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SOLUBILITY PARAMETER APPROACHES FOR PEG: MATHEMATICAL MODELINGS OF SOLUBILITY

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Abstract. Algorithmic methods, as the mathematical application of the principle "like dissolves like", have been applied to interpret the solvent power in poly(ethylene glycol) PEG/solvent systems. The solubility parameters of PEG and solvents have been evaluated with respect to van Krevelen-Hoftyzer (VKH), Hoy, Breitkreutz, Askadskii and Small approaches and their 2-, 3-D graphs have been drawn. By creating the solubility profiles of the polymer in selected solvents, the dissolving capability of these solvents has been discussed. Consequently, solvency power of solvents for PEG decreases below order: THF>chloroform>DMSO>methanol>water.

Keywords: PEG, solubility parameter, algorithmic calculation, mathematical modeling of solubility.

AIM OF STUDY

PEG is bioadhesive and mucoadhesive due to its water solubility, hydrophilicity, high viscosity, ability to form H-bonds and biocompatibility. PEG studies have led to somewhat contradictory results concerning the ability of PEG to be perfectly soluble in dispersed species in some solvents or to form aggregates in these same solvents. Many studies have been carried out in the polymer field but the behavior of PEG in water has been less quantitatively understood [1]. Aim of this study is to improve practical tool which a solvent formulator can use in laboratory to the simplified task [2]. The solubility parameter concept is associated primarily with this aim, and is not sacrifice simplicity for accuracy. Solubility parameters tell only half the story, even if it is usually the most important half [3].

Calculation of Solubility Parameter Components of PEG by Different Algorithmic Approaches

Three-component solubility parameters of PEG are calculated and compared according to VKH [4], Hoy [5] and Breitkreutz's [6] atomic group contribution methods and total solubility parameters of PEG are calculated according to Small's group contribution method and Askadskii's method [7] about molar volumes in terms of van der Waals volumes of the constituent groups here.

TABLE 1. Solubility parameters calculated of PEG

Approaches	δ_t, $(Jcm^{-3})^{1/2}$
Small (method 1, 2, 3)	19.1- 19.2- 18.0
Askadskii	22.0
VKH	22.0
Hoy	21.4
Breitkreutz	25.8

2- and 3-Dimensional Approaches to PEG Solubility

Solvency power of solvents for PEG is compared between the 2-D approach and Hansen's 3-D approach.

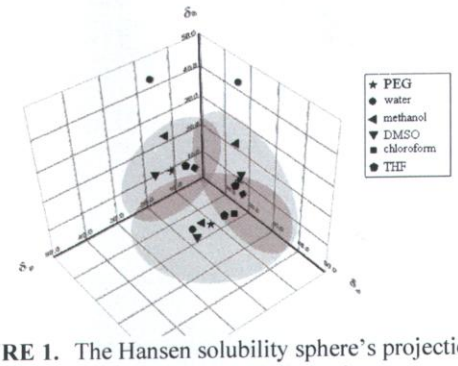

FIGURE 1. The Hansen solubility sphere's projections on three axial planes for PEG and studied solvents.

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