Validation of Supercritical Fluid Extraction Model through COMSOL Multiphysics 5.2

Vibha. Devi, Late Ravindra. Bhargava, Shabina. Khanam
Department of Chemical Engineering
Indian Institute of Technology Roorkee, Uttarakhand, India

COMSOL CONFERENCE 2016 BANGALORE

Introduction:

Supercritical fluid extraction (SFE) technology is one of the best separation technologies, which encourage the society towards the Green Technology as of no harmful residue is emitted during the process. To describe the SFE technology, Sovova,1994 developed a mass transfer based mathematical model which became very successful to describe the SFE technique. Due to the reliable results of this model, many other authors used this model in their research. Sovova et al., 1994 used his own model for Grapes seed extraction and author Mira et al., 1996 and Mira et al., 1999 validated this model for the extraction of essential oil and cuticular waxes from Orange peel.

Name	Sovova et al., 1994	Mira et al., 1996	Mira et al., 1999	Description
x_0	0.144	0.1	0.045	Initial oil content of seed
x_k	0.018	0.06	0.012	Initial oil concentration inside the particles
k_f	$2.2\times10^{-4}\times U^{0.54}$	1.13×10^{-4}	1.13×10^{-4}	Mass transfer coefficient for fluid phase, m/s
k_s	6.6×10^{-10}	2.26×10^{-5}	2.26×10^{-5}	Mass transfer coefficient for solid phase, m/s
y_r	0.00685	0.095	0.008	Solubility
ε	0.33	0.33	0.33	Void fraction of bed
$\dot{q}$	3.8×10^{-3}	1.26×10^{-3}	$1.1.178\times10^{-3}$	Specific flow rate of solvent, 1/s

Computational Methods:

Sovova H., 1994 described the extraction curve into three part. The initial part of curve as ‘Fast Extraction Zone’, last part of curve as ‘Slow Extraction Zone’ and middle part of curve (combination of fast and slow extraction) as ‘Transition Zone’.

Fast Extraction Zone:

$$e = q\times y_r\times[1-\exp(-Z)] \quad \text{for } q < q_m$$

Transition Zone:

$$e = y_r\times(q-q_m\times\exp(((Z\times y_r)/(W\times x_0))\times\log((x_0\times\exp(W\times(q-q_m))-x_k)/(x_0-x_k))-Z))$$

$$\text{for } q_m \le q \le q_n$$

Slow Extraction Zone:

$$e = x_0-(y_r/W)\times\log(1+(\exp((W\times x_0)/y_r)-1)\times\exp(W\times(q_m-q))\times(x_k/x_0))$$

$$\text{for } q \ge q_n$$

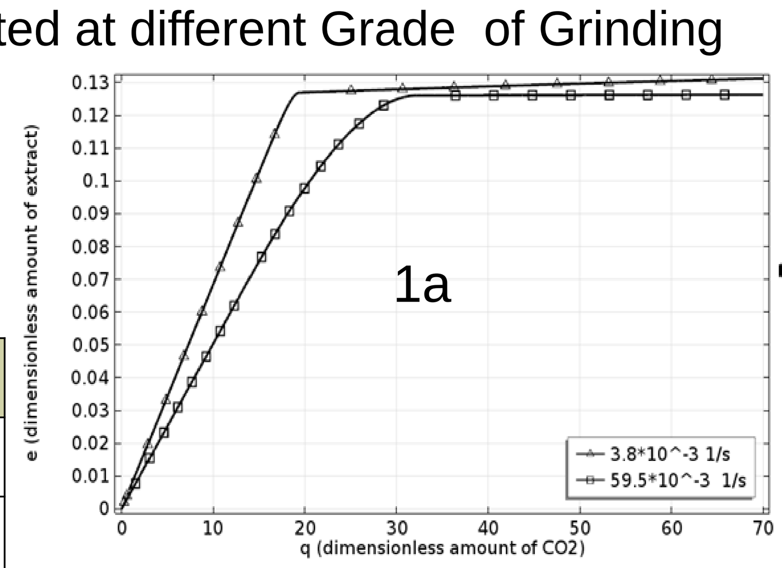
Following steps has been followed to implement these equations in COMSOL multiphysics 5.2 tool:

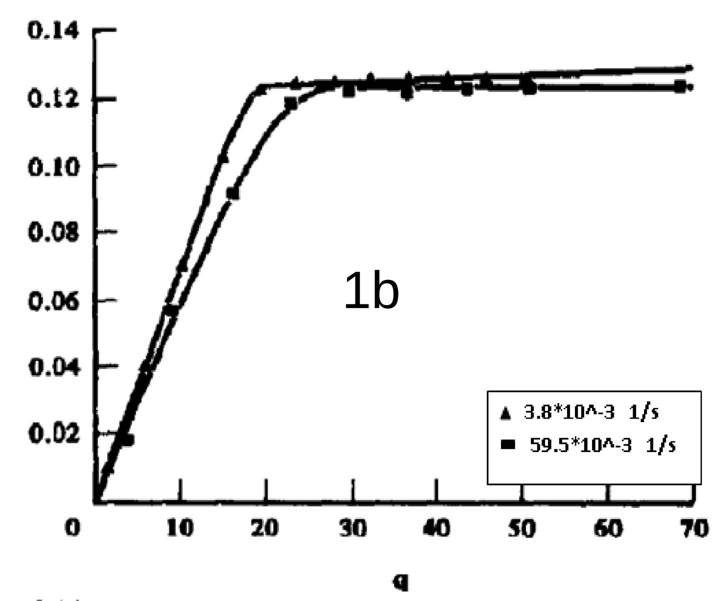
1. *COMSOL multiphysics --› Model Wizard --› Select 1 D space dimension --› No physics selected --› Click done*
2. *COMSOL multiphysics --› Global --› Definitions (Right click) --› Parameter*
3. *COMSOL multiphysics --› Definitions tool bar --› Analytic function* (three times for three analytical function).
4. Define analytic functions and arguments for all three zones;
   Analytic --› Definition --› Expression and Arguments
5. Define conditions of the analytic functions;
   Analytic --› Plot Parameter --› Upper and Lower limit --› Create Plot
6. *Define Parameter Bounds*
   COMSOL multiphysics --› Results --› Data Sets --› Function 1D --› Parameter Bounds
7. *COMSOL multiphysics --› Results --› 1 D Plot Group (Right click) --› Line Graph --› Data (in setting window of Line Graph) --› Data set (Define function 1D)*
8. Define y-Axis data and x-Axis data and plot the results.
9. Add more Line graphs to plot all three equations together.

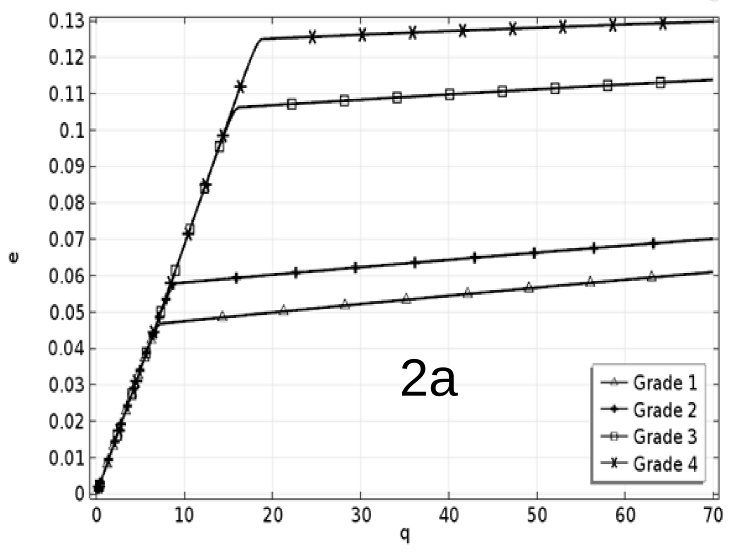
Results:

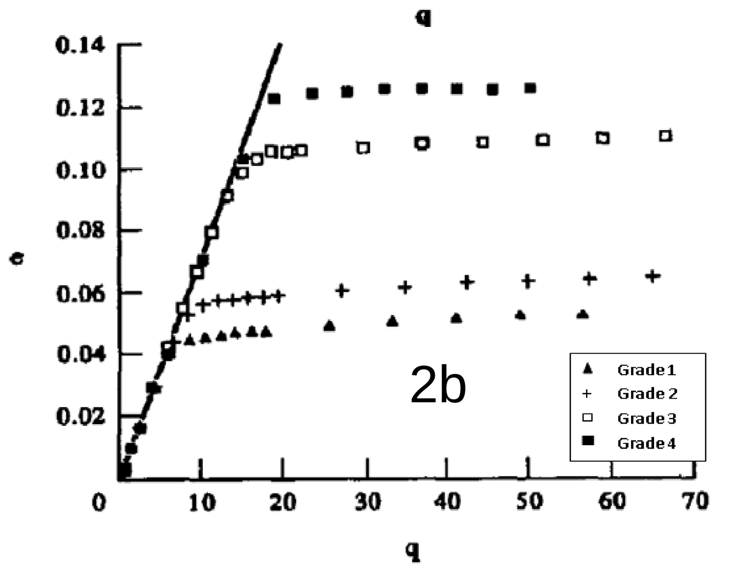
Results obtained from COMSOL multiphysics 5.2 are shown in Left graphs (1,2,3 & 4a) and Results given in research papers are shown in Right graphs (1,2,3 & 4b). Experimental data of all three research papers are given in the table.

Sovova et al., 1994: 1a & 1b are plotted at different specific flow rate of solvent and 2a & 2b are plotted at different Grade of Grinding

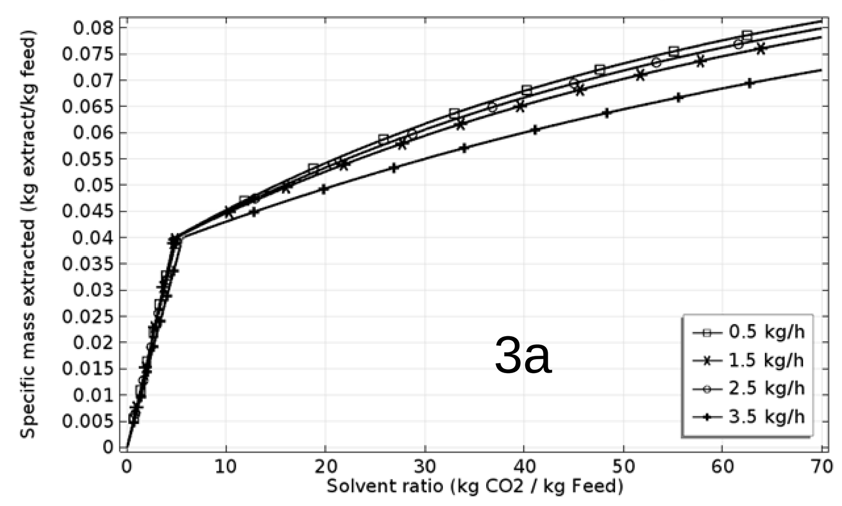


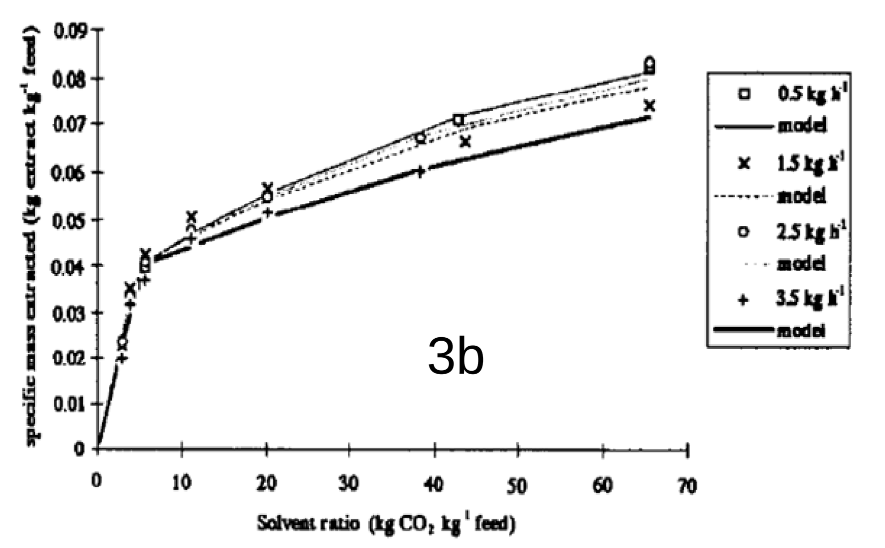




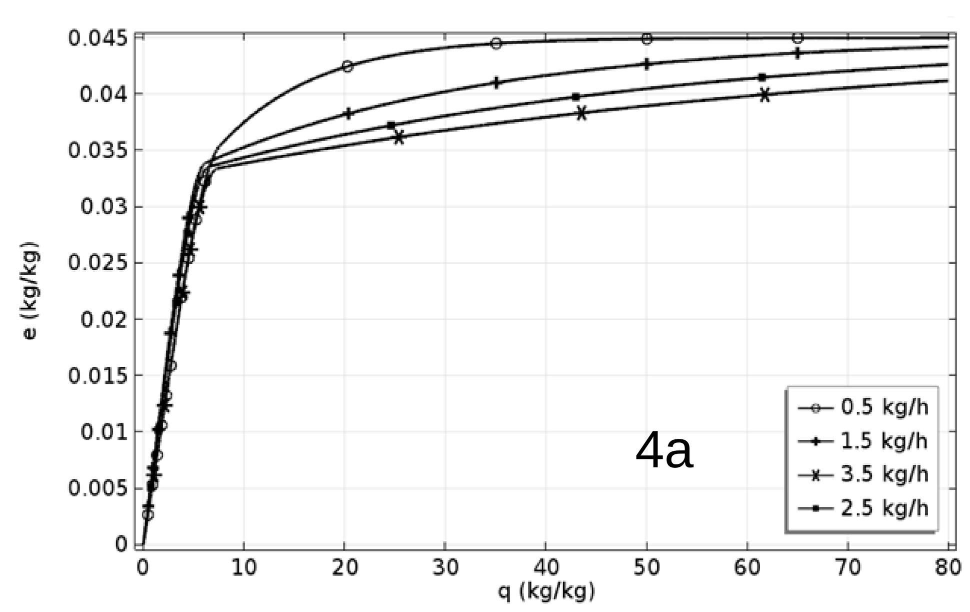


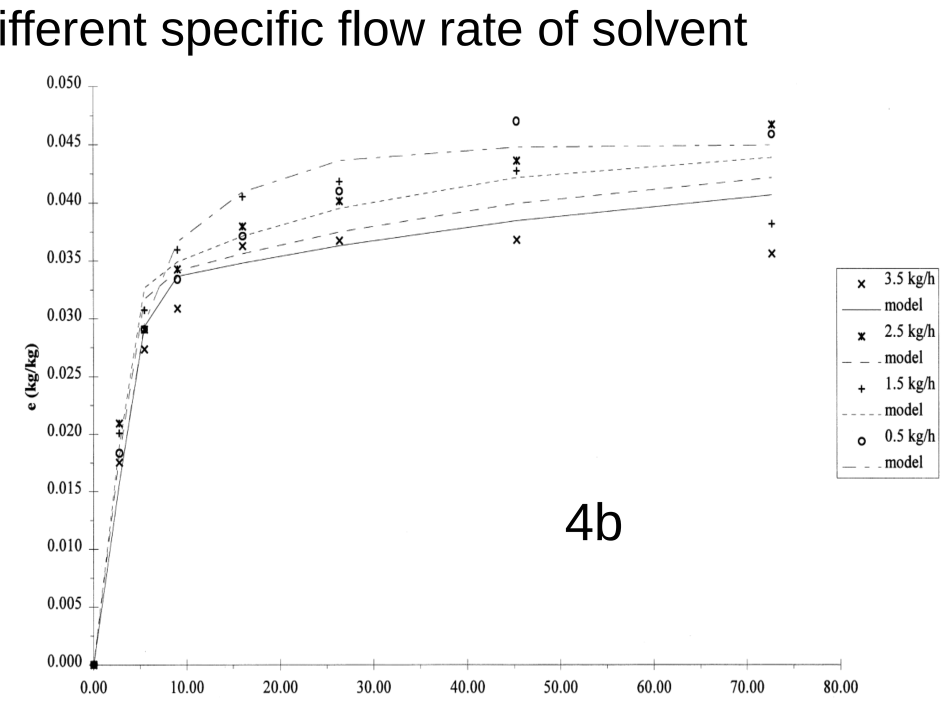
Mira et al., 1996: 3a & 3b are plotted at different specific flow rate of solvent





Mira et al., 1999: 4a & 4b are plotted at different specific flow rate of solvent





Conclusions:

Through the analysis of the results, it can be concluded that COMSOL multiphysics 5.2 is a successful tool for the validation of model equations. The software has very small average absolute relative deviation (AARD) within ± 9.26% error band for Grape seed and ± 4.44% error band for orange peel. COMSOL multiphysics 5.2 can be seen as one of the most reliable modeling software in SFE technique because of its less computation time, comfort handling and better results.

References:

1.Sovova H., Rate of the vegetable oil extraction with supercritical CO2-I modeling of extraction curves, Chemical Engineering Science’ 49: 409-414, (1994)
2.Sovova H., Kucera J., Jez J., Rate of the vegetable oil extraction with supercritical CO2–II extraction of grape oil, Chemical Engineering Science, 49: 415-420, (1994)
3.Mira B., Blasco M., Subirates S., Supercritical CO2 Extraction of Essential Oils from Orange Peel, The Journal of Supercritical Fluids, 9, 238-243, (1996)
4.Mira B., Blasco M., Berna A., Subirates S., Supercritical CO2 extraction of essential oil from orange peel. Effect of operation conditions on the extract composition, Journal of Supercritical Fluids, 14, 95–104 (1999)