MATHEMATICAL MODELLING AND SIMULATION OF MASS TRANSFER IN HORIZONTAL EXTRACTOR

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Abstract. *In this work the coupled model of the processes is presented in horizontal extractor that included 3 zones: of loading, of drainage and extraction field. In this extractor the refined is a porous medium with two types of pores and the liquid miscela form the countercurrent crossed flows. The model has two partial differential equations (2D, transient) for the extraction field that consider: the mass transfer between refined and miscela, the diffusion in the entire extraction field, the transport of miscela between the percolation sections, the influence of loading and drainage zones in processes and, the transient operational regime of extractor. Also the oil loss were considered. The boundary conditions are complex and depend of the field characteristics. The numeric scheme is based on method of lines that shown the good efficiency.*

It is revealed that the calculation of zone stability is depended: of mesh sizes, of integration step, of average velocity and of diffusion coefficients. For conditions of real extractor were executed the numeric investigations to determine the influence of the number of percolation sections on oil losses.

Keywords*: Mathematical model, Extraction, Porous medium, Mass transfers.*

1. Introduction

In general, the applied mathematical modelling to foresee of the oil vegetable extraction began growing in the decade of 50 with “Karnofsky (1949)”, “Coats & Karnofsky (1950)”, that established a oil extraction physical scheme of the laminated flakes. During the extraction, the oil were substituted by solvent that, after the process, it is not drained. The present moment, the industrial vegetable oil extractors "De Smet", "Rotocell", "Crow Model" implanted in the industry of foods are installations of great size but the mathematical modelling of their processes practically doesn't exist. In their extraction fields, the expanded flakes (a porous medium) and the miscela (a liquid that extracts the oil from the flakes) interact in the extraction field through countercurrent crossed flows (CCC) “(Bockisch, 1998; Miyasaka & Medina, 1981)”. In the literature, the mathematical models of the CCC flows, differently of other flows (co-currents “(Chani, Radulovic, & Smoot, 1996)”, countercurrents “(Lasseran & Courtois, 1993; Wronski, & Molga, 1998)”, crusaders “(Qi, & Krishnan, 1996; Wang, Jia, & Davies, 1995)” still were not elaborated. The present moment, in the project and simulation of processes in extractors are used largely at different versions of the multi-state method that for each percolation section the uniform distribution of the oil concentrations is accepted in each component “Foust, et al., (1982)”. This method, in main approach, is not sensitive: a) to the sections dimensions, b) to the components velocity and c) to the porous medium porosities. Therefore, the extractors project and operation is accompanied by a great volume of experimental data that demand financial expenses and considerable time. In this sense the mathematical models of CCC flows that use the diffusion and mass transfer laws, with the space distribution of the extraction field concentrations, could aid.

In the present work a coupled model of the extraction processes is proposed in industrial installation that it uses the CCC flows principles, and it includes the percolation sections sub-models, of drainage and loading zones, and of the trays. Also, the model stability analysis study is presented, and the numeric simulations considering variable the percolation sections number in transient regime.

2. Extraction processes modelling in countercurrent crossed flows

A detailed scheme, with the raw material and miscela flows with the loading and drainage zone, is shown in "Fig. 1". The raw material enters for the tube 1, in the section 1, filling the body of extractor. The solvent enters in the extractor for controller (17) and tube (2), going by the last section, falling in the tray (19); the miscela is moved upward for the tube (13) until arriving in the distributor (12). Later it crosses the penultimate percolation section, falling in the tray (9) and, like this for before, until the tube (3), from where it (enriched of oil) leaves the extraction field and enters in the vaporizer (15); the crumb leaves the drainage section for the dessolventizer (14).

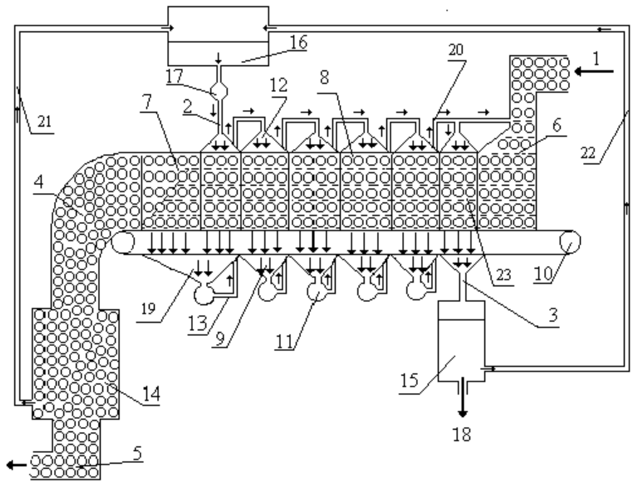

Figure 1 – Process Scheme of a typical extractor "De Smet"

1 - expanded flakes entrance; 2 - solvent inlet in the extraction field; 3 – miscela exit; 4 - porous medium exit; 5 - marc without solvent; 6 - loading zone; 7 - drainage zone; 8 - percolation section; 9 - tray; 10 - transporter; 11 - pumps for miscela distribution; 12 - miscela distributor; 13 - tube with miscela; 14 - marc in DT; 15 - vaporizer; 16 - solvent reservoir; 17 - solvent flow controller; 18 - oil exit; 19 - tray of drained miscela; 20 - tube with miscela distributed to the percolation section and to the loading zone; 21, 22 - tubes with solvent; 23 - first percolation section.

During the loading, the strong miscela fills the spaces between raw material particles and penetrate in pore phase. At the same time, for the force of extraction, the solid phase oil comes out to the pore phase, and quickly, it established the equilibrium among the oil volumetric concentrations in raw material, C^N, and the oil volumetric concentrations of miscela in pore phase, C^p.

The miscela, inside of a percolation section, it moves from top to bottom, in crossed mode with the raw material flow, and cross a section from another contrary this flow, resulting the countercurrent crossed scheme. It has two particularities:

- the drainage miscela flow join up with the main miscela flow (19) "Fig. 1";
- a part of the strong miscela is used in the loading section (6) "Fig. 1", with the raw material entrance (1) "Fig. 1".

Leaning in this description, it can to create the physical model of the typical extractor processes. The main moments of the modeling are present bellow:

1. they are considered the countercurrent crossed flows of the raw material and miscela;
2. the diffusion is considered along the whole extractor, in the vertical and horizontal directions.
3. in the beginning of the filling in, the whole oil is in the solid phase.
4. during the filling in, it happens the strong miscela passage of the second section, with concentration $\overline{C}_2$ of the bulk phase from pore phase, occupying a pores volume fraction (ε_m), and simultaneously, it happens the oil transfer of the solid from pore phase, occupying the other part of the space (ε_p - ε_m).
5. after the filling in, it happens the uniform instantly oil mixture of the spaces ε_m and (ε_p - ε_m) forming the pore phase initial concentration, C^p_{en}, in space ε_p.
6. the amount oil volumetric that leaves (during the percolation) of the particles is substituted by a same amount solvent volumetric. In this case, the miscela volumetric flow, in extractor, is constant and it doesn't depend on the oil transfer processes in bulk phase.
8. the oil drainage stage, in the pore phase of crumb, is lost (it doesn't return to extractor), but bulk phase oil, that went by the drainage zone, returns.
9. The oil volumetric concentrations in solid part and pore phase are in equilibrium for the constant $E^v_d = C^N / C^p$.
10. The porosities ε_b (bulk) and ε_p (pore) are constant during the extraction process.

2.1. Mathematical model for countercurrent crossed flows processes

In agreement with "Fig. 2", the horizontal extractor has some percolation sections, a drainage section, a loading section and trays. The mathematical model was developed in "Veloso et al, (2002)" and "Veloso,(2003)".

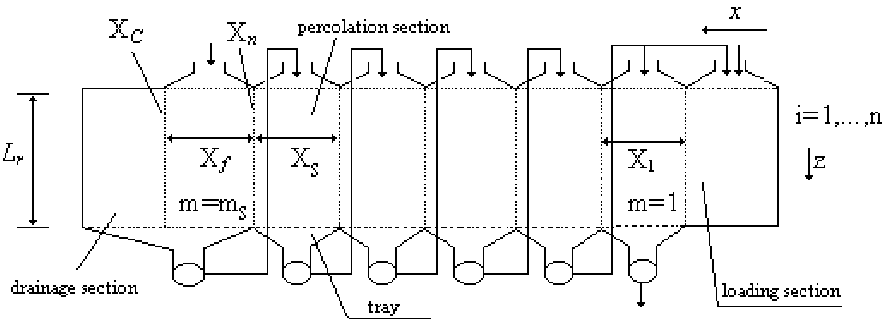

Figure 2. Dimensional scheme of horizontal extractor

2.2.1. Extraction field

In extraction field is had following EDP's:
- for the bulk phase:

$$\frac{\partial C}{\partial \tau} = -V_m \frac{\partial C}{\partial z} + E_S \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2} \right) + \frac{(1-\varepsilon_b)}{\varepsilon_b} k_f a_p \left(C^p - C \right) - u_h \frac{\partial C}{\partial x} \tag{1}$$

- for the pore phase:

$$\frac{\partial C^p}{\partial \tau} = -\frac{k_f a_p \left(C^p - C \right)}{\varepsilon_p + (1-\varepsilon_p) E_d^V} - u \frac{\partial C^p}{\partial x} \tag{2}$$

where C is oil volumetric concentration in bulk phase; C^p is oil volumetric concentration in pore phase; a_p is contact surface between pore and bulk phases, in unitary volume (m^{-1}); E_S is dispersion coefficient (m^2/s) "Cussler, (1997)"; E_d^v is equilibrium volumetric coefficient of oil between the solid phases and pore "Veloso, (2003)"; u is horizontal velocity of the raw material moved by the transporter (m/s); u_h is miscela velocity in the horizontal direction (m/s); V_m is miscela vertical velocity in the percolation sections (m/s); x is bed horizontal coordinate (m); z is bed vertical coordinate (m); k_f is mass transfer coefficient among pore and bulk phases (m/s); ε_b is bed porosity (bulk phase); ε_p is particle interns porosity (pore phase); t is time (s).

2.2.2. Trays sub-model

The equations of concentrations alteration in the trays are deduced with base in the oil conservation law, applied in the volume of the tray. For each tray (except the last) is had:

$$\frac{d\overline{C}_m}{d\tau} = \frac{\int_{X_n}^{X_k} C(x, L_r, \tau)\, dx - \overline{C}_m X_S V_m}{V_b / (H \cdot \varepsilon_b)} \tag{3}$$

where: $m = 2 \ldots (m_S - 1)$; $X_n = X_1 + (m-2) \cdot X_S$; $X_k = X_n + X_S$.

For the last tray, is had:

$$\frac{d\overline{C}_{m_S}}{d\tau} = \frac{\int_{X_n}^{X_C} C(x, L_r, \tau)\, dx + \int_0^{L_r} C(X_C, z, \tau)\, dz - \overline{C}_{m_S} X_S V_m}{V_b / (H \cdot \varepsilon_b)} \tag{4}$$

where: $X_C = X_n + X_f$; $X_n = X_1 + (m_S - 2)\cdot X_S$; H is bed width (m); $\overline{C}_m$ is oil average volumetric concentration in the m-ésima tray; L_r is bed height (m); m_s is number of the extractor sections; V_b is average volume of oil in the trays (m^3); X_n is coordinate of the last percolation section (hexane in) (m); X_S is width of a typical section (m); X_1 is thickness of the first percolation section (m); X_f is thickness of the last percolation section (hexane in) (m).

2.2.3. Initial and boundary conditions

Through the boundary conditions of the miscela flows and of porous medium are interlinked in countercurrent crossed flow. The boundary conditions for bulk phase are:
a) to the right side of extraction field,

$$C(0,z,\tau) = \overline{C}_m(\tau); \quad z = 0,..., L_r; \; m = 2; \quad \tau > 0; \tag{5}$$

b) to the left side of extraction field,

$$\frac{\partial C(X_C, z, \tau)}{\partial x} = 0 \; ; \qquad z = 0,..., L_r; \quad \tau > 0; \tag{6}$$

c) for the upper boundary of field,
- sections $m = 1,..., (m_s - 1)$:

$$C(x,0,\tau) = \overline{C}_{m+1}(\tau); \quad \tau > 0; \tag{7}$$

where: $x = 0, ..., X_1$; if $m = 1$ and $x = (X_1 + (m - 2)\cdot X_S), ..., (X_1 + (m - 1)\cdot X_S)$; if $m = 2, ... (m_s - 1)$;

- for section m_s,

$$C(x,0,\tau) = C_{in} \qquad x = X_1 + (m_s - 1)X_S \tag{8}$$

d) for the bottom boundary of the field:

$$\frac{\partial C(x, L_r, \tau)}{\partial z} = 0 \; ; \qquad x = 0, ..., X_C; \qquad \tau > 0; \tag{9}$$

The boundary conditions for the pore phase on the right hand of the field are:

$$C^p(0,z,\tau) = C^p_{en}(\tau); \qquad z = 0,..., L_r; \quad \tau > 0; \tag{10}$$

The initial values for the entire extraction field are:

$$C(x,z,0) = C_0(x,z) \quad \text{e} \quad C^p(x,z,0) = C^p_0(x,z) \tag{11}$$

for $x = 0,...,X_C$; $z = 0,..., L_r$.

As for the tray: $\overline{C}_m(0) = C^0_m$ for $m = 2,..., m_s$.

During the integration besides the distributions $C(x, z, \tau)$ and $C^p(x, z, \tau)$, the important characteristics are determined:
- flow rate of the oil lost in extractor (m^3/s)

$$F_{ol} = Hu(1-\varepsilon_b)\left[\varepsilon_p + (1-\varepsilon_p)E^v_d\right]\int_0^{L_r}\left(C^p\left(X_f, z, \tau\right)\right)dz \tag{12}$$

- coeficient of the oil losses (*dimensionless*):

$$P_{ol} = \frac{F_{ol}\rho_{ol}}{\left[(1-N_T)M_n + P_{ol}\rho_{ol}\right]} \tag{13}$$

where N_T is mass concentration of oil (*dimensionless*), M_n is mass flow in extractor entrance (*kg/s*) and ρ_{ol} is oil density (*kg/m³*).

- volumetric concentration of the miscela in extractor exit (*dimensionless*):

$$C_s = \frac{\int_0^{X_S} C(x, L_r, \tau)\,dx}{X_S} \tag{14}$$

3. Von Neumann' analysis

According to "Maliska, (1995)", when works with systems of EDP´s nonlinear, where is had delicate coupled (including, in the present case, the integra-differential equations) with complex boundary conditions, it is difficult to prove in advance that a numeric approach is stable and convergent. These difficulties are larger if, in the numeric scheme, a method of high order of precision was used (for instance, Runge-Kutta). For that, considering that the problem is complex, a method of "mathematical experiment" is accepted to determine the safe intervals of parameters alteration of the mesh in the integration domain and the influence of parameters (N_h - number of vertical columns, n - number of lines and h - integration step) in the main characteristics of the processes. In the calculations, the Courant numbers, vertical S_v and horizontal S_h, are the stability indicators "Veloso et al, (2000)" and, with the objective of determining the influence of the dispersion coefficient in the stability limits, the calculations were accomplished for the meshes: G - thick, B - basic and F - fine, varying $E_S = 10^{-6} \ldots 10^{-4}$. In the analysis of the results, the diffusion number was involved given by the expression:

$$S_d = \frac{E_S \Delta t}{\Delta x^2} = \frac{E_S \Delta t}{\Delta z^2} \tag{15}$$

The results evidence the E_S influence in stability limits, to know: to $E_S = 10^{-4}$, the limit, for the Courant number is: $S_v = 0{,}8\ldots\ 0{,}94$; to $E_S = 10^{-5}$, the limit is: $S_v = 1{,}12\ldots\ 1{,}20$ and for you $E_S = 10^{-6}$, $S_v = 1{,}20\ldots\ 1{,}24$ (Tab. 1).

To explain this influence, Von Neumann's analysis was accomplished "Santos, (1998)" in the equation-example:

$$\frac{\partial C}{\partial \tau} = -V_m \frac{\partial C}{\partial x} + E_S \frac{\partial^2 C}{\partial x^2} \tag{16}$$

where was obtained the stability condition:

$$|G| = \left|1 + S_v\left(e^{-i\theta} - 1\right) + 2S_d\left(\cos\theta - 1\right)\right| \le 1 \tag{17}$$

where G is transition factor. For the method to be stable is necessary that the solution remains limited. In the analysis of the inequality "Eq. (17)" is considered that S_v and S_d are positive and θ can assume any value (Tab. 1).

The analysis above was accomplished for the finite differences scheme or (method of lines) for the Euler explicit scheme. But in the algorithm of the horizontal extractor model, was applied R-K4 method. It is known that each numeric scheme, independently of involved EDO's, it possesses an own stability absolute region "Lambert, (1993)".

In "Fig. 3", those regions are shown for the Euler and R-K4 methods. In is observed that the more length is the passage of the negative real axis (ρ), is stable the numeric scheme "Houwen, (1996)".

In other words, the stability interval of the Runge-Kutta method is larger than the Euler method. Maybe this result can explain the increase of the limit of numeric stability $S_v \approx 1{,}2 > 1$, obtained by the "mathematical experiment" considering that the equations system of the model is more complex than to equation-example "Eq. (16)" used in this item.

Table 1. Stability limits of the calculations for different E_S.

$E_S = 10^{-4}$	$n=12$ e $N_h=12$ (G)		$n=20$ e $N_h=20$ (B)		$n=30$ e $N_h=30$ (F)	
	$h_b = 2$	$h_{m+1}=21$	$h_b=2$	$h_{m+1}=11$	$h_b=2$	$h_{m+1}=7$
S_v	0,09	0,94	0,15	0,82	0,22	0,79
S_u	0,006	0,50	0,08	0,44	0,12	0,42
S_d	0,0072	0,075	0,02	0,11	0,045	0,15
C_s	0,3217	-	0,3152	-	0,3179	-
F_{ol} (cm^3/s)	85,48	-	71,42	-	67,80	-
$E_S = 10^{-5}$	$n=12$ e $N_h=12$		$n=20$ e $N_h=20$		$n=30$ e $N_h=30$	
	$h_b = 2$	$h_{m+1}=26$	$h_b=2$	$h_{m+1}=16$	$h_b=2$	$h_{m+1}=10$
S_v	0,09	1,17	0,15	1,20	0,22	1,12
S_u	0,06	0,62	0,08	0,64	0,12	0,60
S_d	0,00072	0,0093	0,002	0,016	0,0045	0,022
C_s	0,3260	-	0,3191	-	0,3260	-
F_{ol} (cm^3/s)	85,59	-	71,47	-	54,76	-
$E_S = 10^{-6}$	$n=12$ e $N_h=12$		$n=20$ e $N_h=20$		$n=30$ e $N_h=30$	
	$h_b = 2$	$h_{m+1}=27$	$h_b=2$	$h_{m+1}=16$	$h_b=2$	$h_{m+1}=11$
S_v	0,09	1,21	0,15	1,20	0,22	1,24
S_u	0,06	0,65	0,08	0,64	0,12	0,66
S_d	0,000072	0,00097	0,0002	0,0016	0,00045	0,0025
C_s	0,3264	-	0,3195	-	0,3222	-
F_{ol} (cm^3/s)	85,61	-	71,49	-	67,84	-

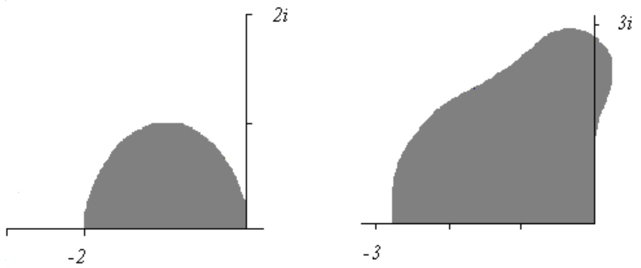

Figure 3. Absolute stability Region for the Euler and R-K methods

4. Variation of the sections number m_S

With the reduction of sections number m_s, the production costs and energy consumption (smaller bombs number) of the extractors are smaller. At the same time, with the decrease of m_s , the oil losses increase. The developed code can help with more safety in the search of the optimum sections number, maintaining the other constant data.

"Figure 4" showing the concentrations C_s evolutions for extractors with different sections numbers. It is observed that the concentrations pass for some maximum while they are in transient regime (the stationary states are reached in $\tau \approx 6000s$). The maximum appear because the amount of oil in the beginning of the process is larger than in the stationary state. Therefore is necessary to remove of the extraction field the oil excess before reaching the stationary state, that drives the formation of the maximum.

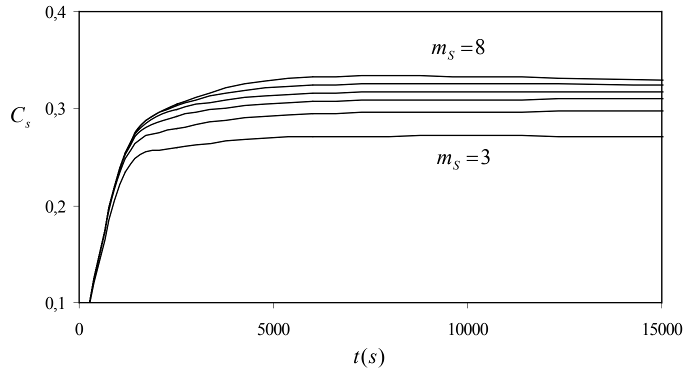

Figure 4. Evolution of the concentrations C_s in function of sections number

It is also observed that for a small sections number the values of C_s are low, and m_s as increases, the concentration C_s increases. "Fig. 5" evidence that, in the stationary regime, with the reduction of the sections number the losses increase, therefore the contact time between the porous medium and the miscela decreases, and therefore, the extraction rate decreases. It is also observed that for m_s = 3 the oil losses are big. But, for m_s > 6, the cost of the extractor and expenses of energy increase, however, the oil losses only reduce a little. Probably for that, in this extractor were established 6 percolation sections.

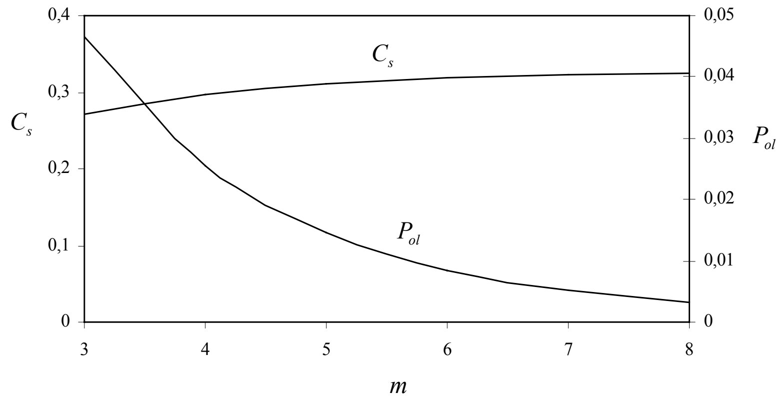

Figure 5. Variation of the concentration C_s and oil losses P_{ol} in function of m_s

"Figure 6" shows the distributions of the concentrations $\overline{C}_m$ for extractors with m_s = 3 to m_s = 8. In this figure is observed that, in the stationary state, the average concentrations in the trays are approximately same but, for m_s = 3, the losses oil are very big for the contact time between the porous medium and the miscela is very small.

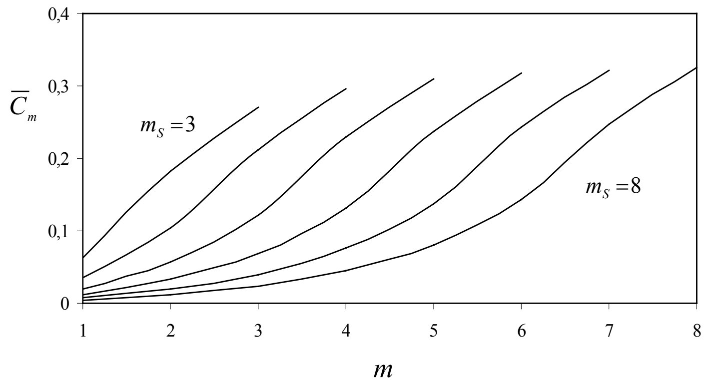

Figure 6. Variations of the average concentrations of trays $\overline{C}_m$ in function of m_s

5. Conclusion

Countercurrent crossed flows model was created, that are characteristic of industrial extractors of the horizontal type. This model is based on the laws of the involved phenomena and in the peculiarities of the flows in porous medium. It foresees the space distributions of the extraction field characteristics main, as well as the oil losses. Therefore is sensitive to the alteration of the porous medium porosity, of the extractor sizes main and of the operational regime parameters. The simulations with the percolation sections number of variable show that, in general, a small sections number leads to a inexpensive extractor with the notable oil losses. On the other hand, a big sections number, turns the extractor an expensive equipment, but with small oil losses. The accomplished simulations confirm that the extractor in study have a optimum sections number equal to six (06).

6. Acknowledgements

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