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Research Article

Mathematical Modeling Study by Supercritical Fluid Carbon Dioxide Extraction of Chamomile by Finite Element Method and Comparison with Finite Difference Method

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Abstract

Today, there will be many challenges ahead of chemical engineers to reach materials that could be less pollution and drawbacks of production and more and more pure, so there is any of these characteristics such as it comes to attract as the goal in the use of materials, various design process and the creation of new products for healthier lives and clean environment, in terms of other using clean energies and energy consumption. One of the innovations which started by the Baron Charles (the first person that changes in the fluid critical phase studied) above the concept of fluid in critical condition. In this paper we examine around the oil extraction plant chamomile by the fluid critical carbon dioxide, different way sand different numerical modeling methods used in this article. The fact that the use of the fluid in extracting oils from oil seeds and medicinal herbs would save of the materials very important because the process of extracting at less than other separating processes.

Keywords: Supercritical fluids; Chamomile; Modeling; Finite element

Introduction

In this section we briefly review some of the characteristics of supercritical fluid can move on a solvent supercritical fluid (SCF) it is likely that multi-component compounds with a focus on differences in volatility components (The outstanding feature of distillation) and Significant differences in the interaction between the components and solvents SCF (in other words, the outstanding features liquid extraction), we isolated. When a critical point is a matter of getting the temperature up too dense, towards the infinite desire for density or molar volume so that it is significantly changed in a critical region, a bit in terms of the density of the liquid and the gas is typical of similar capacity increased so much that solubility is dependent on the pressure of their own shows. Solubility is a fundamental variable capacity supercritical fluid separation process can be based on it. Garlic is a supercritical fluid in the vapor-liquid equilibria conditions are less than the critical point is that the vapor phase and liquid phase separation above is placed in the lower level. increases with

Figure 1: From left to right the process of change and achieving phase of the zone supercritical.

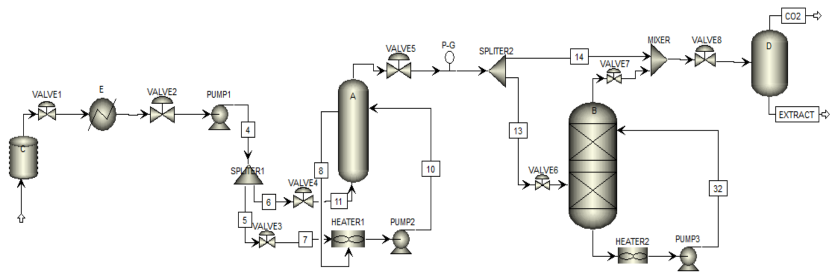

Figure 2: Schematic by supercritical fluid extraction device.
A: Tank; B: Extraction column; C: Carbon dioxide reservoir; D: Sample containers; E: Condensing

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temperature and pressure to gradually liquid density decreased and gas density increases in critical point with two phases density is against each other and the level of Separation two phases is impossible. Fluid in terms of pressure and temperature above critical point is called the fluid critical (Figure 1).

The most important issue in the design of a supercritical extraction process, solvent is selected. By selecting the appropriate solvent reduces operating costs and increases the purity of the products. Solvent should be inexpensive, non-toxic and have high solubility. By taking this thing and something else about drugs and food sensitivities to temperature and pressure of the solvent is very important. Therefore, one of the supercritical fluid carbon dioxide extraction is very useful for this type of critical situation due to very good (31.6°C and 73.4atm) compared with supercritical fluids other than the appropriate pressure and temperature is much lower and the pressure and temperature, especially suitable for the extraction of food much to help us [1].

Chamomile plant permanent vegetation and small and almost 30cm height which car you go in the fields and roadsides. Chamomile has a warm and dry nature of the chicory family, and yarrow. This plant has many pharmaceutical properties and also refers to the mobile pharmacy skin beneficial properties of chamomile can be used as anti-inflammatory, relieve skin wounds, relieve eczema , anti-acne and pimples, burn repair, cosmetology, hair care, golden blonde hair and skin disinfectant noted [2]. Numerical solution to the finite element method the data in this paper. This article first review the results of the numerical solution to the finite element method with laboratory results, paper, and validate the results of the finite element numerical solution with the results of the method of limited to resolve differences. Below you can see a schematic of the device extracted by supercritical fluid (Figure 2).

Mathematical Modeling

All experiments in a fixed bed of chamomile as stationary phase and supercritical fluid carbon dioxide as the fluid phase were carried out. The aim of these experiments, the extraction of essential oils is derived from chamomile and gain efficiency. Chamomile plant solutes to simulate the extraction process, the system of partial differential equations that are derived using a mass balance, can be used. Model assumptions are as follows:

1. The solid particles are perfectly spherical and the size and due to the small diameter solid particles, changes in the concentration of particles in the form of concentrated (lumped) will be considered.
2. Change the concentration and temperature during extraction process is negligible.
3. Changes in concentration, centrifugal extractor, is negligible.
4. Porosity remains constant throughout the extraction process.
5. The physical properties of supercritical fluids, extracted over time and is constant throughout the bed.

With these assumptions, as well as writing a mass balance, differential equation governing the fluid phase after just no written as follows: [2-12]

$$\frac{\partial C_f}{\partial \tau}-\frac{1}{\mathrm{Pe}_b}\frac{\partial c_f}{\partial z^2}+\frac{\partial c_f}{\partial z}+\frac{1-\varepsilon}{\varepsilon}\frac{3\mathrm{L}}{\mathrm{R}_p}\frac{\mathrm{Bi}}{\mathrm{Pe}_p}\left(\mathrm{C}_f-\mathrm{C}_s\right)=0 \quad (1)$$

The following initial and boundary conditions:

$$\text{At } \tau = 0 \rightarrow C_f = 0 \quad (2)$$

$$\text{At } z = 0 \rightarrow C_f = 0 \quad (3)$$

$$\text{At } z = 1 \rightarrow \frac{\partial c_f}{\partial z} = 0 \quad (4)$$

Similarly to the solid phase can be mass balance differential equation as a dimensionless follows:

$$\frac{dq}{đ} = -3\frac{k_f}{v}\frac{L}{R_p}(C_c - C_f) \quad (5)$$

With the initial condition of the following:

$$\text{At } \tau = 0 \rightarrow q = q_0 \quad (6)$$

In the above equations q and c_s can be assumed equilibrium conditions associated with the equilibrium constant k is as follows:

$$q = kc_s \quad (7)$$

The Model Parameters

Supercritical temperature and pressure, weight average molecular tests in this study were obtained from the chamomile plant. CO_2 viscosity of the equation of state of Soave / Redlich / Kwong calculated. In this study, density obtained using the relationships Jossi [3].

To determine the molecular diffusion coefficient D_{AB} existing relationships in the book properties of gases and liquids are used: [3]

A solvent and solute B

$$D_{AB} = \alpha + 10^{+5}\left(\frac{T}{M_A}\right)^{0.5}\exp\frac{0.3887}{0.23-\upsilon_{rB}}$$

$$\upsilon_{rB} = \frac{\upsilon_B}{\upsilon_{cB}}, \quad \upsilon_B = \frac{ZRT}{P} \quad (8)$$

$$\alpha = 14.882 + 0.005908\frac{T_{cB}VcB}{M_B} + 2.0821\times10^{-6}\left(\frac{V_{cB}T_{cB}}{M_B}\right)^2 \quad (9)$$

The external mass transfer coefficient (k_f) and if Hatami and colleagues calculated using the formula in the book we Treybal mass transfer: [13-22]

$$K_f = \frac{Sh.D_{AB}}{d_p}$$

In this regard D_{AB} (molecular diffusion coefficient), Sh (Sherwood) and dp(particle diameter) are dimensionless number. To calculate the Sherwood number of Hatemi and colleagues presented a paper that: [20]

$$Sh = 0.0306\ Re^{0.83}\ Sc^{0.33}$$

In this regard, Re and Sc are dimensionless numbers Re and Sc are calculated using the following equation:

$$Re = \frac{2R_\rho V_\rho f}{\mu_f}, \quad Sc = \frac{ì_f}{\rho f D_{AB}}$$

In this regard μ_f fluid viscosity and fluid density ρ_f

Numerical Solution

In this study, the equations governing the extraction process with the finite difference method and finite element numerically solved and compared. Finite Difference Method of form governing the system

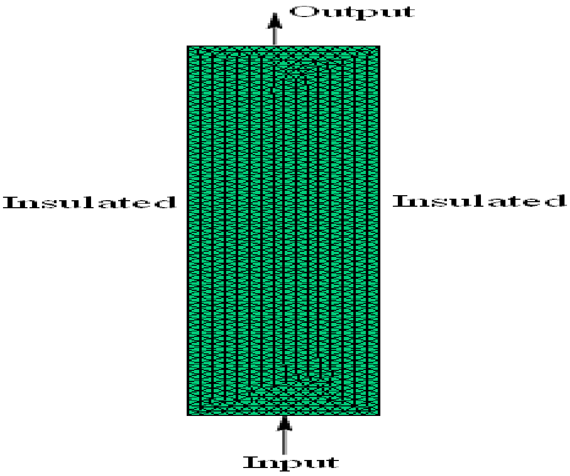

Figure 3: Area of supercritical fluid simulation software.

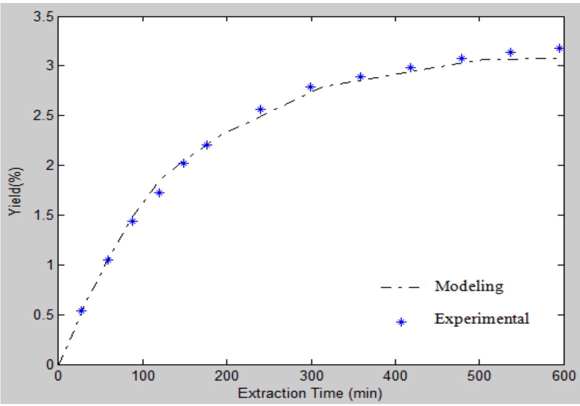

Figure 4: Supercritical fluid at a pressure of 10 MPa and 313 percent efficiency Kelvin.

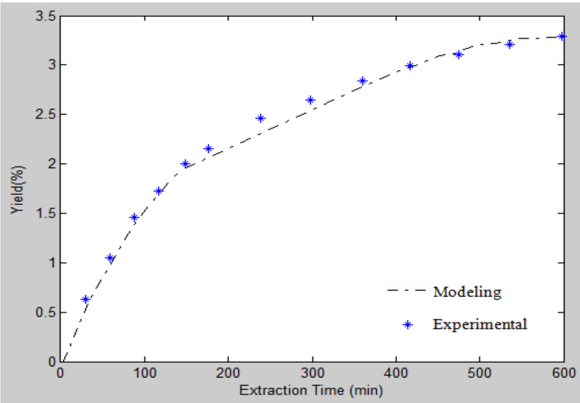

Figure 5: Supercritical fluid at a pressure of 10 MPa and 303 percent efficiency Kelvin.

uses differential equations, integral equations of the form used if the finite element method. Typically integral form to complex geometry in a multi dimensional problems is a better option compared to differential form. Finite element method, when the physical properties of materials are variable or second boundary condition (Neumann boundary condition) in question is present; it can be used simpler than finite difference. To solve equations using finite difference method MATLAB software for solving equations using finite element software Flex PDE was used. Flex PDE a mathematical software created by PDE Solutions Inc, which differential equations governing the issue by the finite element method to solve. 1 to 7 simultaneous equations are solved with software Flex PDE. Area intended for solving the governing equations, the software Flex PDE (Figure 3).

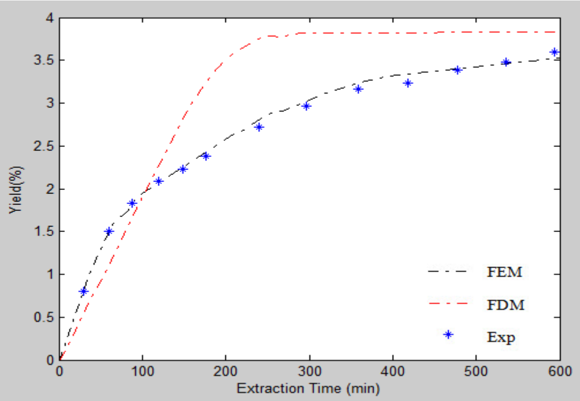

Figure 6: Comparison of the finite element method, finite difference method with experimental data for the pressure of 16 MPa and 313 °K.

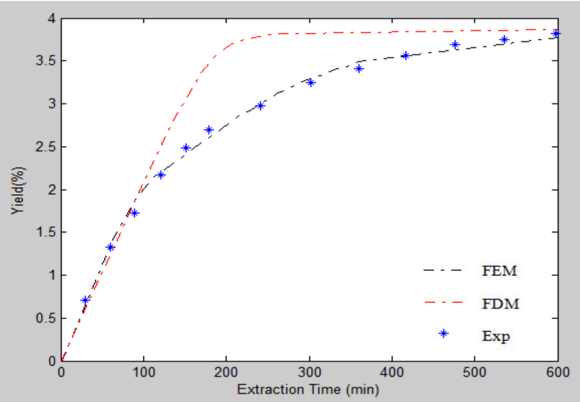

Figure 7: Compare the finite element method compared to the finite difference method with experimental data for the pressure of 16 MPa and 303 K.

Table 1: Process Parameters for SFE of chamomile.

Parameter	Value
T(K)	313
P(Mpa)	25
Q $(kgs^{-1})\times10^5$	11.55
D_{ext}(cm)	0.0542
L(m)	0.1254
dp(mm)	0.3
ε	0.8297
$\rho_s(kgm^{-3})$	1417

Validation

As can be seen in Figures 4 and 5 experimental data with the results of finite element modeling and numerical solution of high compliance. The difference Figure 4 and Figure 5 at the operating temperature is supercritical extraction process.

Discussion

In this paper, the mathematical model presented to the finite difference method and finite element solution and were compared with experimental results. This compares to the pressure of 16 MPa and 313 K in Figure 6 and Figure 7 for the pressure of 16 MPa and 303 K show. As you can see, the finite element method, finite difference

Table 2: Composition and physical properties of chamomile extract.

Substance	Molecular formula	Mole fraction	Mw $(gmol^{-1})$	K)Tc)	Pc(bar)	Zc	w
Beta-farnesene	$C_{15}H_{24}$	0.1473	204	704.14	16.88	0.223	0.499
7-Methoxycoumarin	$C_{10}H_8O_3$	0.0232	176.17	737.77	40.93	0.322	0.683
Palmitic acid	$C_{16}H_{32}O_2$	0.042	256.43	887.59	14.08	0.185	1.055
Linoleic acid	$C_{18}H_{32}O_2$	0.0377	280.45	951.23	13.19	0.174	1.047
Alpha bisabolol oxide B	$C_{15}H_{25}O$	0.0787	221	831.95	20.93	0.225	0.475
Alpha bisabolol	$C_{15}H_{26}O$	0.0417	222	857.36	19.51	0.217	0.877
Alpha bisabolol oxide A	$C_{15}H_{26}O_2$	0.1054	238	838	22.59	0.241	0.5
En-in-dicycloether	$C_{13}H_{12}O_2$	0.5239	200	884.54	35.18	0.285	0.436
Extract		1.0000	212.01	847.01	26.24	0.26	0.53

Table 3: Molecular diffusion coefficient of extract in supercritical fluid, viscosity and density of supercritical fluids as a function of temperature and pressure.

T(K)	MPa)P)	$Dm^{*}10^{8}(m^{2}s^{-1})$	$\mu\times(10^{5}kgm^{-1}s^{-1})$	$\rho(kgm^{-3})$
303.15	10	0.907	5.866	722.718
	12	0.807	6.504	775.637
	16	0.694	7.486	844.997
	20	0.626	8.315	893.227
313.15	10	1.364	4.340	564.567
	12	1.065	5.310	666.664
	16	0.847	6.456	768.099
	20	0.740	7.308	830.250
	25	0.657	8.228	885.939

Table 4: Transport and dimensionless parameters calculated during modeling.

$Q^{*}10^{5}(kgs^{-1})$	T(k)	P(Mpa)	$D_l^{*}10^{8}(m^{2}s^{-1})$	Re(-)	Sc(-)	Sh(-)	Pe_b(-)	$Kf^{*}10^{5}(ms^{-1})$	K(-)
3.33	303.15	10	2.205	0.19	8.949	0.121	385.336	3.665	43.1
		20	1.899	0.134	14.878	0.12	361.973	2.511	14.3
3.33	313.15	12	2.317	0.21	7.479	0.12	397.58	4.262	33.2
		16	2.081	0.172	9.923	0.12	384.192	3.375	31
6.67	303.15	10	5.799	0.38	8.949	0.172	293.481	5.183	20.8
		12	5.503	0.343	10.397	0.171	288.141	4.6	21.6
		16	5.182	0.298	12.771	0.171	280.899	3.95	12.8
		20	4.995	0.268	14.878	0.17	275.688	3.55	11
	313.15	10	6.97	0.514	5.638	0.171	312.559	7.783	28.6
		12	6.093	0.42	7.479	0.17	302.807	6.033	18.2
		16	5.437	0.345	9.923	0.169	292.61	4.783	16.4
		20	5.178	0.305	11.898	0.169	386.079	4.167	8.6
11.55	313.15	25	3.903	0.22	14.147	0.152	218.818	3.317	13.6

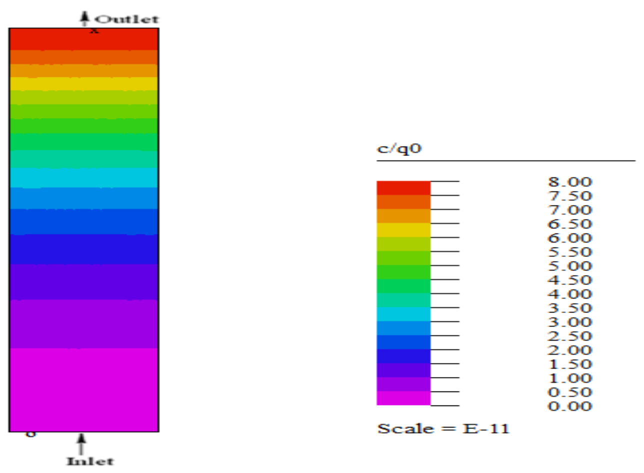

Figure 8: Contour concentration dimensionless fluid phase at the time of 600 minutes.

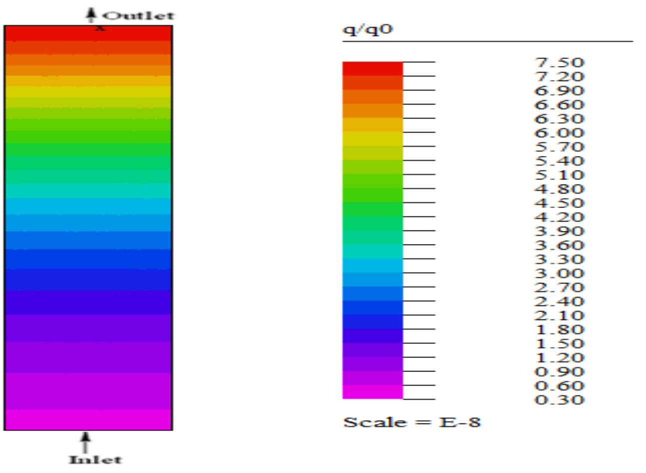

Figure 9: Cantor concentration without the solid phase at the time of 600 minutes.

method towards a better agreement with the experimental data (Table 1-4).

Contours concentration dimensionless fluid phase and solid phase, respectively, are shown in Figures 8 and 9. In this contour increasing trend with increasing concentrations of the substrate is visible.

With a view to Cantor, shown in Figure 8, a witness and increase of oil plant chamomile at the top of the bed of the movement of the fluid critical of the foot to the top of the bed.

with a view to Cantor, shown in Figure 9 witnessed a greater degree of gathering, oil seeds chamomile at the top of the bed, because of the influence of the crisis and fluid motion at the beginning of the process, and also at the beginning of the bed, more than and influence, a move that is at the top of the bed, So the oil chamomile at the top of the bed, it would be better to gradually until the amount of oil at the top of the bed of the fluid passing through a crisis also decreases over time.

Conclusion

In this paper, a detailed survey of supercritical fluid extraction, carbon dioxide, mathematical modeling and simulation software are addressed. In this paper to the modeling approach has been focused on that topic time in this way, the modeling of the key points, including the modeling approach. Overall the concept of the fluids critical pointed to the two time static and dynamics of great significance. As in the simulations observed in time to gradually static and dynamic in time to return almost remains constant. Other tips found in this simulation using the finite element method instead of using the finite difference method is that the results are better this way. Particular advantage of this method of application in the complex geometries and much higher accuracy and compliance with the experimental data of this approach than in the difference is very limited. Because of the finite element method is regular networking and simulations in any one of these elements is done regularly, With the correct definition of boundary conditions and initial conditions can produce better results than the finite difference method. Another important result in this paper is to reduce yields at constant pressure, with an increase in temperature. The results of the finite element method in an article available independent of the grid will be announced.

Nomenclature

C_f	oil concentration in the supercritical fluid phase (kg m^{-3})
C_s	solute concentration in the supercritical fluid phase on the surface of solid (kg m^{-3})
d_p	particle diameter (m)
D_{ax}	axial dispersion coefficient (m^2 s^{-1})
D_{ext}	extractor diameter (m)
DAB	molecular diffusion coefficient (m^2 s^{-1})
F	feed mass (g)
K	extract equilibrium constant between the solid and fluid phases
k_f	external mass transfer coefficient (m s^{-1})
L	extractor length (m)
M	Molecular weight (g mol^{-1})
P	pressure (bar)
P_{eb}	Péclet number for the bed, (L υ D_{ax}^{-1})
Q	solvent flow rate (kg s^{-1})
Q	solute concentration in the solid phase (kg m^{-3})
R_p	particle radius (m)
Re	Reynolds number (ρ υ d_p μ^{-1})
S_c	Schmidt number (μ ρ^{-1} DAB^{-1})
S_h	Sherwood number ($d_p k_f$ DAB^{-1})
T	temperature (K)
T	time (min)
TcB	critical temperature of the solvent (K)
υB	molar volume of the solvent (cm^3)
υcB	critical volume of the solvent (cm^3 mol^{-1})
υrB	residue volume of the solvent (cm^3 mol^{-1})
V	molar volume (cm^3 mol^{-1})
V	superficial fluid velocity (m s^{-1})
Y	extraction yield
Z	dimensionless axial coordinate along the bed, x L^{-1}
Greek letters	
M	Viscosity (kg m^{-1} s^{-1})
P	Density (kg m^{-3})
E	extractor void fraction
T	dimensionless time, (t v L^{-1})
Subscripts	
C	Critical
Ext	Extractor
F	Fluid
P	Particle
S	surface of particle
0	Initial

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