**1. Introduction**

Chemical and petroleum, pharmaceutical, food, biotechnology, biomedical, nuclear, material and polymer processing industries can be mentioned as example of industries use Supercritical fluid (SCF) technology for extraction and separation widely (Cabral et al. 2007; Dong et al. 2010; Park and Bae, 2002; Giorgi et al. 2000; Srinivasan et al. 2002; Said-Galiyev et al. 2003; Guney and Akgerman, 2002; Subramanian et al. 1997; Guzel and Akgerman, 2000; Macnaughton et al. 1996; Murga et al. 2002; Ajzenberg et al. 2000; Jafari Nejad et al. 2011; Jafari Nejad et al. 2012). In fact, in recent years, this technology has attracted considerable attention and widely applied.

Supercritical fluids, particularly supercritical carbon dioxide which is one of the most common SCF, have unique physical and chemical properties and usually low toxicity. This process is categorized as rapid processes due to high diffusivity and lower viscosity in SCF mediums. By setting the operating condition i.e. temperature, pressure and density, which itself results in a variation in solvating power as indicated by Tabernero et al (Tabernero et al. 2010), a desired selectivity can be obtained. Of the most interesting properties of supercritical carbon dioxide are the relatively low critical temperature and pressure of 304 K and 73.7 bar, low costs, nontoxicity, no flammability, and recyclability with no environmental hazard (Saus, 1995; Fasihi et al. 2004).

The design of SCF processes will be facilitated and possible provided that the solubility data and mathematical modeling of these solubility data are available and known (Lucien and Foster, 2000; Bae and Hur, 1996; Haarhaus et al. 1995; Joung et al. 1998). In fact, a better understanding of the process can be achieved by the mathematical modeling in any process of interest (Asgarpour Khansary et al., 2014), and here it can be used for the representation of solubility at interested pressures and temperatures.

The mathematical modeling of solubility data of solutes in supercritical fluids process can involve three main categories;

1. A single solute in a supercritical fluid,
2. Mixed solutes in a supercritical fluid, and
3. A single solute in mixed supercritical fluids or supercritical fluid plus an organic solvent.

Also, based on the method of mathematical modeling, different equations for representation of solubility data in supercritical carbon dioxide can be obtained. Generally, these models are classified into two groups; theoretical or semi-empirical equations such as models based on equations of state, and empirical equations such as density based equations.

Using theoretical models such as cubic equation of state requires complicated computational procedures and methods, and also the knowledge of the solid properties including critical properties, acentric factor, molar volumes and sublimation pressure, which often cannot be easily determined experimentally and should be calculated using some group contribution method. It's obvious that uncertainty and errors on numerical values of the solute properties can affect solubility predictions (Garnier et al. 1999). The physical basis of these models can be regarded as one the most important reasons why such models may appear in some literatures.

To overcome some of the mentioned obstacles, most researchers tend to use empirical models such as density-based models of Chrastil, Bartle, M´endez-Santiago–Teja and etc., Or the Ziger–Eckert semi-empirical model. These models are based on the simple error minimization and use only density of pure supercritical carbon dioxide and operational pressure and temperature. Thus, there is no need to calculate critical and thermo physical properties of the involved solutes. Several equations have been presented by different authors, covering from three to six parameters, which are necessary to determine solids solubility.

In this paper, after reviewing most efficient published solubility models in literature, a new accurate model for solute solubility in supercritical carbon dioxide has been proposed. These density based correlations have been presented in the following section in detail. The accuracy and performance of proposed model and previous models are critically verified and examined using a large number of solute solubility in supercritical data (more than 2400 data points), collected from literatures for the calculations. For an in-depth comparison, four statistical parameters have been defined. The results demonstrated that, using the proposed empirical model, much accurate solubility calculations could be achieved with readily available independent variables temperature, pressure and density of pure supercritical . Thus, the proposed model could be used for solubility calculation at interested pressures and temperatures in industry.

**2. A Brief Literature Review and Presentation of New Model**

Conveniently, using the density of the supercritical solvent, the solute solubility data can be correlated and modeled. Historically, by assuming association of one molecule of solute with k molecules of solvent and a complex formation, Chrastil (1982) derived an equation that relates the solubility of solute in a supercritical fluid with the density of the pure supercritical fluid and the absolute temperature as shown by **Eq. 1** in **Table 1**.

In Chrastil Model (**Eq. 1**), and  are the model constants which are obtained from experimental data fitting by means of an efficient error minimizing technique such Least Square Method, Objective Function minimization using Evolutionary Algorithms (Genetic Algorithm, etc.) which are widely available in literatures (for an example of GA application refer to Asgarpour Khansary and Hallaji Sani, 2014). It’s worthwhile to mention that is an association number and represents the average number of molecules in the solvated complex, the constant  depends on vaporization and solvation enthalpies of the solute, and the constant  depends on molecular weight of the solute, molecular weight of supercritical fluid and also . Also in **Eq. 1**, (), is the solubility of the solute in the supercritical phase and (), density of pure supercritical phase.

A similar expression of Chrastil type model was proposed by Kumar and Johnston (1988) in which the linear expression between and  was expressed as shown in **Eq. 2**. In fact, Kumar and Johnston (1988) found that the linear relationships between  versus and in some cases between  and are depended on the system. In the same year, del Valle and Aguilera (1988) developed and proposed another model by addition of one term to the Chrastil's model as indicated by **Eq. 3**.

Based on the theory of dilute solutions, a simple linear expression was proposed by Méndez-Santiago and Teja (2000) for the solubility of solutes in a supercritical fluid in which unlike previous models, effect of pressure was considered directly (**Eq. 4**). In this model, mole fraction of solute solubility was used. Bartle et al. (1991) proposed a simple density-based semi empirical model (**Eq. 5**) where is reference standard pressure,  reference density assumed as of 1 bar and 700, respectively. Again, it’s worthwhile to mention that the parameter  is related to the enthalpy of sublimation of the solute.

Another model for the mole fraction solubility of a solute () as function of pressure and temperature was proposed by Yu et al. (1994). In this model (**Eq. 6**),  represents the mole fraction of the solvent, here supercritical carbon dioxide. As the model uses a function of the dependent variable,  as an independent variable , the  value should be known in order to calculate  at a given temperature and pressure.

Following Sung and Shim (1999) and Gordillo et al. (1999), Jouyban et al. (2002) proposed another efficient empirical model for solubility calculation in supercritical carbon dioxide (**Eq. 7-9** respectively).

Using experimental data for pure supercritical carbon dioxide at various temperatures and pressure and by fitting collected data from international thermodynamic tables of the fluid state carbon dioxide (Angus et al. 1976), they also proposed an empirical correlation for pure supercritical carbon dioxide as indicated by **Eq. 9.b**. Models proposed by Adachi and Lu (2008), Garlapati and Madras (2009, 2010), and Jafari Nejad et al. (2010) are of the most recent models for solubility of a solute in supercritical fluids (SCFs). These models equations are listed in **Table 1** as **Eq. 10-13** respectively.

**Table 1**. Empirical Models for Solute Solubility Representation in Supercritical Fluids.

Reviewing these models of solute solubility data in supercritical fluids, it can be concluded that following fundamental relations exist which can be regarded as rules of thumbs for new models developments;

1. Non-linear relationship between  and pressure in isothermal conditions,
2. Non-linear relationship between  and temperature in isobaric conditions,
3. Non-linear relationship between and temperature when density is constant,
4. Non-linear relationship between  and density in isothermal conditions,
5. Linear relationship between  and .

Considering the relations mentioned and in order to provide more accurate solubility calculations, development of an accurate model was investigated during this research. Then following empirical equation (**Eq. 14**) is proposed after critical comparisons to other models in literature.

 (14)

Here,,and  are the proposed model constants. The feasibility and applicability of our proposed model investigated by means of a substantial solubility data collected from the available literatures as presented in **Material and Methods** section.

**3. Material and Methods**

A large number of solubility data, more than 2400 data points, have been collected from literature. The details of these solubility data including references, temperature and pressure ranges, and number of data points for each system are listed in **Table 2**.

**Table 2.** The details of studied solute in supercritical carbon dioxide.

For comparison of the models, the Surface Fitting Toolbox (**sftool**) of MATLAB software (R2009a) was used in which for a comprehensive and depth comparison between the fitted models and real behavior of the experimental data four parameters have been defined i.e. **SSE**, **R2**, **R2-adj** and **RMSE** which are shortly described below. It most noted that all collected data from literature have been assumed correct.

The total deviation of the predicted values () from the models to the experimental values () can be measured by sum of squares due to error of the fit (**SSE**) as defined by **Eq. 15** where  are weight values that in this study are assumed as unity.

 (15)

**R-square (or R-sq, R2)** is the square of the correlation between the solubility values and the predicted solubility values. This parameter (**Eq. 16**) measures how successful the model is in explaining the variation of the data. In other words, it is the square of the correlation between the experimental values and the predicted values.

 (16)

Where, **SSR** means the sum of squares of the regression and **SST** the total sum of squares as described in **Eq. 17-18**. Here, **SST** = **SSR** + **SSE** and  is the average of all data.

 (17)

 (18)

**Adj R-sq** is defined to handle the models have many constants. In fact, when the number of models coefficients increase, R-square will increase but the model may not improve in a practical sense. This parameter (**Eq. 19**) is the degrees of freedom adjusted R-square. In this Equation n is number of data and m is number of coefficient in the model.

 (19)

**RMSE** is the model standard error and the standard error of the regression. It is an estimation of the standard deviation of the random component in the data and can be defined as **Eq. 20**.

 (20)

It’s worthwhile to know that;

1. A **SSE** value closer to zero indicates a fit that has a smaller random error component and is more useful for prediction,
2. An **R-sq.** value closer to 1 indicates that a greater proportion of variance is accounted for by the model
3. An **Adj R-sq.** value closer to 1 indicates a better fit however it can take on any value less than or equal to 1, and
4. A **RMSE** value closer to 0 indicates a fit that is more useful for prediction.

For each system, listed in **Table 2**, the solubility data together with operating condition (supplementary file “**SampleDATA.mat**”) were supplied in sftool Toolbox, and models were introduced using “Custom Equation” option of the Toolbox (supplementary file “**Empirical.sfit**”). As mentioned in previous section and also seen in **Table 1**, there’re models which requires the parameter solubility () instead of the mole fraction (). As in most literature the solutes data were reported in terms of mole fraction (), the solubility of solute is calculated from mole fraction solute solubility data, by means of **Eq. 21** where subscript SCF indicate supercritical fluid molecular weight in. The result of comparisons of all models for all materials of study (for all data points) are provided in the following section.

 (21)

**4. Result and Discussion**

The proposed model and models in the literature have been critically compared by four predefined parameters. The accumulative average values of **SSE**, **R-square**, **Adj R-sq.**, and **RMSE** for each model are summarized in **Table 3**, in order to achieve general judgment and conclusion about models performance and accuracy in predicting solubility data. Also, for the first 30 system in **Table 2**, individual values of these four variables are provide in **Table 4-7** as an example and more information.

**Table 3**. Accumulative Average of comparative parameters values obtained from models for all 2400 data points.

From **Table 3**, it can be seen that the proposed model has the smallest value of SSE and RMSE, and also the highest values for R-square and Adj R-sq. This means that the proposed model is considerably reliable, and the predicted solubility has more agreement with experimental data in comparison to other models.

Jouyban et al. model is ranked as second on the basis of obtained values, it also reveals accurate results in solubility calculations over other models. This model can be rearranged in terms of temperature and pressure with regard to the **Eq. 9.b**, however it is out of scope of this study. In no doubt, Jouyban’s model was one the best models published for prediction and correlation of solubility data in supercritical carbon dioxide so far.

Jafari Nejad et al. model also reveals good agreement with the experimental data according to R-square and Adj R-sq. values, but RMSE and SSE values suggest that this model must be employed after the proposed and Jouyban et al. models, also even after Yu et al, Gordillo, Adachi and Lu, Sung and Shim, and Bartle models. The reason would be the simple and inefficient power form of the model, which will fail in predictions if there's unsmooth data or very scattered data. Thus more care should be taken using this model.

Models with little number of coefficients are preferable as they reduce the computation time, so the numbers of coefficients play an important role in empirical correlations. In other words Chrastil, Sung and Shim, Bartle, and Jafari Nejad have similar accuracy according to R-square value but for example Jafari Nejad model having four coefficients has greater RMSE and SSE value over Chrastil and Bartle models, which show the priority of these models in comparison to this model.

**Table 4**. R-square Value obtained for models.

**Table 5**. Adj R-sq. Value obtained for models.

**Table 6**. SSE Value obtained for models.

**Table 7**. RMSE Value obtained for models.

The worst results are obtained from using Méndez-Santiago and Teja, del Valle and Aguilera, and Kumar and Johnston models. Sorting all models with regard to the performance and accuracy comparison from the largest (the best in prediction) to smallest, we got the list: 1. Proposed, 2. Jouyban, 3. Gordillo, 4. Adachi and Lu, 5. Yu et al., 6. Chrastil, 7. Sung and Shim, 8. Bartle, 9. Jafari Nejad, 10. Garlapati and Madras (2009), 11. Garlapati and Madras (2010), 12. Kumar and Johnston, 13. del Valle and Aguilera, and 14. Méndez-Santiago and Teja.

The results demonstrated that, by using the proposed empirical model, much accurate solubility calculations could be achieved with readily available independent variables temperature, pressure and density of pure supercritical . Thus, the proposed model could be used for solubility prediction at interested pressures and temperatures.

**5. Conclusion**

A new model proposed for representation of solute solubility in supercritical fluids and validated by more than 2400 experimental data point collected from literature. The comparison between proposed model and published models shows that the proposed model gives much more accurate results in solubility calculations than previously published models. The proposed model has great and considerable agreement with the experimental data, so it’s strongly recommended to be used to facilitate and accelerate industries in where a knowledge and estimation of solute solubility is required at interested operating conditions.

**6. Further Information**

A 3D graphical overview of some models performance generated for system No. 11 due to the largest data points (69 points) are provided in **App. A** as informative material. In **App. B**, the coefficients of all studied models together with the new model for a number of systems have been provided. The systems in **App. B** are all the dyes listed in **Table 2**, as these are of the most interest of the authors’ field of research (Chemical Engineering). The **Graphical Abstract** has been provided to illustrate the behavior of studied models for a randomly selected system.

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