Simulation of Supercritical Fluid Extraction Process using COMSOL

PRIYANKA[1], SHABINA KHANAM[2]

Department of chemical engineering, IIT Roorkee, Roorkee, Uttarakhand 247667.

Introduction: Supercritical fluid extraction process (SFE) is a technique that exploits the solvent power of supercritical fluids at temperatures and pressures near the critical point. A mathematical model is developed by Reverchon,1996 for SFE of sage leaves and solved with experimental data as show in table 1. Mathematical model can be solved by using a approach of Equation based modeling.

Parameter	Value	Units
Flow rate (Q)	8.83	g/min
Porosity (ε)	0.4	Pa.s
Superficial viscosity	$0.455*10^{-3}$	m/s
Fluid phase coefficient (k_f)	$1.91*10^{-5}$	m/s
Volumetric partition coefficient (k_p)	0.2	
Diffusivity (D_i)	$6.0*10^{-13}$	m^2/s

Table 1. Experimental conditions and process parameters

Computational Methods: Reverchon,1996 proposed model based on differential mass balances performed along the extraction bed.

$$uV\frac{\partial c}{\partial h} + \varepsilon V\frac{\partial c}{\partial t} + A_p K(q - q^*) = 0$$

$$(1-\varepsilon)V\frac{\partial q}{\partial t} = -A_p K(q - q^*)$$

$$c = k_p . q^*$$

With initial and boundary condition

$$c = 0, \quad q = q_0 \quad \text{at } t = 0$$

$$c(0,t) = 0 \quad \text{at} \quad h = 0$$

These equations were added by taking Mathematical interface: (i)The Coefficient form PDE interface for eq. (1) and (ii) Domain ODEs and DAEs for eq. (2). Time dependent study and 1D geometry is taken to solve the equations as shown in Figure 1.

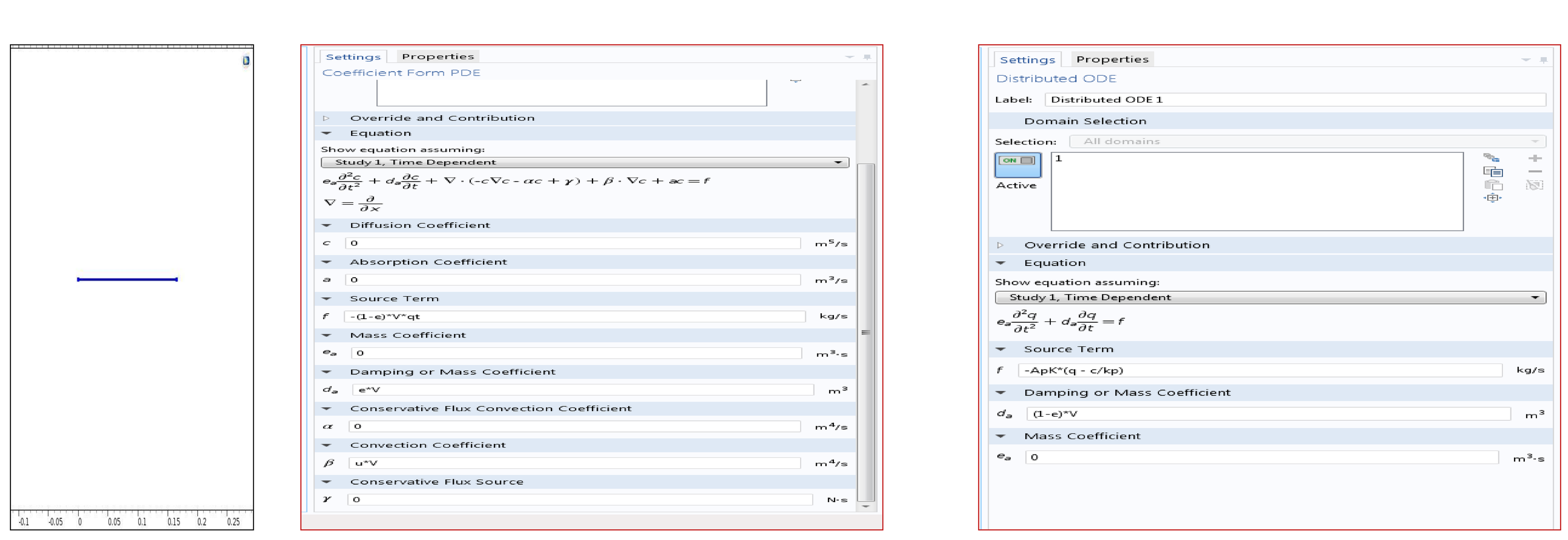

Figure 1. 1D Geometry and mathematical interfaces

Results: Results are computed considering four different particle size and plotted between extraction yield (amount of oil extracted*100/amount of oil available in seed) and extraction time. While comparing the literature results (Figure 2) with COMSOL multiphysics (Figure 3), extraction yield results for 0.25, 0.5 and 0.75 mm particle size are same as found in literature and shows that almost total amount of oil available are extracted by the extraction process. However, extraction yield observed is lesser than that of literature for the particle size 3.1. The reason for a lesser extraction yield could be that model is not supporting the extraction of large particle size solute.

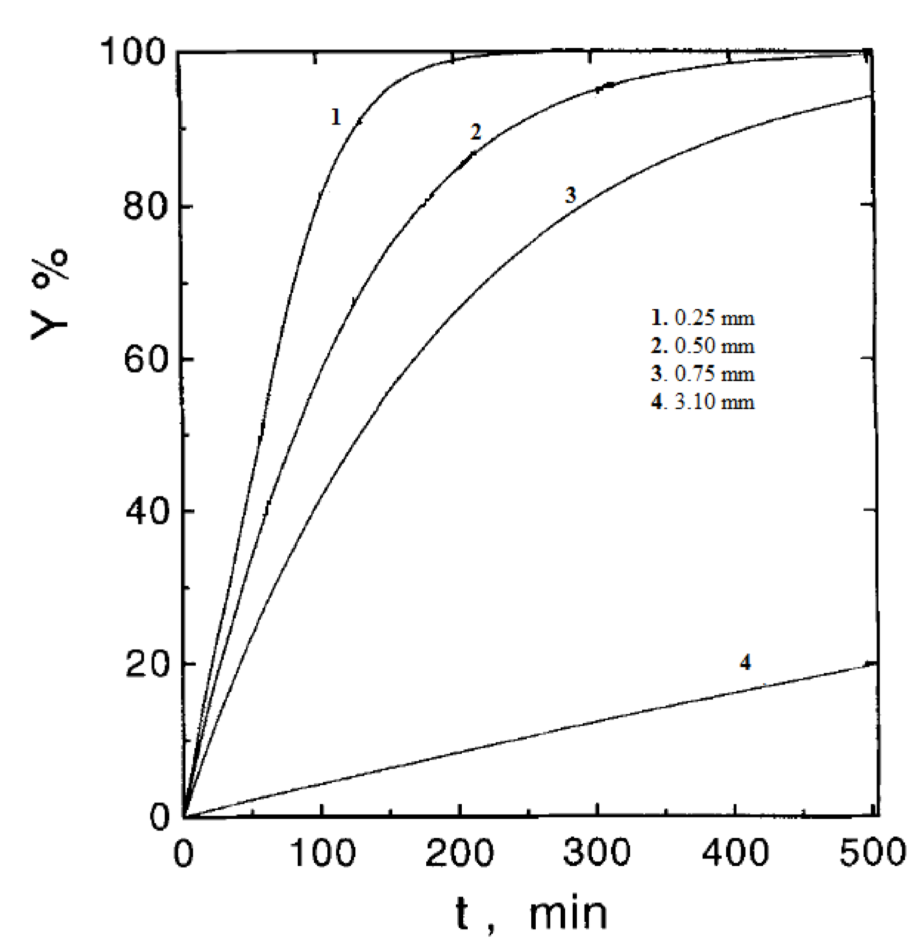

Figure 2. Results given by Reverchon,1996

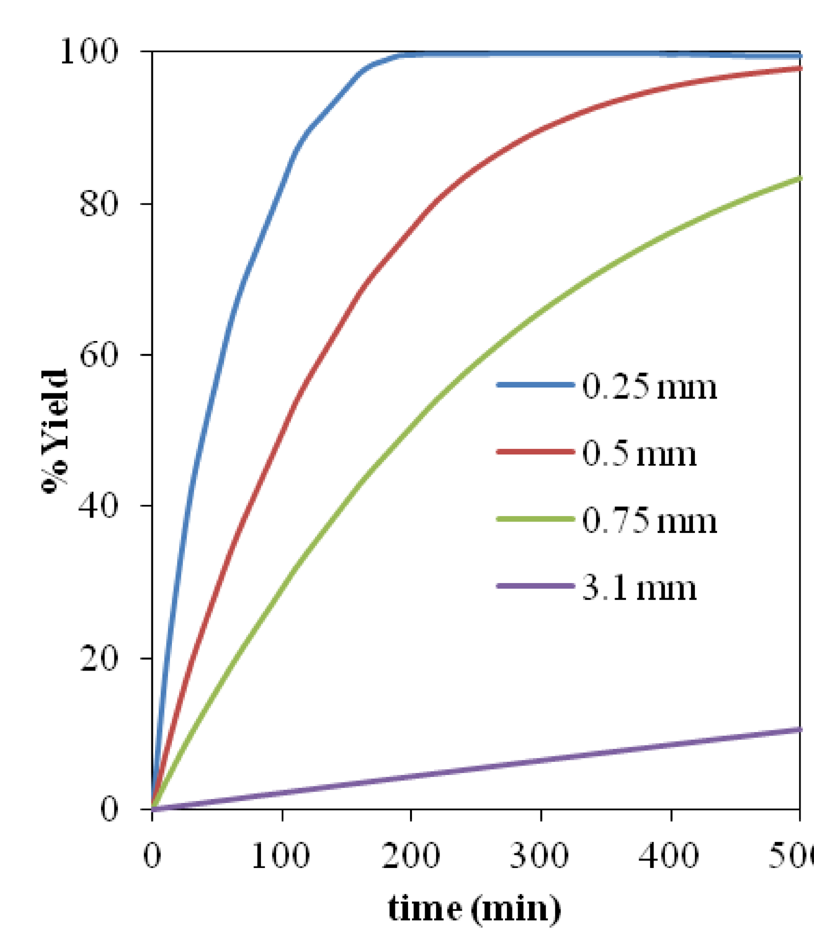

Figure 3. Results from COMSOL multiphysics

Conclusions: Model equations are successfully solved with the help of Equation based modeling approach. Computation time taken by the COMSOL multiphysics is 12 s which is far lesser than other software packages and larger memory usage also requires for Runge- kutta method which is used in literature to solve the model equations.

References:

1. E. Reverchon, Mathematical Modeling of Supercritical Extraction of Sage Oil, Bioengineering, Food, and Natural Products, Vol. 42, No. 6 (1996).
2. Eduardo L.G. Oliveira et al., Review of kinetic models for supercritical fluid extraction, *chemical engineering research and design*, **89**,1104-1117 (2011).
3. Mamata Mukhopadhyay, Extraction and processing with supercritical fluids, *J Chem Technol Biotechnol*, **84**, 6-12 (2008).

Excerpt from the Proceedings of the 2015 COMSOL Conference in Pune