MODELING FOR VERIFICATION OF THE SOYBEAN OIL CONTENT IN HEXANE MISCELLA USING DENSIMETER

MODELAGEM PARA VERIFICAÇÃO DO TEOR DE ÓLEO DE SOJA EM MISCELA DE HEXANO UTILIZANDO DENSÍMETRO

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ABSTRACT: Soybean is one of the most important crops in Brazil since the grain and its primary derivatives (bran and oil) are exported to several countries and widely used in various industrial segments, contributing to the national economy. The extraction of crude oil by hexane solvent is the most applied method in industries, with miscella being the intermediate result of this process. The yield and efficiency of the extraction are verified by analyzing the concentration of oil present in it. The analytical method used by industries in general consists of solvent evaporation, which requires about two hours to obtain results. The research aimed to build a mathematical model to calculate the oil concentration from the temperatures and specific masses of the solvent, soybean oil and miscella, measured with a densimeter and thermometer, optimizing the time and cost of this analysis. In addition to savings for the industry, with faster results, the operator can act in the process and prevent the error and losses from continuing if the result points to failure in the operational regime. To validate the mathematical model, the results obtained in the modeling were compared with those obtained by the hexane solvent evaporation method, which were very approximate from the industry perspective. The mean absolute difference between the results of the methods was 0.21% in samples with oil concentration below 38%. It is concluded that the method can be implemented as a tool to optimize the analysis of soybean oil concentration in the hexane miscella.

Keywords: Soybean, Soybean oil extraction, Hexane miscella, Mathematical model, densimeter.

Resumo: A soja é uma das culturas mais importantes do Brasil, visto que o grão e seus derivados primários (farelo e óleo) são exportados para diversos países e amplamente utilizados em vários segmentos industriais, contribuindo para a economia nacional. A extração do óleo bruto de soja pelo solvente hexano é o método mais aplicado nas indústrias, sendo a miscela o resultado intermediário deste processo. O rendimento e a eficiência da extração são verificados analisando a concentração de óleo presente na mesma. O método analítico utilizado pelas indústrias em geral consiste na evaporação do solvente, que leva cerca de duas horas para obter resultados. A pesquisa teve como objetivo construir um modelo matemático para calcular a concentração de óleo a partir das temperaturas e massas específicas do solvente, óleo de soja e miscela, medidos com densímetro e termômetro, otimizando o tempo e custo desta análise. Além da economia para a indústria, com resultados mais rápidos, o operador pode atuar no processo e evitar que o erro e prejuízos continuem caso o resultado aponte falha no regime operacional. Para validar o modelo matemático, os resultados obtidos na modelagem foram comparados com os obtidos pelo método de evaporação do solvente hexano, que foram bastante aproximados do ponto de vista industrial. A diferença média absoluta entre os resultados dos métodos foi de 0,21% nas amostras com concentração de óleo abaixo de 38%. Conclui-se que o método pode ser implementado como uma ferramenta para otimizar a análise da concentração de óleo de soja na miscela de hexano.

Palavras-chave: Soja, Extração de óleo de soja, Hexano miscella, Modelo matemático, densímetro.

Introduction

Soybeans (Glycine Max L.) belongs to the dicotyledonous class and legume family. It is a grain with a unique chemical composition, rich in protein and oil, with approximately 40% protein, 35% carbohydrates, 20% oil, and 5% ash (on a dry basis) (Hofmann, 2012).

The soybean crop is one of the most important in the country since the grain and its derivatives are widely used in several industrial segments. Brazil is the world's largest producer of grain, according to *CONAB* (2020), with 124.845 million tons harvested and a planted area of 36.950 million acres. Followed by the United States with a production of 96.67 million in an area of 30.332 million acres (USDA, 2020). Soybean is mainly intended for the production of animal feed (in the form of husk or bran) or for human consumption (refined oil). However, the legume is also used in the manufacture of paints, in the adhesives industry, in foam formulators, fertilizers, fiber manufacturing, cosmetics and in the pharmaceutical industry. (*Fundação Cargill*, 2009).

Hexane is the most used solvent in soybean oil extraction, as it easily dissolves the oil; it has a homogeneous composition and a narrow boiling temperature range; is immiscible in water; and has a low latent heat of boiling (Mandarino; Hirakuri; Roessing, 2015). The liquid mixture of soybean oil and hexane that comes out of the extractor is called a miscella.

The relationship between the amount of solvent and raw material used, according to Bley (2007), plays an important role in the industry, which works in a continuous system. Also according to the author, the greater the amount of solvent per volume of raw material that enters the extractor, the greater the energy expenditure for pumping the miscela and distillation (separation of oil and solvent).

The analysis of oil concentration present in the miscella is very relevant since it represents the extraction yield. If the percentage of oil in the miscella is below normal (expected standard) it means that oil retained in the raw material residue is being lost, causing damage to the industry. The greater the financial loss, the longer it takes to find the aforementioned inefficiency (Bley, 2007).

Our work is justified because the traditional method for checking the oil concentration in the miscella consists of a laboratory procedure of hexane evaporation and oven drying, which can take two hours or more to obtain a reliable result. During this time the losses can be considerable, if the final results do not reach the expected standard, not to mention the maintenance costs of permanently connected electric stoves (Hahn, 2020).

Based on the above, the objective of this work was to build a mathematical model to calculate the oil concentration from physicochemical characteristics such as temperature and specific mass of the solvent, soybean oil and miscella, measured with a densimeter and thermometer, optimizing the time and cost of this analysis, which represents an important innovation for industries that can optimize the analysis of oil concentration in miscella using a densimeter and a mathematical model. Thus, we present the research subsequently, initially approaching some theoretical aspects.

In order to achieve the objectives we use a methodology. Thus, in terms of nature, this study was considered applied and with a quantitative approach since, according to Nascimento and Souza (2016), the applied research seeks knowledge to solve specific problems and the quantitative approach seeks to validate hypotheses through analysis, this analysis of process variables using statistical techniques

Theoretical development

Extraction of soybean oil with hexane solvent

N-hexane is a mixture of hydrocarbons produced from the distillation of naphtha, where its distillation range comprises temperatures between 62 and 74 °C and is highly flammable (Portantilo, 2011).

Most of n-hexane used in industry, according to Pubchem (2020), is mixed with similar chemicals called solvents, being of main use to extract vegetable oils from crops such as soybeans. And being used on a large scale, this mixture of solvents is directly linked to cost reduction.

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Table 1 shows the physicochemical data of hexane, according to Pubchem (2020).

Table 1 - Physical-chemical characteristics of n-hexane.

Chemical formula	**C6H12**
Molar mass	86.18 g/mol
Boiling point (1atm)	69 ºC
Density (20 ºC)	0.66 g/cm³
Flash point	- 22 ºC
Ignition temperature	240 ºC
Melting point	- 94.3 ºC
Steam pressure (20 ºC)	160 hPa
Kinematic viscosity (20 ºC)	0.50 mm²/s
Solubility	0.0095 g/L
Storage temperature	5 – 30 ºC

Source: (Pubchem, 2020)

Table 2 shows the specific masses as a function of hexane temperature, according to Perry and Green (2007).

Table 2 - Specific mass of hexane at different temperatures.

Temperature in Kelvin [K]	**Specific mass [mol/dm³]**	**Temperature in Celsius [°C]**	**Specific mass [kg/m³]**
255	8.0472	-18	693.5
270	7.8927	-3	680.2
285	7.7363	12	666.7
300	7.5774	27	653.0
315	7.4151	42	639.0
330	7.2487	57	624.7

Source: (Perry; Green, 2007).

The oil is obtained by extracting hexane with an organic chemical solvent through the percolation of the solvent through the bed of solids, that is, the solvent is squirted onto the bed composed of soy blades that move horizontally in the extractor, in countercurrent with the hexane (Mandarino; Roessing, 2001; Tomazin, 2008). These seeds, after being prepared in flakes, are placed in a suitable environment together with the solvent in order to transfer of the oil from the solid phase to the liquid phase. (Milligan & Tandy, 1984).

In this way, the oil present in the soybean is solubilized and dragged out of the solid material. In this step, two by-products result: the solids cake (mixture of soybean ran, hexane, water, and residual oil) and the miscella, which is the liquid mixture of oil and hexane at a concentration of approximately 32% by mass of oil. After extraction, solvent recovery is necessary, so the solids cake goes to desolventization and the miscella to distillation (Mandarino; Roessing, 2001; Tomazin Junior, 2008).

The miscella that has a higher concentration of oil in its composition is called a fat/strong miscella, so it has a higher specific mass in relation to the lean/weak miscella, which in turn has a lower concentration of soybean oil and a grater amount of hexane solvent in its composition. The weak miscella is obtained in the first bath of pure solvent that the raw material receives inside the extractor (Hahn, 2020).

Preceding mathematical model

The model proposed by Hahn (2020) is based on the principle of conservation of the masses of the components of the miscella, performing a calculation of the mass fractions of oil and hexane from their specific masses and considering steady state, ideal and constant volume, the variables of specific heat at constant pressure (Cp) and specific heat at constant volume (Cv).

The deduction steps are described below, according to Hahn (2020), to arrive at his model. Assuming that the process operates continuously in steady state, the global mass balance adapted for the soybean oil extraction process is given by Equation 1.

$$m_S + m_H = m_M + m_{SI} \tag{1}$$

being m_S the soybean mass (kg), m_H the hexane mass (kg), m_M the miscella mass (kg) and m_{SI} the inert solids mass (kg).

For the miscela mass composition, we have Equation 2:

$$m_M = m_{Ol} + m_H \tag{2}$$

being m_{Ol} soybean oil mass (kg).

For the volumetric composition of miscella, we have Equation 3:

$$V_M = V_{Ol} + V_H \tag{3}$$

being V_M the miscela volume (m³), V_{Ol} the oil volume (m³) and V_H the hexane solvent volume (m³).

Considering that the specific mass (ρ) in kg/m³ of the miscella is the ratio between its mass and its volume, we have Equation 4.

$$\rho_M = \frac{m_M}{V_M} \tag{4}$$

being ρ_M the specific mass of the miscella (kg/m³), m_M the mass of the miscella (kg) and V_M the volume of the miscella (m³).

From Equation 4, isolating V_M, Equation 5 is obtained:

$$V_M = \frac{m_M}{\rho_M} \tag{5}$$

Since the volume of the miscella results from the sum of the hexane and oil volumes, replacing V_M from Equation 4, by the sum demonstrated in Equation 3, gives Equation 6:

$$\rho_M = \frac{m_M}{V_{Ol}+V_H} \tag{6}$$

Thus, the ratio of Equation 5 applied to the volumes of oil and hexane of Equation 6, gives rise Equation 7.

$$\rho_M = \frac{m_M}{\frac{m_{Ol}}{\rho_{Ol}}+\frac{m_H}{\rho_H}} \tag{7}$$

being ρ_M the specific miscela mass (kg/m³), m_M the miscela mass (kg), m_{Ol} the soybean oil mass (kg), ρ_{Ol} the soybean oil specific mass (kg/m³), m_H hexane mass (kg) and ρ_H hexane specific mass (kg/m³).

Also according to Hahn (2020), hexane and crude soybean oil have different specific masses, in this way, when we combine these two liquids to form a miscella, the resulting specific mass for this solution depends on the present amount (mass fraction) of each of the components in the mixture.

Considering that the percentage is a centesimal fraction, the mass of the miscella (mM) of Equation 7 was replaced by the number 100. Likewise, the mass of oil (m_{Ol}) and that of hexane (mH), gave rise to the concentrations of oil and hexane relative to the total 100. With this, the mass fractions of oil and hexane assume the percentage value of each in the mixture, resulting in Equation 8.

$$\rho_M = \frac{100}{\frac{C_M^{Ol}}{\rho_{Ol}} + \frac{C_M^{H}}{\rho_H}} \tag{8}$$

being ρ_M the specific mass of the miscella (kg/m³), ρ_{Ol} the specific mass of soybean oil (kg/m³), ρ_H the specific mass of hexane (kg/m³), C_M^{Ol} the mass concentration of soybean oil present in the miscella (%) and C_M^H the percentage of hexane in the miscella.

Bearing in mind the specific weights of the miscella, solvent, and soybean oil, to calculate the percentage oil in the sample, this must be the only variable. For this the percentage of solvent (C_M^H) in Equation 8 was replaced by the difference between the total (100%) and the percentage of oil (C_M^{Ol}), resulting in Equation 9.

$$\rho_M = \frac{100}{\frac{C_M^{Ol}}{\rho_{Ol}} + \frac{100 - C_M^{Ol}}{\rho_H}} \tag{9}$$

Finally, performing the base change by inverting numerator and denominator, Hahn (2020) obtained Equation 10, which represents the previously proposed model.

$$\rho_M = \left[\left(\frac{C_M^{Ol}}{\rho_{Ol}} + \frac{\left(100 - C_M^{Ol}\right)}{\rho_H}\right)/100\right]^{-1} \tag{10}$$

being ρ_M the specific miscela mass (kg/m³), C_M^{Ol} soybean oil concentration presents in miscella (%), ρ_{Ol} the soybean oil specific mass (kg/m³) and ρ_H the hexane solvent specific mass (kg/m³).

The model by Hahn (2020) model showed goods results when verifying oil concentration by density, however, it is limited by requiring that the miscella, oil and hexane be measured at the same temperature of 20 °C to use it.

As a result, the present work improved the model proposed by Hahn (2020), employing differential calculation and allowing the collection of the specific mass of the samples at any temperature, in a compatible range between room temperature and the collections in industrial extractors.

Methodology

Research ranking

With reference to the classificatory principles of Gil (2017), the research can be differentiated in terms of nature, methods or approach, in terms of objectives and procedures.

Thus, in terms of nature, this study was considered applied and with a quantitative approach, since, according to Nascimento and Souza (2016), applied research seeks knowledge to solve specific problems and the quantitative approach seeks to validate the hypotheses through the analysis of process variables using statistical techniques.

Since the problem presented is a current reality of the industries and using mathematics it can be solved, becoming a landmark in the modeling of industrial processes, also allowing it to be extended it to other oilseeds.

Regarding the objectives, the research was classified as exploratory as it deepens the knowledge of the characteristics of a given phenomenon according to Richardson (2017), as well as explanatory because, according to Neuman (2019), it aims to describe processes. And it was classified as descriptive because it determines, according to Cervo, Bervian e Silva (2006) and Gil (2017), through the confrontation of variables, the factors or causes that determine or influence the manifestation of certain phenomena. Regarding the technical procedures, they were classified as bibliographic based on the basis raised.

Experimental Methodologies

From the samples of crude soybean oil and commercial hexane, the rates of variation of the specific masses, as a function of temperature, oil and hexane, were determined using densimeters and thermometer, comparing them with data from the literature to be used as input data in the model, which is deduced and explained later in this chapter.

Also, from the hexane and oil samples, 10 miscella samples of different concentrations were simulated in the laboratory, measuring the temperature and specific mass of each and, using the proposed model, the mass percentage of oil present in each of them was calculated. Next, the same samples were subjected to the heating and evaporation method of hexane in order to determine the oil concentration. This procedure aimed to compare the results obtained by the two methods and assess whether the model is viable, validating it or not.

To verify the specific mass of hexane, crude soybean oil and miscella, temperatures in the range of 17 ºC to 53 ºC were used. The upper limit (53 ºC) was defined as a function of the volatility and evaporation point of hexane and the temperature used in the industrial extraction process. The lower limit of 17ºC guarantees a wide range to validating the model and carrying out measurements in industrial laboratories, being below the average regional ambient temperature. Another factor that was considered is the rate of change in the specific mass of soybean oil, which, in theory, is no longer linear at temperatures below 16ºC, according to preliminary tests.

Rate of change: specific mass x temperature

In this procedure, 4 diving densimeters calibrated and certified by the National Institute of Metrology, Quality and Technology – INMETRO were used, with an acuracy of 0.0005 g.mL^{-1}. The densimeters used were: a densimeter for specific masses between 0.65 and 0.7 g.mL^{1}, one between 0.7 e 0.75 g.mL^{-1}, another between 0.75 and 0.8 g.mL^{-1} and another between 0.9 e 0.95 g.mL^{-1}. The results were converted to kg/m^{3}.

Approximately 750 mL of crude soybean oil was used and placed in an oven set at approximately 53°C for two hours. Then, using three 250 mL beakers, 230 mL of oil were added to each, the temperature was measured, and the sanitized densimeter was inserted into each sample doing the reading. The procedure was repeated for other temperatures between 17 °C and 53 °C, and also, for commercial hexane samples, totaling 10 measurements of each.

Then, applying the Ordinary Least Squares Method, the equations were found that relate the variation of the specific mass, as a function of temperature, for soybean oil and hexane. The variation rates extracted from the equations found were used in the mathematical model, as well as the average density (triplicate) and temperature of a hexane sample and an oil sample.

Determination of temperature and specific mass in miscella

Miscella samples were simulated from the approximate concentrations of 2, 5, 10, 15, 20, 25, 30, 35, 40 and 45% of oil in relation to hexane. Each sample had its specific mass measured at a different temperature, between 17 and 53 ºC, at approximately regular intervals of 2 to 4 ºC. To reach the lower temperatures, the samples were placed in a thermal box with ice, sealing the amber conditioning flasks of the samples. For higher temperatures, in an amber flask, the samples were taken to an oven, regulating the desired temperature.

According to procedure 2.1, the density and temperature of each simulated sample were measured. Both temperature and specific mass were used as input data for the model, which calculates the mass content of oil present in the sample.

Determination of oil concentration in miscella by evaporation

A flat-bottomed flask was weighed on an analytical balance. Then, a 100 mL sample of soybean oil miscella was added, weighing again. Subsequently, the flask was placed on a heating plate, with a fume hood on, evaporating the solvent. Soon after the flat-bottomed flask was left for 2 hours in the oven at 105 °C, to eliminate any remaining solvent. The flask rested in a desiccator for 30 minutes and was weighed on an analytical balance, recording the value. Thus, the heating and cooling procedure of the sample was repeated until reaching constant weight.

Finally, using Equation 11, the concentration of soybean oil (%) present in the sample was calculated.

$$C_M^{ol} = \frac{(m_{Ol} - m_b) \times 100}{(m_M - m_b)} \tag{11}$$

Being C_M^{ol} soybean oil concentration in the miscella (%), m_{Ol} the mass of the flask with soy oil obtained from the miscella (g), m_b the masso of the empty flat-bottomed flask used (g) and m_M the mass of the flask with the soy miscela sample (g).

Analysis and discussion of the experimental results and the mathematical model

Mathematical Model

Bearing in mind the specific mass of commercial hexane and crude soybean oil, it is possible to calculate the mass fractions of each of these components, and consequently, the percentage of each in the mixture, based on the specific mass of the miscella. Therefore, it is necessary that the measurement of the mass/volume ratio of oil, hexane and miscella be made at the same temperature. Or, that the equation used calculates and harmonizes the different temperatures, using the rates of variation of the specific masses as a function of temperature.

The temperature variation increments the model proposed by Hahn (2020). His Equation (10), can be rewritten as:

$$\rho_M = 100/\left(\frac{C_M^{Ol}}{\rho_{Ol}} + \frac{(100 - C_M^{Ol})}{\rho_H}\right) \tag{12}$$

Considering steady state, ideal and constant volume the variables of specific heat at constant pressure (C_p) and specific heat at constant volume (C_v).

From Equation (12), we introduce the temperature variable into the specific mass of the miscella, and the difference in relation to the temperatures of the crude soybean oil and hexane, so that measurements can be carried out at any temperature, for the miscella and anyone of the mixture components.

The model needs to determine what is the variation that these temperature differences cause in the specific mass of the oil and hexane when homogenizing them with the miscella temperature. Thus, the difference between the temperatures at which the oil and the miscella had their specific masses measured must be multiplied by the rate of variation (derivative) of the specific mass of the oil as a function of temperature, equating the temperatures and changing the initial specific mass of oil. The same reasoning applies to the hexane solvent.

From the above, in the specific masses of oil and hexane, in Equation 10, the variation that the difference between the temperature of the miscella and oil and between the miscella and hexane causes is added, when all temperatures are equal to that of the miscella. This result in Equation 13.

$$\rho_M^T = 100/\left(\frac{C_M^{Ol}}{\rho_{Ol}+(T_{Ol}-T_M).\frac{d\rho_{Ol}}{dT}}+\frac{(100-C_M^{Ol})}{\rho_H+(T_H-T_M).\frac{d\rho_H}{dT}}\right) \tag{13}$$

Being ρ_M^T the specific mass of the miscella (kg/m³) for the temperature of T °C, C_M^{Ol} the concentration of soybean oil present in the miscella (%), ρ_{Ol} the specific mass of soybean oil (kg/m³), ρ_H the specific mass of the hexane solvent (kg/m³), T_{Ol} , T_H and T_M , respectively, the temperature of the oil, hexane and miscella when measuring their specific mass, $\frac{d\rho_{Ol}}{dT}$ the rate of change of the specific mass of soybean oil as a function of temperature, and $\frac{d\rho_H}{dT}$ the rate of change of the specific mass of hexane as a function of temperature.

When the data for the specific mass of crude soybean oil and its temperature, the specific mass of the miscella and its temperature, the specific mass of the hexane and its temperature, and the derivatives of the specific masses as a function of temperature are inserted into Equation 13, the same should return the percentage mass concentration of oil present in the miscella sample (C_M^{Ol}). To do so, it is necessary to isolate this variable on the left side of the equation, whose deduction follows:

$$\rho_M^T = \frac{100}{\left(\dfrac{C_M^{Ol}}{\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}} + \dfrac{(100 - C_M^{Ol})}{\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}}\right)} \tag{13}$$

$$\left(\frac{C_M^{Ol}}{\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}} + \frac{(100 - C_M^{Ol})}{\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}}\right) = \frac{100}{\rho_M^T} \tag{14}$$

$$\left(\frac{\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right].C_M^{Ol} + \left[\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right].(100 - C_M^{Ol})}{\left[\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right].\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}\right) = \frac{100}{\rho_M^T} \tag{15}$$

$$\left[\rho_H + (T_H - T_M).\frac{d\rho_H}{dT}\right].C_M^{Ol} + 100.\left[\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right] - C_M^{Ol}.\left[\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right] = \frac{100.\left[\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right].\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}{\rho_M^T} \tag{16}$$

$$C_M^{Ol}.\left[\left(\rho_H + (T_H - T_M).\frac{d\rho_H}{dT}\right) - \left(\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right)\right] = 100.\left[\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right].\frac{\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}{\rho_M^T} - 100.\left[\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right] \tag{17}$$

$$C_M^{Ol}.\left[\left(\rho_H + (T_H - T_M).\frac{d\rho_H}{dT}\right) - \left(\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right)\right] = 100.\left[\rho_{Ol} + (T_{Ol} - T_M).\frac{d\rho_{Ol}}{dT}\right].\left[\frac{\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}{\rho_M^T} - 1\right] \tag{18}$$

And finally, we arrive at Equation (19) that isolates and calculates the oil concentration in the miscella:

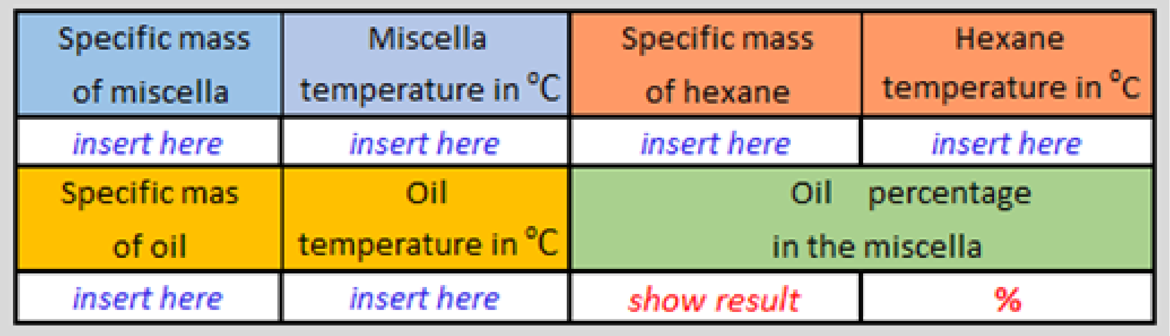
$$C_M^{Ol} = \frac{100.\left[\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right].\left[\dfrac{\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}{\rho_M^T} - 1\right]}{\left[\left(\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right) - \left(\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right)\right]} \tag{19}$$

And finally, we arrive at Equation (19) that isolates and calculates the oil concentration in the miscella:

$$C_M^{Ol} = \frac{100.\left[\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right].\left[\dfrac{\left[\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right]}{\rho_M^T} - 1\right]}{\left[\left(\rho_H + (T_H - T_M).\dfrac{d\rho_H}{dT}\right) - \left(\rho_{Ol} + (T_{Ol} - T_M).\dfrac{d\rho_{Ol}}{dT}\right)\right]} \tag{19}$$

The model was implemented in a *Microsoft Excel* spreadsheet, as shown in Figure 1, which received the experimental data of specific masses and temperatures and calculated the oil concentration in the miscella, to compare with the data obtained, also experimentally, through the traditional method of evaporation.

Figure 1 - Microsoft Excel spreadsheet for calculating the oil concentration.



Specific mass of miscella	Miscella temperature in °C	Specific mass of hexane	Hexane temperature in °C
insert here	*insert here*	*insert here*	*insert here*
Specific mas of oil	Oil temperature in °C	Oil percentage in the miscella	
insert here	*insert here*	*show result*	%

Source: The autor.

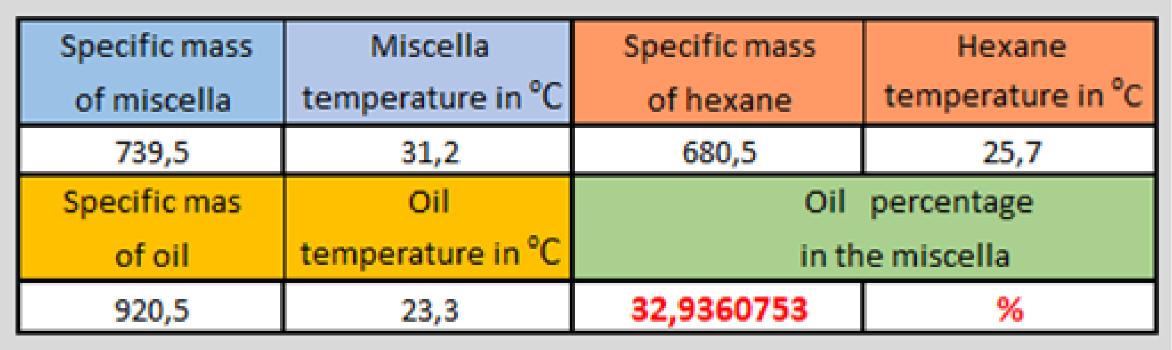
For example:

The industry is using hexane of 680.5 Kg/m^3 measured ate 25.7 °C and produces oil of 920.5 Kg/m^3 of specific mass at 23.3 °C.

To check the process efficiency, it took a sample of miscela at 31.2 °C that has 739.5 Kg/m^3 of specific mass.

What is the oil concentration of the sample? Answer of model: 32.9 %

Figure 2 – Simulation of the example.



Specific mass of miscella	Miscella temperature in °C	Specific mass of hexane	Hexane temperature in °C
739,5	31,2	680,5	25,7
Specific mas of oil	Oil temperature in °C	Oil percentage in the miscella	
920,5	23,3	**32,9360753**	%

Source: The autor.

Determination of the rate of change: specific mass x temperature

The specific mass of the oil and hexane was verified at different temperatures, according to item 2.1.1, in order to obtain reliable results to compare with the existing literature and use in the mathematical model.

Figure 3 represents the values found for the specific masses at 10 different temperatures, with a collection range between 17 and 53 °C, from a sample of crude soybean oil collected in the industry.

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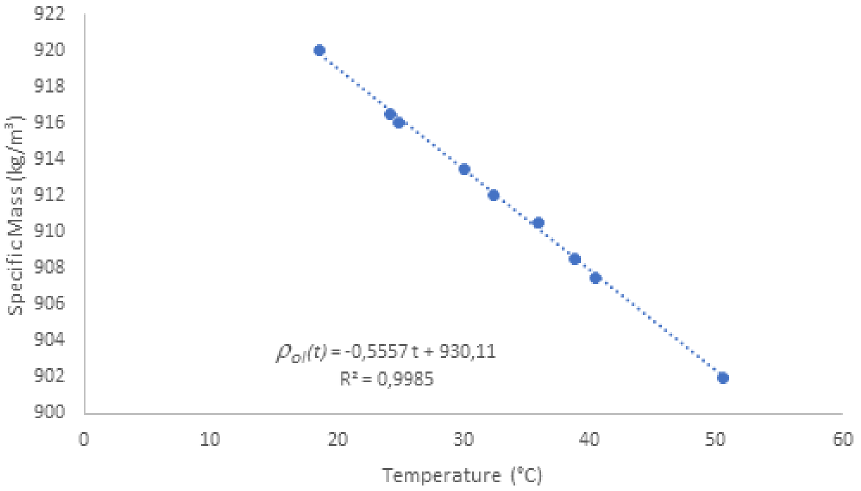
Figure 3 - Graph of the variation of the specific mass of crude soybean oil in relation to temperature.



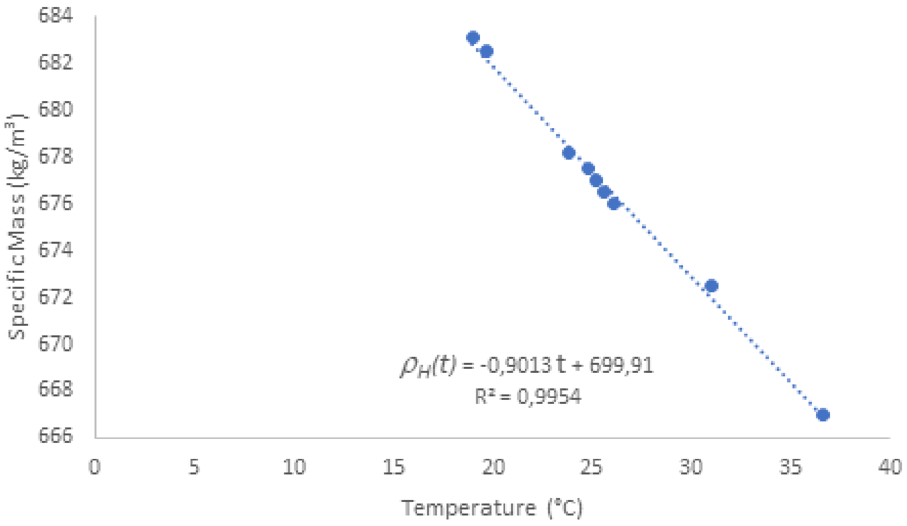
Source: The autor.

Note that the coefficient of determination R² was 0.9985, indicating a high degree of linearity because it is very close to 1, as well as justifying that the function fits the set of points. Analyzing the function obtained, we can express the derivative of the specific mass of crude soybean oil as a function of temperature as -0.56 $kg/m^3.°C^{-1}$, this means that the specific mass of crude soybean oil varies approximately -0.56 kg/m^3 for each degree Celsius as the temperature increases.

The same experiment was performed by Hahn (2020), where the equations point to an average of -0.58 $kg/m^3.°C^{-1}$. The results found in both studies are very close, practically coincidental, since they differ by 0.02 kg/m^3 of oil.

In the same way, the variation of the specific mass of a sample of hexane solvent sample collected in the industry was analyzed. Also, at 10 different temperatures, with a collection range between 17 and 53 °C, as shown in Figure 4.

Figure 4 – Graph of the variation of the specific mass of the industrial hexane solvent in relation to temperature.



Source: The autor.

It is observed that the coefficient of determination R² was 0.9954, very close to 1 as well, indicating a high degree of linearity and justifying that the function fits the phenomenon. Thus, from the resulting equation, we can express the derivative of the specific mass of hexane as a function of temperature as -0.901 $kg/m^3.°C^{-1}$, this means that the specific mass of hexane varies approximately -0.901 kg/m^3 for each degree Celsius as the temperature increases.

The data in Table 2, extracted from Perry and Green (2007), allow the calculation of the rate of variation as a function of temperature at -0.9 $kg/m^3.°C^{-1}$. Thus, the result found in the present research can be considered coincident with the literary result, one corroborating the other.

The rates of change of oil and solvent as a function of temperature are fundamental as they make up the mathematical model, allowing the reading of the specific mass of the miscella at any time after collection.

Considering the results obtained, the variation rates used in the model were -0.56 and -0.901 $kg/m^3.°C\text{-}^1$, for soybean oil and hexane, respectively.

Determination of oil concentration in micelles using the proposed model

The results obtained using the densimeter, thermometer and mathematical model are listed in Table 1. The specific masses, temperature and percentage of oil concentration of each Nth sample represent the arithmetic mean of the experiments carried out in triplicate.

Table 1 – Percent oil concentration in the miscella calculated by the model with the specific mass and temperature input data.

Sample	Specific Mass (kg/m^3)	Temperature (°C)	Concentration (%)
1	687.2	17.4	1.67
2	693.5	19.1	6.04
3	696.0	24.0	9.78
4	701.5	32.7	16.71
5	716.0	29.4	22.61
6	715.5	37.6	25.85
7	727.0	42.5	33.30
8	733.0	45.6	37.30
8	740.0	46.8	40.80
10	745.0	52.8	45.11

Determination of oil concentration in miscella through solvent evaporation (traditional method)

Each of the 30 samples used to measure the specific masses and temperatures (Table 1), after this step they were submited to evaporation to verify the percentage of oil present in them by the traditional method currently used in industries. The values obtained and presented in Table 2 also reflect the arithmetic mean of three samples, for each of the concentrations.

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Table 2 – Oil concentration obtained by the solvent evaporation method.

Sample	Miscella Mass (g)	Oil Mass (g)	Concentration (%)
1	105.6963	1.8984	1.78
2	96.9924	5.9605	6.14
3	96.2401	10.0405	10.41
4	101.0919	16.9502	16.76
5	98.0206	22.1281	22.56
6	90.8958	23.3914	25.71
7	98.1237	32.5203	33.13
8	100.0473	36.9838	36.97
8	100.6458	39.7203	39.45
10	97.2584	42.6983	43.90

Comparison of results and validation of the modeling

When comparing the data obtained by the proposed model with the results of the traditional evaporation method, as shown in Table 3, it appears that two of them are approximate and the other eight can be considered practically coincident, from the perspective of results sought by the industry.

The two results referring to the most concentrated miscella showed the greatest difference between the two methods, 1.35% and 1.21%.

The other samples had, on average, a variation of 0.21% between the absolute results obtained. This small difference has little or no significance in an industry reading. For example, a strong miscella has a concentration of 33% or 33.2%, for the industry, it means a minimally and desconsiderable difference.

Table 3 – Oil concentration calculated by the model and solvent evaporation method.

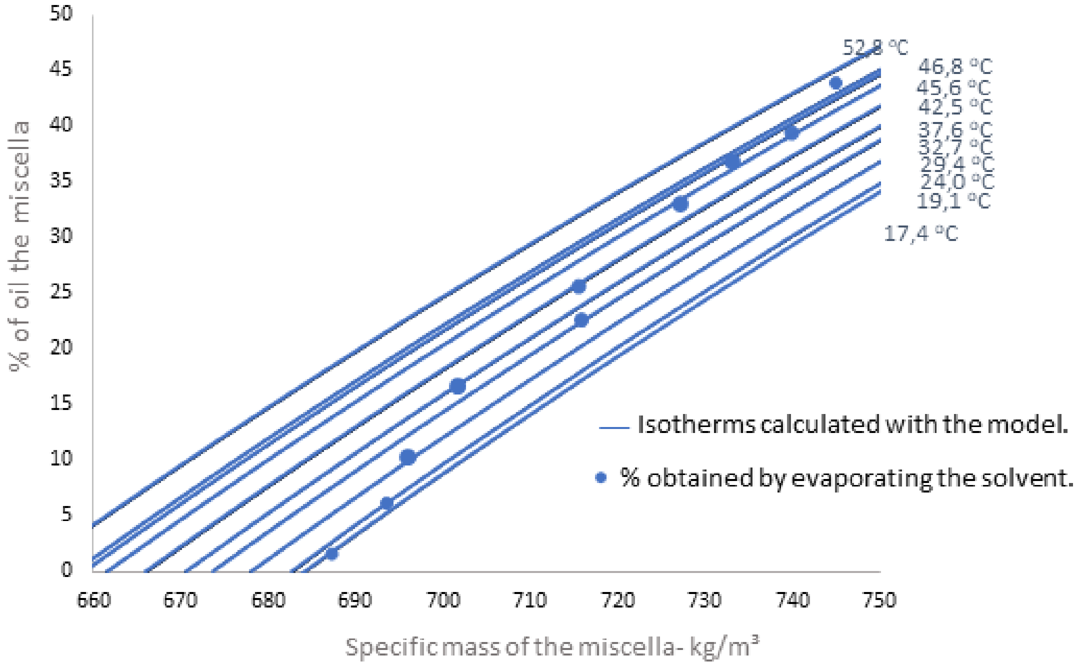
Sample	Modeling Result (%)	Evaporation Method (%)	Differences of the Methods
1	1.67	1.78	-0.11
2	6.04	6.14	-0.10
3	9.78	10.41	-0.63
4	16.71	16.76	-0.05
5	22.61	22.56	0.05
6	25.85	25.71	0.14
7	33.39	33.13	0.26
8	37.30	36.97	0.33
8	40.80	39.45	1.35
10	45.11	43.90	1.21

The graphical analysis (Figure 5) also allows to corroborate the good results obtained in the modeling. For each of the temperatures at which the miscella samples were analyzed (Table 2), isothermal curves were drawn using the mathematical model.

It means that - for the hexane and soybean oil used in the research - each of the curves mirrors the specific mass ratio of the miscella x oil concentration in it for the studied temperature.

The oil concentrations in the same miscella, obtained by evaporation the solvent (Table 3), are inserted and shown by the points (●).

Figure 5 – Comparative graph between results of oil percentage in miscella obtained with the mathematical model and with the solvent evaporation method.



Source: The autor.

Is it noted that the miscella with oil concentrations above 40% have the greatest differences in results between the two methods. Coincidentally, they are those samples analyzed at higher temperatures. Although the differences are small, it is suspected that the use of a densimeter and thermometer, not simultaneously, may have influenced this variation, as some time is lost between the introduction and stabilization of both and the reading of the equipment. This is because when the temperatures of the samples are high, they tend to lose heat during the experiment, as they vary until they stabilize at room temperature.

It is thought that the differences observed in the two miscellas at higher temperatures could be mitigated with the use of a more accurate digital densimeter with a coupled thermometer, which allows simultaneous measurements.

However, miscellas with oil concentrations greaterer than 40% are not common in the continuous industrial process, nor is there a need to manipulate the miscella at such high temperatures (50 ºC). In the collection of samples, heat loss occurs, as well as in the time lapse until sending to the laboratory and subsequent manipulation.

Another important issue to note is that the usual solvent evaporation method is also an error-prone experimental procedure. From this point of view, the hottest miscellas subjected to this method, likewise, may present less accurate results, given the volatility of hexane.

Nevertheless, the results obtained for temperatures below 46°C and concentrations below 40% are very promising. Coincident results would be practically impossible, since both methods have, in whole or in part, experimental components.

In short, as already illustrated in Table 5, the method proposed in this work presents similar results to the traditional method and perfectly adjusted to the needs of the industries. This assertion allows us to say that it is feasible to verify the percentage of soybean oil in hexane miscella, using a densimeter and the proposed mathematical model.

Thus, the developed method allows for a reduction of more than two hours in the verification time of the oil concentration in the miscella. This results in energy and labor savings, as well as speeding up the adjustment of the extraction system, if the analysis shows results outside the desiberable standards.

Conclusion

This study addressed a small fraction of the oil extraction process, but it had a bottleneck to be optimized: time and cost in the analysis of soybean oil concentration in the hexane miscella.

In this context, the objectives of the work were: to verify the rates of variation, as a function of temperature, of the specific masses of crude soybean oil and hexane, and to build a mathematical model to calculate the oil concentration from the specific masses of the solvent, soybean oil and the miscella verified at temperatures consistent with the industrial collection and analysis.

The specific mass variation rates in relation to temperature determined were -0.9 $kg/m^3.°C^{-1}$ for hexane and -0.56 $kg/m^3.°C^{-1}$ for crude soybean oil, and served as input data for the model.

In the end, the proposed method obtained results similar to the experimental results of the usual industrial method. In the eight samples of oil concentrations ≤ 37.3% the average absolute variation was 0.21% between the two methods. In two samples, with concentrations above 40%, the differences between the methods were 1.21% and 1.35%. It should be noted that these concentrations greater than 40% are not achieved in strong miscella of industry.

Thus, the method implemented in this research can be perfectly used as a tool in the process to optimize the analysis of soybean oil concentration in hexane miscella, using densimeter and the mathematical model developed. This way, it is possible to shorten the analysis time by more than two hours, with lower energy and labor costs and, above all, it makes it possible to anticipate the change in the extraction way, in case the result is incompatible with what was expected

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