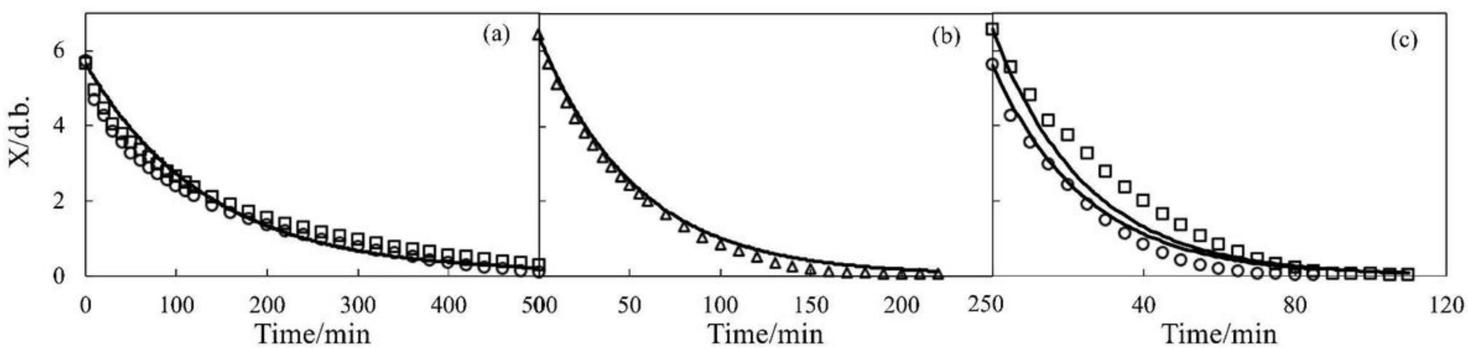

Figure 2

Drying kinetics of the bed of guaco leaves. (a) 40 ºC, (b) 55 ºC, (c) 70 ºC. The continuous line represents predicted values, and individual points are measured values (2.2 m/s, 3.2 m/s, and 4.2

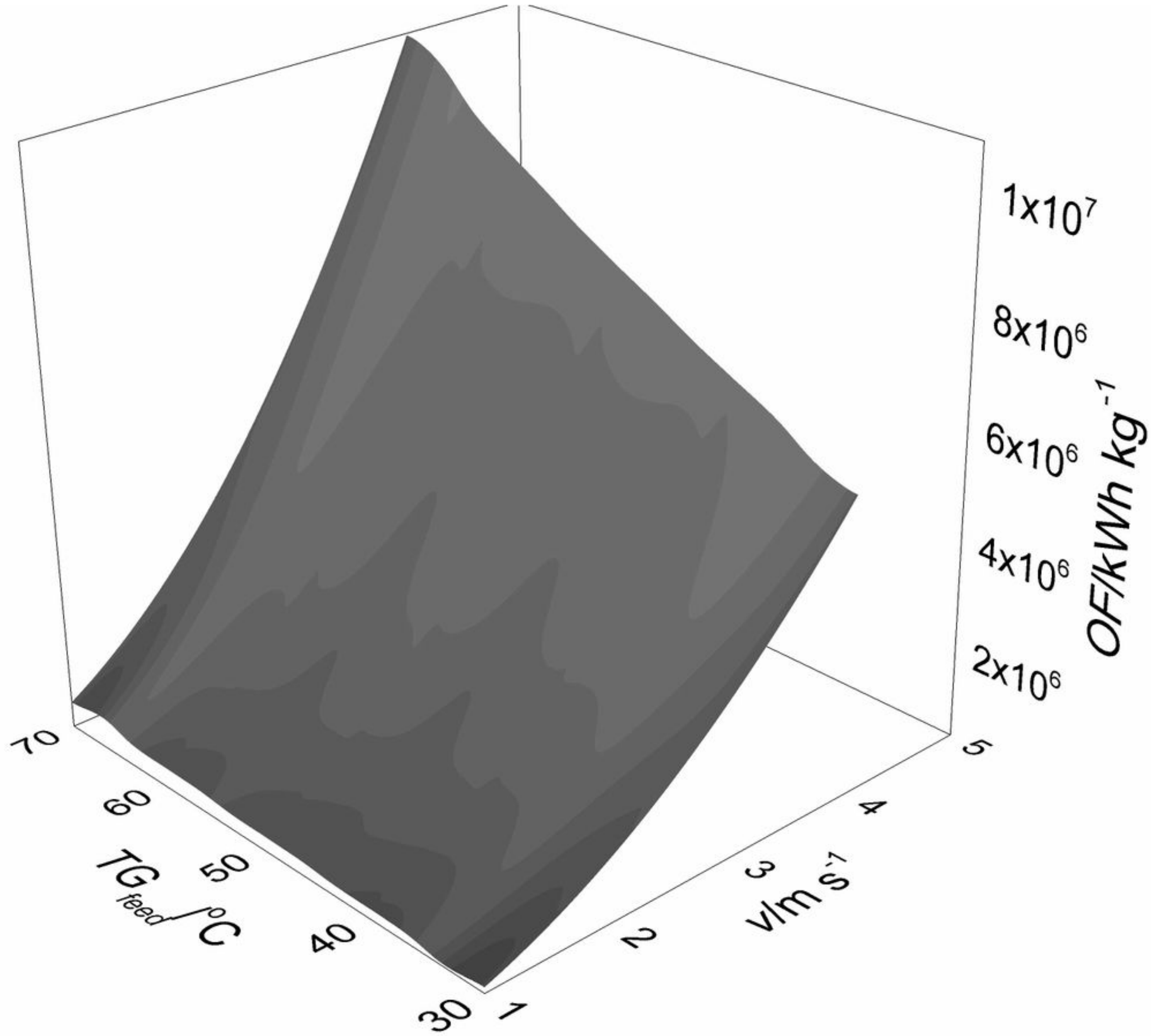

Figure 3

Energy consumption per mass of oil extracted as a function of drying air conditions

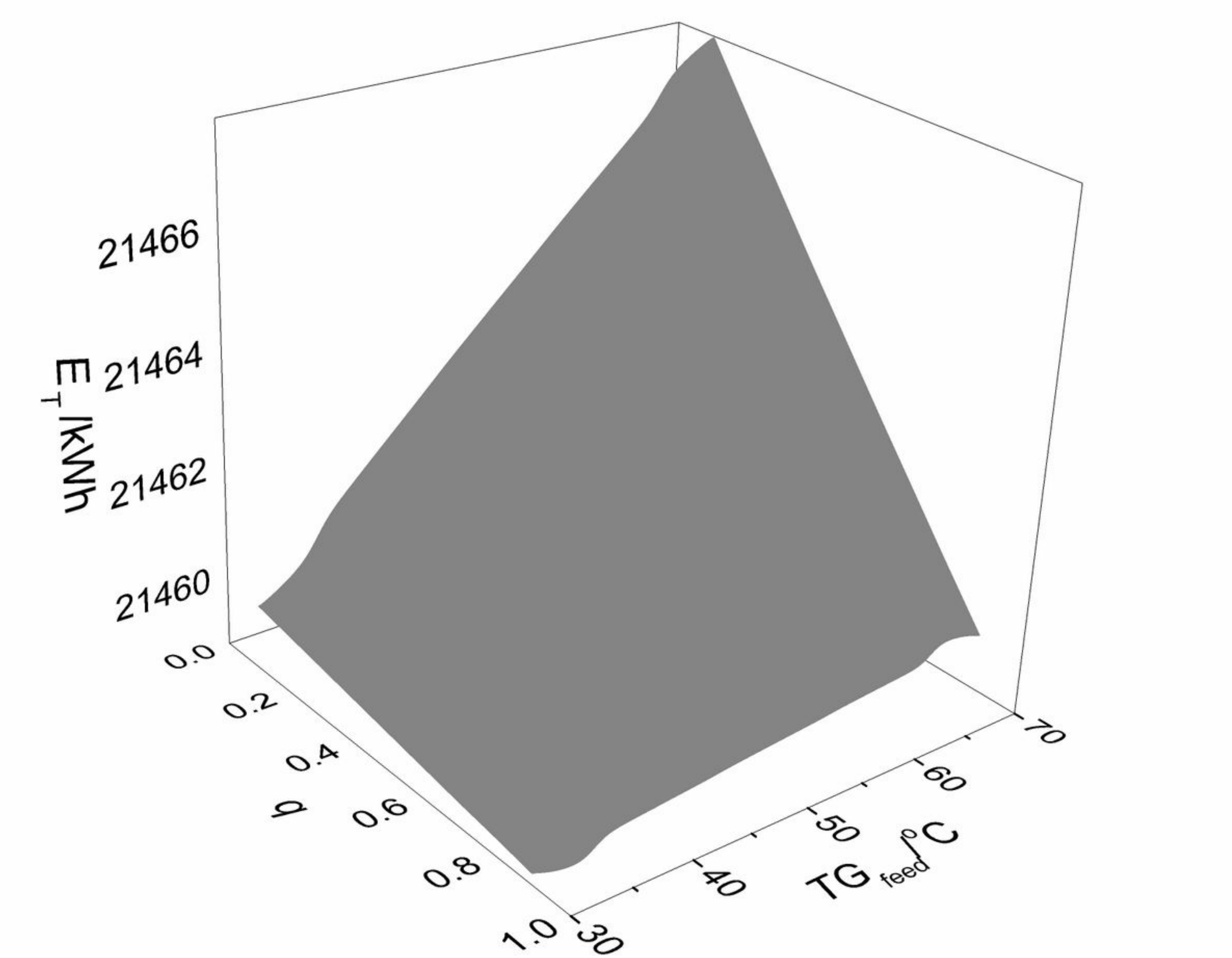

Figure 4

Energy consumption as a function of recirculation rate and drying temperature

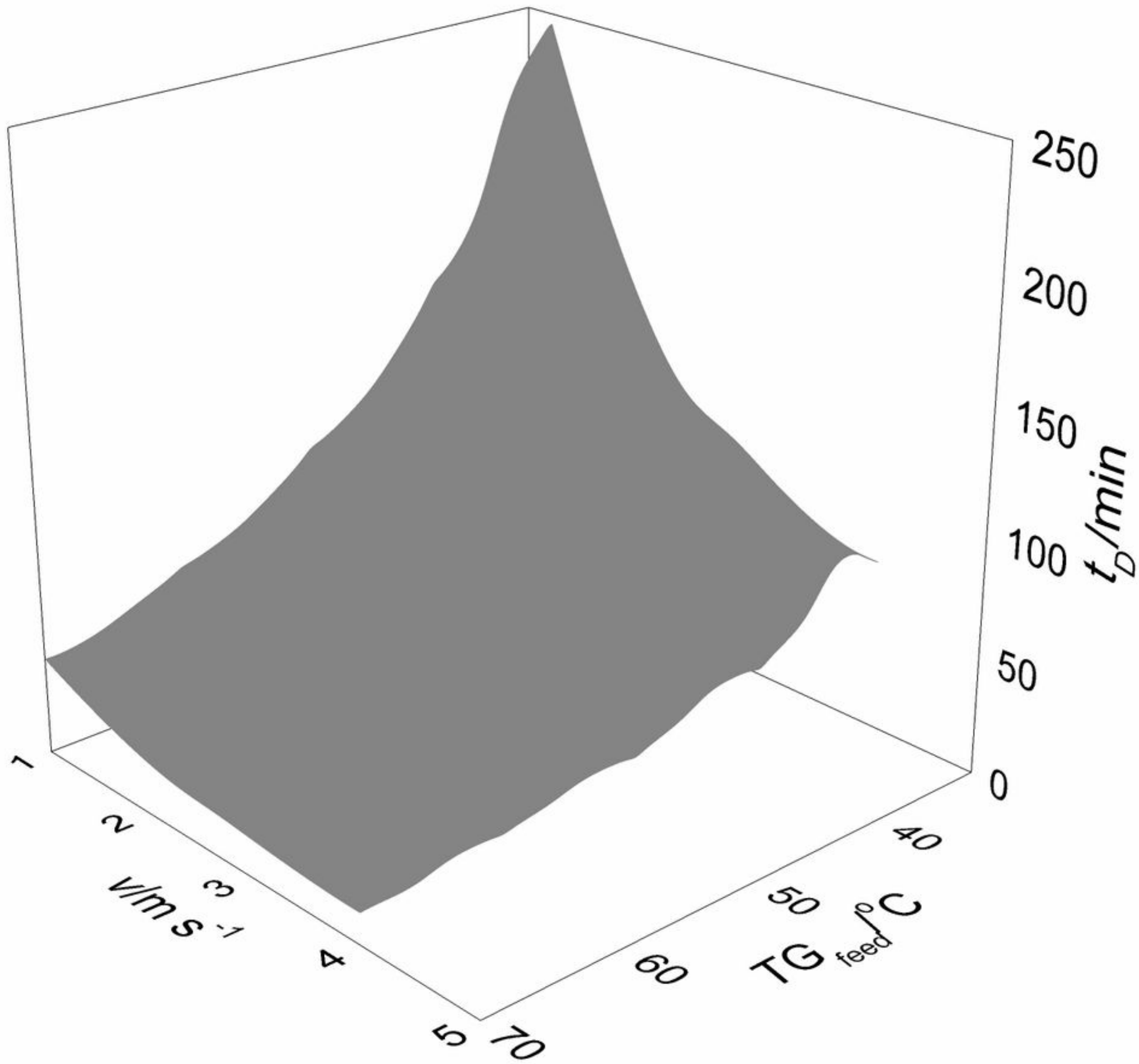

Figure 5

Drying time as a function of drying air speed and temperature

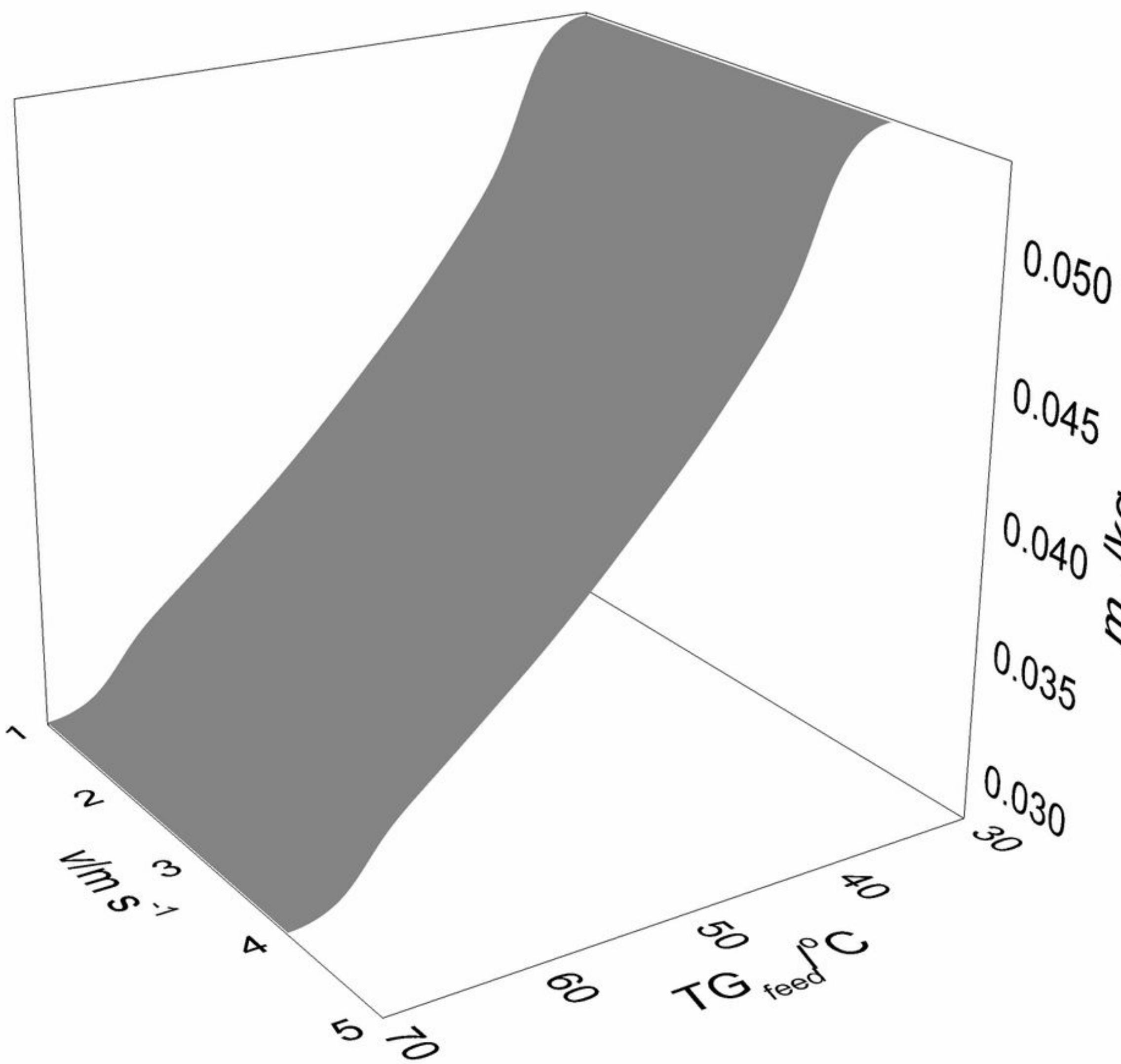

Figure 6

Extracted mass oil as a function of drying air speed and temperature