

Simulation of a Mathematical Model of SFE Process through COMSOL Multiphysics



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Introduction: Supercritical fluid extraction (SFE) has been named as ‘Green’ technology due to its compatibility with the environment during the effective and efficient extraction of various plants products (i.e. Seeds, Leaves, Stems, Flowers, Roots, Fruits and Herbs). In this work, COMSOL Multiphysics 5.2 was used to solve a mathematical mass transfer based model (Stastova et al., 1996) which is a modified model of Sovova H., 1994 by introducing the term ‘Grinding efficiency’. The solved model was validated with the results reported by Duba and Fiori, 2015, during the SC-CO₂ extraction of Grape seeds oil. The solved model’s mechanism is based on DDD (Desorption-Dissolution-Diffusion) phenomenon, explained by three analytic equations which represents three different regimes of whole extraction curves. Analytic function in COMSOL Multiphysics 5.2 software was used to solve each mathematical equation and then compiled all of them to get a complete profile of SC-CO₂ extraction.

Mathematical model:

The proposed model (Stastova et al., 1996), first time explained the effect of grinding efficiency term in the BIC concept hypothesized by Sovova H., 1994 and it is based on differential mass balance in solid and solvent phase along the extraction bed as shown in Fig.1.

Assumptions:

- Fixed bed.
- Plug flow of the solvent exists in the bed.
- Axial dispersion is neglected.
- Solute accumulation in the solvent is neglected.
- Solvent is solute free at the entrance.
- Temperature and pressure are regarded as constant.
- Solid bed is homogeneous w.r.t. to particle size and initial distribution of solute.
- Solute is deposited in plant cells and protected by cell walls.

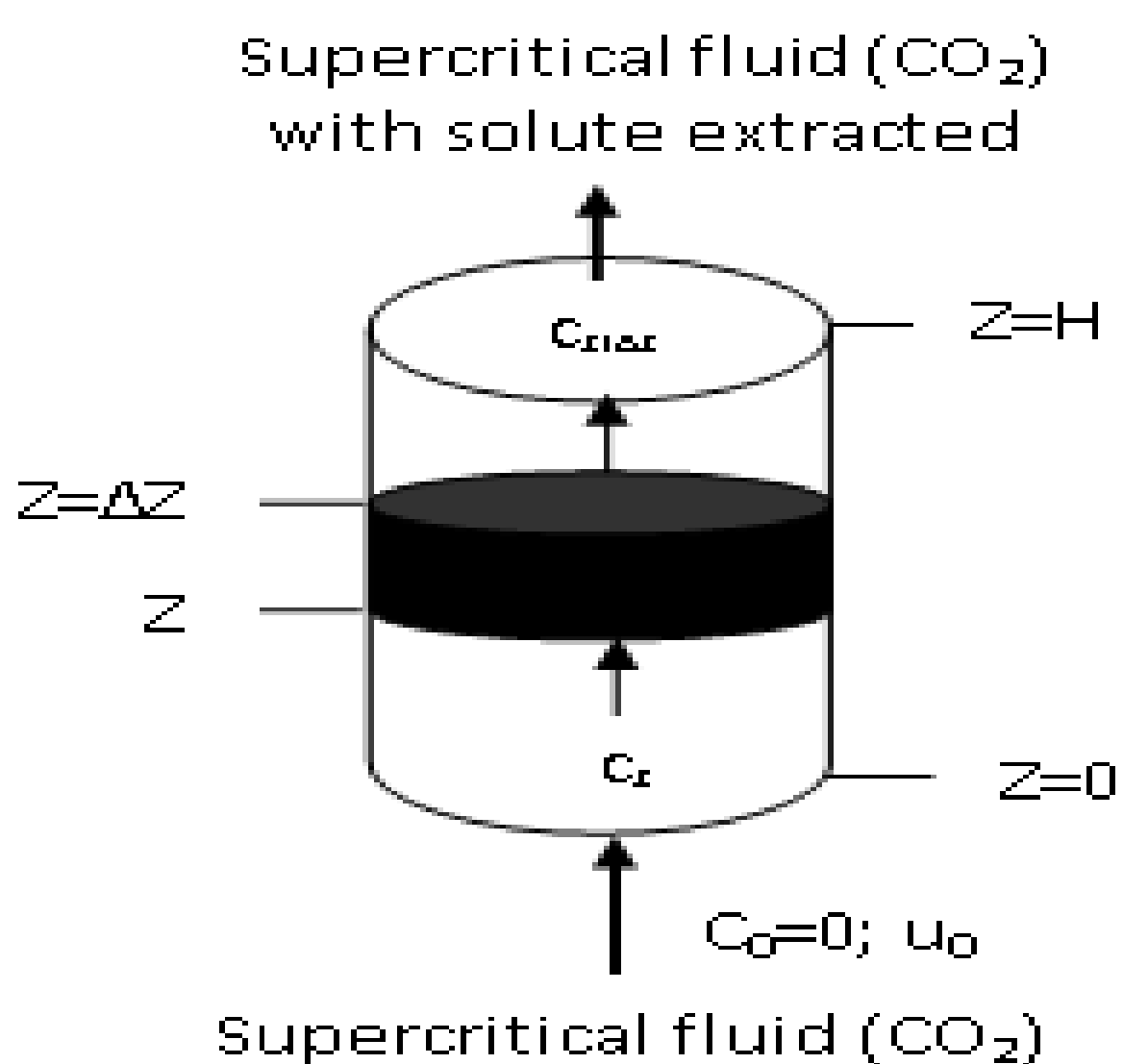


Fig.1:Schematic representation of extracting bed.

Three analytical equations, representing the three periods during SC-CO₂ extraction of grape seed oil. First period:

$$E = Nx_0 \phi(1 - \exp(-Z)) \quad \text{for } \phi < \frac{G}{Z} \quad \dots\dots\dots (1)$$

Second period:

$$E = Nx_0 \left(\phi - \frac{G}{Z} \exp(Z(h_k - 1)) \right) \quad \text{for } \frac{G}{Z} \leq \phi < \phi_k \quad \dots\dots\dots (2)$$

Third period:

$$E = Nx_0 \left(1 - \frac{1}{Y} \ln(1 + (\exp(Y) - 1) \exp(Y(\frac{G}{Z} - \phi))(1 - G)) \right) \quad \text{for } \phi \geq \phi_k \quad \dots\dots\dots (3)$$

Operating conditions:

Duba and Fiori, 2015 demonstrated the effects of different parameters (P, T, Q, dp and ep) during the SC-CO₂ extraction of grape seed oil from grape as shown in Table below:

P (bar)	200	300	400	500	Fixed parameters
	4.20 (y _s , mg/g)	7.60	10.4	13.0	T = 40 °C
	8.51 (Q, g/min)	8.43	8.32	8.59	ε _p = 0.41
	0.71 (G)	0.76	0.72	0.72	x ₀ = 0.120
	1.2*10 ⁻² (kfa0, 1/s)	9.8*10 ⁻³	8.29*10 ⁻³	6.61*10 ⁻³	Error % = -12.398 to +18.154
	3.49*10 ⁻⁵ (ksa0, 1/s)	3.45*10 ⁻⁵	7.18*10 ⁻⁵	9.7*10 ⁻⁵	AARD % = 7.26 to 9.629
T (°C)	35	40	50		Fixed parameters
	12.8 (y _s , mg/g)	13.0	13.4		P = 500 bar
	8.28 (Q, g/min)	8.59	8.70		ε _p = 0.41
	0.70 (G)	0.72	0.77		x ₀ = 0.120
	3.02*10 ⁻³ (kfa0, 1/s)	6.61*10 ⁻³	5.06*10 ⁻³		Error % = -2.499 to +5.819
	6.44*10 ⁻⁵ (ksa0, 1/s)	9.7*10 ⁻⁵	6.19*10 ⁻⁵		AARD % = 2.252 to 3.049
Q (g/min)	4.71	7.45	8.43	10.22	Fixed parameters
	0.42 (d _p , mm)	0.43	0.41	0.43	T = 40 °C
	0.52 (G)	0.62	0.57	0.78	P = 350 bar
	3.84*10 ⁻³ (kfa0, 1/s)	6.98*10 ⁻³	1.002*10 ⁻²	1.27*10 ⁻²	y _s = 8.60 mg/g
	2.3*10 ⁻⁵ (ksa0, 1/s)	5.04*10 ⁻⁵	8.87*10 ⁻⁵	9.73*10 ⁻⁵	ε _p = 0.41
					x ₀ = 0.120
					Error % = -16.357 to +17.813
					AARD % = 4.706 to 6.732
d _p (mm)	0.41	0.45	0.59	0.75	Fixed parameters
	7.34 (g/min)	7.19	7.46	7.31	T = 50 °C
	0.81 (G)	0.67	0.55	0.39	P = 500 bar
	3.26*10 ⁻³ (kfa0, 1/s)	4.27*10 ⁻³	2.42*10 ⁻³	6.11*10 ⁻³	y _s = 13.4 mg/g
	4.98*10 ⁻⁵ (ksa0, 1/s)	2.44*10 ⁻⁵	2.56*10 ⁻⁵	1.98*10 ⁻⁵	ε _p = 0.41
					x ₀ = 0.167
					Error % = -1.351 to +15.733
					AARD % = 1.607 to 7.439
(ε _p)	0.41	0.32	0.23	0.10	Fixed parameters
	0.38 (d _p)	0.47	0.43	0.47	T = 50 °C
	8.84 (g/min)	8.38	8.63	8.43	P = 500 bar
	0.81 (G)	0.72	0.86	0.93	y _s = 13.4 mg/g
	6.33*10 ⁻³ (kfa0, 1/s)	4.87*10 ⁻³	5.49*10 ⁻³	1.77*10 ⁻³	x ₀ = 0.167
	9.63*10 ⁻⁵ (ksa0, 1/s)	1.14*10 ⁻⁴	1.08*10 ⁻⁴	2.33*10 ⁻⁵	Error % = -1.451 to +5.912
					AARD % = 2.012 to 2.997

Table 1: Operating conditions and estimated model adjustable parameters for different operating parameters (P, T, Q, p, ep) during SC-CO₂ extraction of grape seed oil.

Steps followed during computation in COMSOL:

- Selecting, 1 D space dimension then click ‘model’ a Model Builder pop-up window appears. Parameters were given in option ‘Parameters’ under the Definitions.
- Three analytic functions (an1, an2, an3) were chosen in which all three analytic equations were inserted with an argument ‘t’ which varies from lower limit to upper limit according to the conditions given to each equation.
- Now, create a plot of each equation. After clicking ‘create plot’ of each equation , different functions (1D1, 1D 1a, 1D 1b) and three 1D plot groups (group1, group2, group3) appears as the new data sets and different 1D plot groups respectively under the section ‘Results’ of the model builder.
- Now, these three groups of pots were combined to get a complete nature of the model. Similarly, after putting the value of different operating conditions, estimated model adjustable parameters and operating parameters, new solution could be achieved.

Results: Results obtained by solving model equations using COMSOL Multiphysics 5.2 were compared with the available results obtained through MATLAB 7.0 in the literature as shown in Figures below:

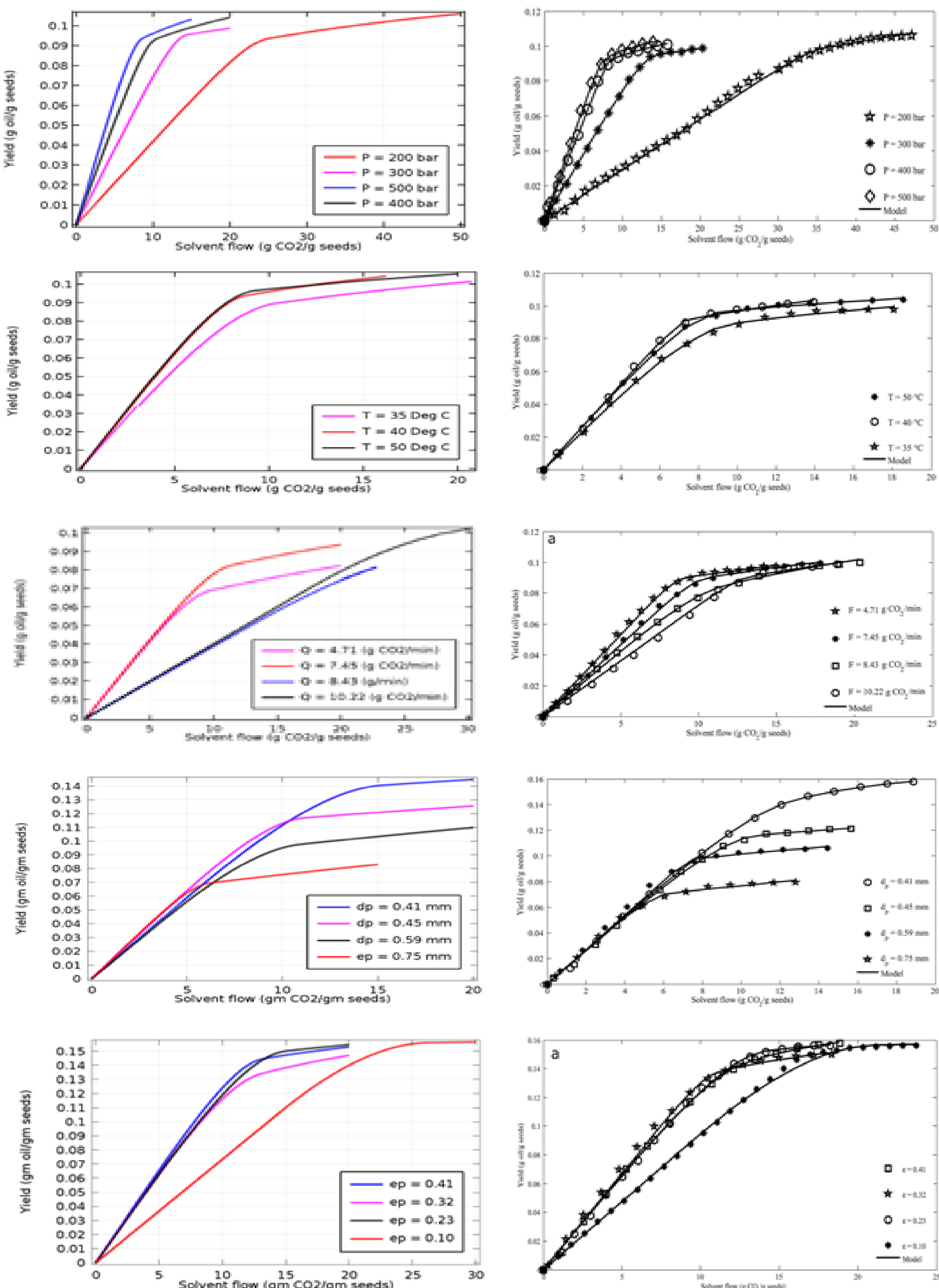


Fig 2. A comparison between results obtained from COMSOL multiphysics 5.2 (left side) with MATLAB solutions (right side) reported by Duba and Fiori , 2015 in literature.

Conclusions:

Results obtained through COMSOL Multiphysics 5.2 shows a good agreement with the MATLAB results found in literature with acceptable error % band and AARD % in each parametric conditions. From the results it is clear that COMSOL Multiphysics 5.2 superior in terms of time consumption in computation and could be a great option to solve analytic equations.

References:

- Duba K.S., Fiori L., "Supercritical CO₂ extraction of grape seed oil: Effect of process parameters on the extraction kinetics." J. of Supercritical Fluids 98 (2015) 33–43
- Sovova H., Rate Of The Vegetable Oil Extraction With Supercritical CO₂-I. Modelling of Extraction Curves." Chemical Engineering Science, 49, 409-414 (1994).
- Stastova J., Jez J., Bartlova M., Sovova H., "Rate Of The Vegetable Oil Extraction With Supercritical CO₂-III. Extraction from Sea Buckthorn." Chemical Engineering; Science, Vol, 51, No. 18, Pp. 4347 4352, 1996.