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Dedicated to the memory of
Professor Cristofor I. Simionescu (1920–2007)

IMPROVEMENT OF SUNFLOWER OIL EXTRACTION BY MODELLING AND SIMULATION

Dorina BRĂTFĂLEAN, Vasile Mircea CRISTEA,* Paul Şerban AGACHI and Dan Florin IRIMIE

"Babes Bolyai" University, Faculty of Chemistry and Chemical Engineering,
11 Arany Janos Street, 400028 Cluj-Napoca, Roumania

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The paper describes the results obtained by modelling and simulation of sunflower oil extraction. The methods used for lipid extraction have been the conventional ISO extraction Soxhlet method (SO) and the mechanical oil press method (PO). These methods have been investigated on 14 Roumanian genotypes of sunflower seeds (10 inbred lines and 4 sunflower hybrids). Genetic material was obtained from the Agricultural Research and Development Institute Fundulea, Roumania. The sunflower seeds variability proved to be responsible for the quantity of the extracted oil. A difference in the oil extraction yield has been detected between Soxhlet and mechanical extraction. Compared to the mechanical press extraction, the Soxhlet oil extraction yield is higher. The diffusion coefficient through the seed, mainly depending on particle pores, has been fitted with experimental observations in the SO extraction. The yield of the oil extraction by oil press method has been investigated as depending on a set of parameters such as: feed stream, mechanical energy, speed of rotation, moisture and particle size. The oil press extraction yield has a large variability among the 14 investigated sunflower genotypes. It ranges from the minimum value of 66.3% for the LC-L3 type to the maximum value of 94.2% for the LC-L10 type. Based on the quantitative analysis of the extracted fat, the study reveals the fact that assessment of the sunflower seed genotype depends on the extraction methods, PO or SO, used in the investigation.

INTRODUCTION

Among species of oleaginous plants grown in Roumania, a high-ranking position place is held by the sunflower genotypes.[1] The sunflower seed, named achene, is formed by a seed wall covering the endosperm and embryo, the cells being filled with oil globules and protein corpuscles. Sunflower seed is considered an important lipid and protein source due its high nutrition composition. Seeds consist in complex matrices for which some characteristics such as particle size, moisture, core penetration etc., have a decisive influence on extraction.[2] Most of the lipids (75-85%) are easily extractable by the simple use of the suitable organic solvent, but the rest of the lipid matter is strongly bonded to the matrix of seed.[2] The general strategy of analyzing the complex processes of chemical or physical extraction follows a set of the common sense steps. The first step consists in preparing the experimental methods, establishing the process parameters, analyzing the variables and their relationships in order to provide a simple but consistent relationship set. The second step performs the mathematical modeling of the process. In the next step the evaluation of the model fitness to the real process behavior is made. During the last step, the simulation and model interpretation are performed on the obtained results. The mathematical model development is aimed to establish a set of the equations that can be subsequently used for simulating the evolution of the extraction process. The interest is to determine the time varying concentrations of the extracted compounds, based on the model parameters particular to a certain solid and solvent system in which the compounds are distributed.

* Corresponding author: mcristea@chem.ubbcluj.ro

The research work consisted in two types of experimental extraction processes and associated mathematical model development. The first method is the Soxhlet extraction (SO). The model of integral diffusion was used for describing the transport of lipid from the solid into the liquid phase. The partial differential equations of the mathematical model were solved using a specific algorithm, implemented in Matlab simulation software. Based on experimental data, relevant relationships between main variables have been developed for the mechanical oil press extraction (PO) method.

EXPERIMENTAL

Samples

The sunflower seeds of different genotypes were provided by the National Agricultural Research and Development Institute of Fundulea. Ten inbred lines and four hybrids have been considered in this study. The genotypes are presented in Table 1.

Table 1

Roumanian sunflower hybrids and inbred lines

Genotype	LC-L1	LC-L2	LC-L3	LC-L4	LC-L5	LC-L6	LC-L7
Type of variety	Semi-precocious	Semi-precocious	Precocious	Tardif	Semi-precocious	Semi-Tardif	Semi-tardif
Genotype	LC-L8	LC-L9	LC-L10	H1	H2	H3	H4
Type of variety	Semi-precocious	Precocious	Tardifs	Simple hybrid	Simple hybrid	Simple hybrid	Simple hybrid

Extraction of total lipids (TL)

a. Soxhlet method[3]

Approximately 10g of dry sunflower seed at harvesting maturity was sampled for each variety and prepared for the Soxhlet extraction. The conventional extraction procedure followed in this research was performed according to the International Organization for Standardization procedures.[3] SO-extraction involves the gravimetric determination of the oil using the light petroleum extract from oilseeds. The petroleum extract is called “oil content”. The decorticated seed material was weighed and then placed in a cellulose extraction cartridge. The cartridge was plugged with cotton-wool and then placed in the Soxhlet extractor containing 250mL of petroleum ether. The extraction time has been of 6h for each sample. The oils were recovered by distilling the solvent in a rotary evaporator at 40°C.

b. Mechanical press oil method[4]

The second procedure consists in mechanical pressing of 300g sunflower seeds of each genotype. The study was performed to investigate the efficient energy use in PO-extraction. The oil screw press was used in this study.[4] The yield of oils extracted by press method depends on the following set of parameters: feed stream Q_R , specific mechanical energy EMS, speed of rotation RS, moisture and particle size R.

Mathematical modeling and simulation

a. Soxhlet method

Since the controlling process for the transferred species through the solid spherical particle is the diffusion, the appropriate mathematical model for the Soxhlet extraction is considered to conform to this mass transfer mechanism.[5] The following assumptions have been taken into consideration: the solvent is intensely stirred and consequently is considered totally mixed; initially, the transferred species (lipids) are uniformly distributed in the solid particle; the flux of the transferred species at the particle’s surface is controlled by the intense mixing of the liquid phase; the liquid volume associated to the spherical particle is considered finite. During the extraction process the total lipids are transferred from the solid system to the liquid solvent, with kinetics depending on the lipids diffusion coefficient in the solid phase. The diffusion coefficient through the crust depends on particle pores. Consequently, the transport is characterized by the diffusive transport equation.[5,6] Taking into account the considered model, the following partial differential equation with associated initial and boundary conditions, has to be solved:

$$\begin{cases} \dfrac{\partial c_s}{\partial \tau} = D\left(\dfrac{\partial^2 c_s}{\partial r^2} + \dfrac{2}{r}\dfrac{\partial c_s}{\partial r}\right) \\ \tau = 0 \quad 0 < r < R \quad c_s = c_{s,0} \\ \tau > 0 \quad r = 0 \quad \dfrac{\partial c_s}{\partial r} = 0 \\ \tau > 0 \quad r = R \quad -4\pi R^2 D\dfrac{\partial c_s}{\partial r} = V\dfrac{\partial c_1}{\partial \tau} \end{cases} \tag{1}$$

where c_s is the lipid fat concentration in the solid particle, c_l is the lipid fat concentration in the liquid phase and R is the radius of the spherical particle.

A linear equilibrium relationship $c_l=k\cdot c_s$ has been further considered, where k is the distribution constant of the transferred species between the solid system and the liquid solvent.[5, 6]

Using the variable separation method for solving equation (1) the explicit solution, presented sequentially in the equations (2), (3) and (4), may be obtained by:

$$\frac{c_s - c_{s,\infty}}{c_{s,0} - c_{s,\infty}} = -\frac{2\cdot\upsilon\cdot R}{3r}\sum_{n=1}^{\infty}\sin\alpha_n\cdot\frac{\left(3+\upsilon\cdot\alpha_n^2\right)^2+9\alpha_n^2}{\alpha_n^2\left(\upsilon^2\cdot\alpha_n^2+3\cdot\upsilon+9\right)}\cdot e^{-\frac{\alpha_n^2 D}{R^2}\cdot\tau}\sin\frac{\alpha_n r}{R} \quad (2)$$

$$1-\frac{c_s - c_{s,\infty}}{c_{s,0} - c_{s,\infty}} = 1+\frac{2\cdot\upsilon\cdot R}{3r}\sum_{n=1}^{\infty}\sin\alpha_n\cdot\frac{\left(3+\upsilon\cdot\alpha_n^2\right)^2+9\alpha_n^2}{\alpha_n^2\left(\upsilon^2\cdot\alpha_n^2+3\cdot\upsilon+9\right)}\cdot e^{-\frac{\alpha_n^2 D}{R^2}\cdot\tau}\sin\frac{\alpha_n r}{R} \quad (3)$$

$$\frac{c_{s,0} - c_s}{c_{s,0} - c_{s,\infty}} = 1+\frac{2\cdot\upsilon\cdot R}{3r}\sum_{n=1}^{\infty}\sin\alpha_n\cdot\frac{\left(3+\upsilon\cdot\alpha_n^2\right)^2+9\alpha_n^2}{\alpha_n^2\left(\upsilon^2\cdot\alpha_n^2+3\cdot\upsilon+9\right)}\cdot e^{-\frac{\alpha_n^2 D}{R^2}\cdot\tau}\sin\frac{\alpha_n r}{R}\,. \quad (4)$$

Table 2 presents the roots of the transcendental equation (5) needed for the explicit solution (4) computation, considering different values for υ, where $\upsilon=3V/(4\pi R^3 k)$, and V is the totally mixed liquid volume surrounding the spherical particle of radius R.

$$\mathrm{tg}\alpha_n = \frac{3\alpha_n}{3+\upsilon\cdot\alpha_n^2} \quad (5)$$

Table 2

Roots of the transcendental equation (5), (first six solutions of the characteristic equation)[5]

υ	α_1	α_2	α_3	α_4	α_5	α_6
∞	3.14	6.28	9.42	12.56	15.71	18.84
9.00	3.24	6.33	9.45	12.59	15.72	18.86
4.00	3.34	6.39	9.50	12.62	15.75	18.88
2.33	3.46	6.73	9.55	12.66	15.78	18.95
1.00	3.72	6.68	9.71	12.79	15.89	19.00
0.666	3.87	6.82	9.84	12.89	15.98	19.08
0.25	4.18	7.22	11.24	13.27	16.32	19.39
0.111	4.33	7.46	11.54	13.61	16.68	19.76
0	4.493	7.72	11.9	14.06	17.22	20.37

The concentration distribution was calculated for finite contact time between the solvent (ether petrol) and the solid phase. The mathematical model and the subsequent analysis have been performed based on the experimental data obtained for each sunflower genotype.

b. Mechanical press oil method

For the second case, of the mechanical oil press extraction, the experimental data have been also used for fitting the model that describes the mechanical press operation.[6,7] The oil extraction yield (efficiency) was determined on the basis of the residual oil content of the cake, as presented in equation (6):

$$\eta = \frac{Q_G C_{max} - Q_R C_{cake}}{Q_G C_{max}} 100 \quad (6)$$

where η [%] is the oil extraction yield of the mechanical press extraction, Q_G [kg/h] is the feed flow rate, C_{max} [%] is the total lipids concentration of the seeds, Q_R [kg/h] is the cake outlet flow rate, and C_{cake} [%] is the lipids content in the cake.

The specific mechanical energy EMS [W·h/kg] may be computed according to the equation (7):

$$\mathrm{EMS} = \frac{P}{Q_G} \quad (7)$$

where P [W] represents the motor power described by

$$P = \left[\frac{460\times I\times 0.95\times RS}{600}\right] \quad (8)$$

with I [A] the electrical intensity and RS [rpm] the screw rotation speed. 460 [V] and 600 [rpm] are used to describe the efficiency of the extruder.[7]

Again, the mathematical model and the analysis have been performed based on the experimental data of each sunflower genotype.

RESULTS AND DISCUSSION

a. Soxhlet method

The obtained results show the values of the oil extracted by solvent extraction and the cake fat content of the sunflower seeds. The oil content ranged from the value of 41.93% for the LC-L6 genotype to the value of 49.12% for the R-H2 genotype in the case of the experimental data, while the oil content ranged from the value of 43.41% for the LC-L 6 genotype to the value of 49.55% for the R-H2 genotype in the case of the simulation data. For all cases, the extract was dependent on the sunflower seeds genotypes. Table 3 summarizes lipophilic extract weight as percentage of the total seed weight. The percentage of lipids in Roumanian hybrids is under 45% (47.13% for R-H3 and 49.12% for R-H2). Large variations have been observed in fat content of sunflower seeds, both for the experimental and simulation data.[8]

The concentration profile has been investigated by simulation, for different values of the operating variables and for each genotype. Simulation results are in good agreement with experimental data of the Soxhlet extraction. Figs. 1 and 2 show the space distribution of the oil content in the spherical particle of radius $R=1.5\cdot10^{-3}$ [m], at different moments of time during the extraction process, for the LC-L6 and R-H2 genotypes.

Figs. 1 and 2 reveal the different behavior of the investigated varieties. The large variability of the extracted oil among the investigated sunflower genotypes may be explained by different values of the diffusion coefficient.[8] Comparative oil concentration results obtained by experiment and by simulation, using the SO extraction method are shown in Table 3, for different investigated sunflower genotypes.

Meaning of the variables presented in Table 3 is given by the following: C_{max} is the maximum oil concentration in the seeds; C_{exp} is the experimental result of oil concentration in the seeds; C_{sim} is the oil concentration in the seeds, obtained by simulation; D is the diffusion coefficient; C_{rexp} is the experimentally obtained oil concentration in the cake; C_{rsim} is the oil concentration in the cake, obtained by simulation and computed as the mean value of the oil concentrations in the center $c_{s,r=0}$, at the surface $c_{s,r=R}$, and in the middle of the radius $c_{s,r=R/2}$ of the solid particle.

For the SO extraction method the experiments have been carried out at the constant temperature of T=40°C, according to the ISO procedures.[3]

It may be concluded that a large variability of oil extraction yield from the different investigated sunflower seeds was detected by the Soxhlet extraction method.

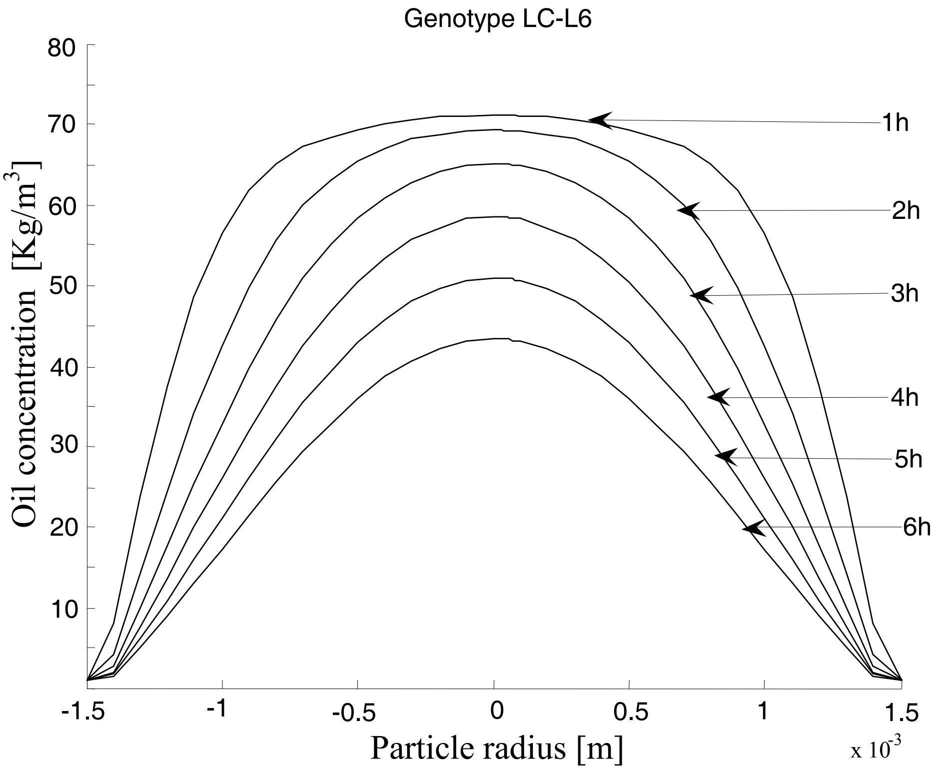

Fig. 1 – Space distribution of oil concentration inside the particle, at different extraction moments, for LC-L6 genotype.[8]

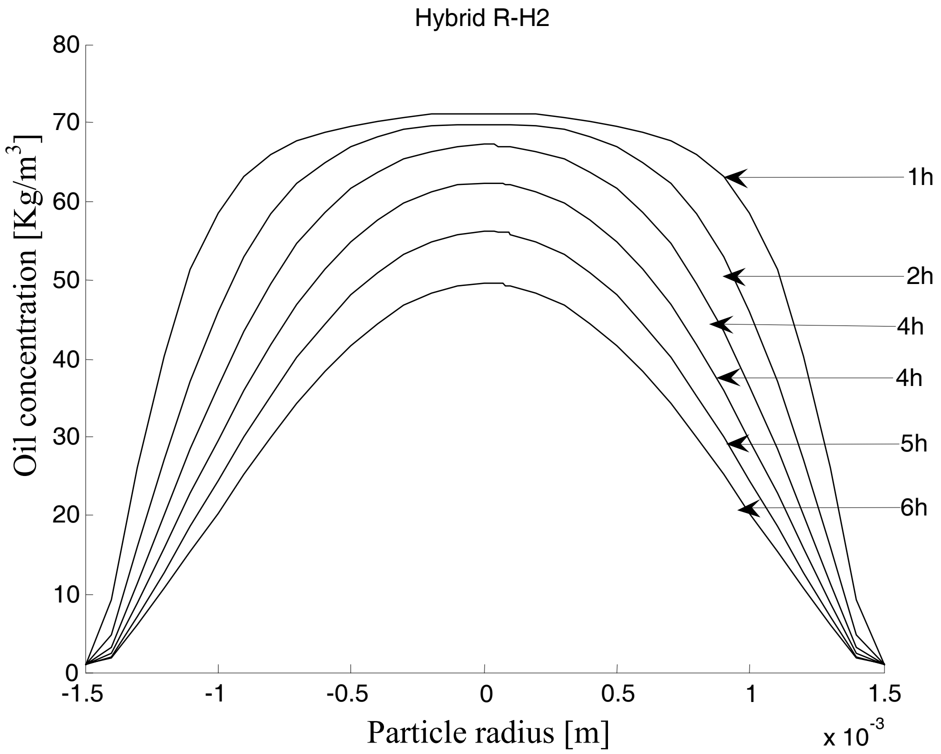

Fig. 2 – Space distribution of oil concentration inside the particle, at different extraction moments, for R-H2 genotype.[8]

Table 3

Experimental and simulated oil concentrations obtained using the SO extraction method

Item no.	Genotypes	Type of variety	C_{max} [%]	C_{exp} [%]	C_{sim} [%]	D [m^2/s]	C_{rexp} [%]	C_{rsim} [%]	k
1	LC-L1	Semi-precocious	47.70	46.79	47.17	1.00E-07	0.907	0.53	1.0194
2	LC-L2	Semi-precocious	48.80	47.80	48.41	9.70E-12	1.000	0.39	1.0209
3	LC-L3	Precocious	43.70	42.98	43.41	1.09E-06	0.720	0.29	1.0168
4	LC-L4	Belated	46.40	46.06	45.93	1.03E-11	0.340	0.47	1.0074
5	LC-L5	Semi-precocious	46.11	45.95	45.91	1.03E-11	0.150	0.19	1.0033
6	LC-L6	Semi-belated	44.50	41.93	43.46	1.09E-11	2.570	1.04	1.0613
7	LC-L7	Semi-belated	45.60	45.13	45.11	1.05E-11	0.470	0.49	1.0114
8	LC-L8	Semi-precocious	49.60	48.05	48.54	9.67E-12	1.552	1.06	1.0323
9	LC-L9	Precocious	44.80	44.05	44.7	1.06E-11	0.750	0.11	1.0170
11	LC-L10	Belated	45.80	45.21	45.56	1.04E-11	0.595	0.24	1.0132
11	R-H1	Simple hybrid	48.90	47.75	47.87	1.00E-11	1.150	1.03	1.0241
12	R-H2	Simple hybrid	50.11	49.12	49.55	9.43E-12	0.980	0.55	1.0200
13	R-H3	Simple hybrid	49.55	47.13	49.25	9.50E-12	2.420	0.30	1.0513
14	R-H4	Simple hybrid	49.12	48.95	48.75	9.62E-12	0.170	0.37	1.0035

b. Mechanical oil press method

The obtained results show the values of the oil extraction yield by pressing with the screw press. They range from the value of 19% to the value of 36 % after filtration, as presented in Table 4. The oil extraction yield of the mechanical oil press method is varying form the value of 66.35% for the LC-L3 genotype to the value 94.21% for the LC-L10 genotype. Small waste was observed for the LC-L3 genotype with the value of 2.75%, as oil concentration after filtration has the value of 19.28%. In this case only 44.11% from the total oil content in the seed was extracted by mechanical oil press.[9]

The hybrids have rich oil content ranging from the value of 48.90% for the R-H1 genotype to the value of 50.11% for the R-H4 genotype, but by press extraction the percent of extracted oil varies between the values of 22.82% for the R-H3 genotype to the value of 34.00% for the R-H1 genotype. Yield of oil extracted by the oil press method depends on the sunflower genotypes, as it is shown in Table 4.

Table 4

Oil concentrations obtained using the PO extraction method[9]

Item no.	Genotypes	Type of variety	C_{max} [%]	C_{gross} [%]	$C_{filtrate}$ [%]	C_{cake} [%]	Oil yield [%]	Waste [%]	EMS [W·h/Kg]
1	LC-L1	Semi-precocious	47.70	37.89	31.77	9.81	87.71	1.65	32.24
2	LC-L2	Semi-precocious	48.80	27.76	22.85	21.04	70.12	2.45	64.48
3	LC-L3	Precocious	43.70	23.48	19.28	20.22	66.35	2.76	64.48
4	LC-L4	Belated	46.40	35.41	31.24	11.99	85.39	1.65	45.14
5	LC-L5	Semi-precocious	46.11	40.01	36.46	6.09	92.55	1.19	45.14
6	LC-L6	Semi-belated	44.50	31.91	26.34	12.59	79.19	2.14	70.93
7	LC-L7	Semi-belated	45.60	40.44	36.14	5.16	93.61	1.08	38.69
8	LC-L8	Semi-precocious	49.60	29.24	22.60	20.36	72.06	2.04	51.59
9	LC-L9	Precocious	44.80	35.79	30.81	9.01	87.69	1.25	64.48
11	LC-L10	Belated	45.80	41.63	30.92	4.17	94.21	1.87	51.59
11	R-H1	Simple hybrid	48.90	39.97	34.00	8.93	89.65	1.56	45.14
12	R-H2	Simple hybrid	50.11	45.30	26.95	4.80	95.04	2.70	38.69
13	R-H3	Simple hybrid	49.55	35.80	22.82	13.75	83.20	2.55	38.69
14	R-H4	Simple hybrid	49.12	42.77	28.21	6.35	92.95	2.20	38.69

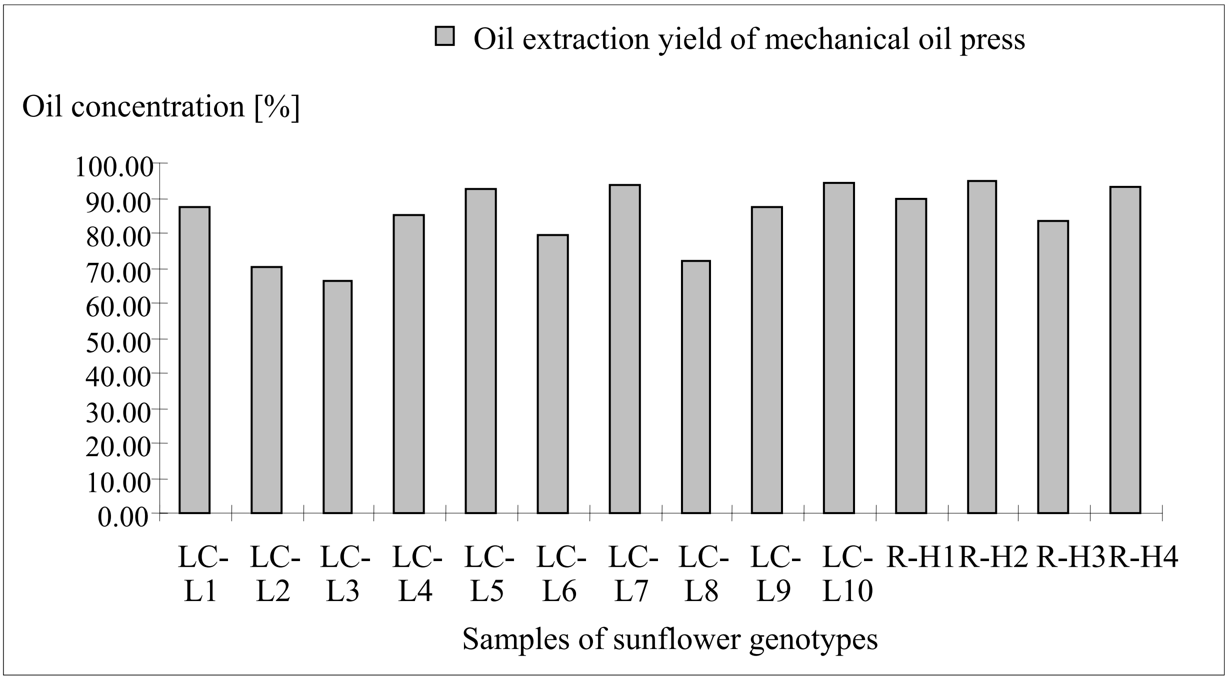

Fig. 3 – The oil extraction yield of the mechanical oil press extraction for the different investigated sunflower genotypes.[9]

Meaning of the variables presented in Table 4 is given by the following: C_{max} is the maxim concentration of oil content in the seeds; C_{gross} is the oil concentration before filtration; $C_{filtrate}$ is the oil concentration of the filtrate; C_{cake} is the oil concentration remaining in the cake after oil press extraction.

A large variability of the extracted oil quantity was detected by mechanical oil press method, too. The oil extraction yield of the mechanical oil press, for all the investigated sunflower genotypes, is presented in the Fig. 3.

For the oil press extraction method the experiments have been carried out at the mean temperature value of T=40°C.

CONCLUSIONS

The results obtained using both experimental and simulation approaches have led to the following conclusions. Sunflower seed genotypes can be classified taking into account the extracted oil quantity. A large variability of oil extraction yield was detected when comparing the two extraction methods. The Soxhlet extraction yield is higher compared to the mechanical press extraction yield.[10] Quantitative analysis of the extracted fat showed that the extraction method, SO or PO, influences the evaluation of the sunflower seeds genotypes. The quantity of organic solvent used for de-fatting the cake material depends of the lipids content. The developed mathematical model provides information on the time and space oil extraction development inside the spherical seed particle and in the associated liquid solvent surrounding it. Further investigations may be carried out using different types of solvents. The presented application may be developed for similar approaches of other oleaginous plant genotypes. The value of the diffusion coefficient inside the seed particle, determined from experimental data, may be further involved in the optimization of the industrial process of oil extraction as well as for obtaining desired quality of the cake that is used with efficient results as poultry food.[11]

NOMENCLATURE

c_l - oil concentration in the liquid phase surrounding the particle[5] [kg/m^3]
c_s - oil concentration in the solid particle [kg/m^3]
c_{s0} - initial oil concentration in the solid particle [kg/m^3]
$c_{s\infty}$ - final oil concentration in the solid particle [kg/m^3]
$c_{s,r=R}$ - oil concentration at the surface of the spherical particle [kg/m^3]
$c_{s,r=R/2}$ - oil concentration at the half radius of the spherical particle [kg/m^3]
$c_{s,r=0}$ - oil concentration in the center of the spherical particle [kg/m^3]
C_{cake} - oil concentration remaining in the cake after oil press extraction [%]
C_{exp} - experimental result of oil concentration in the seeds [%]
$C_{filtrate}$ - oil concentration of the filtrate [%]
C_{gross} - oil concentration before filtration [%]
C_{max} - maximum oil concentration in the seeds [%]
C_{sim} - oil concentration in the seeds obtained by simulation [%]
C_{rexp} - oil concentration in the cake, obtained by experiment [%]
C_{rsim} - oil concentration in the cake, obtained by simulation [%]
D - diffusion coefficient [m^2/s]
EMS - specific mechanical energy [Wh/kg]
H1 … H4 - investigated sunflower hybrids
I - electrical current intensity [A],
k - distribution constant between the solid and liquid phase
LC-L1 … LC-L10 - investigated sunflower inbred lines
P - motor power of the mechanical press [W]
PO - mechanical oil press extraction method
Q_G - feed flow rate [kg/h]
Q_R - the cake outlet flow rate [kg/h]
r - distance along the radius of the solid particle [m]
R - the radius of the spherical particle [m]
RS - oil-press screw rotation speed [rpm]
SO - Soxhlet extraction method
T - temperature [°C]
V - constant volume of liquid surrounding the solid particle [m^3]
α_n - eigenvalues of equation (5)
η - oil extraction yield for the mechanical oil press extraction method [%]
τ - time [s]

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