IGC determinations of solubility parameter for characterization of pharmaceutical excipients

Katarzyna Adamska, Adam Voelkel

Poznań University of Technology, Institute of Chemical Technology and Engineering, pl. M. Skłodowskiej-Curie 2, 60-965 Poznan, Poland

The solubility parameter concept is an important tool to interpret some relations between materials e.g. their compatibility, miscibility, adsorption. The close values of the solubility parameter of two materials indicate their similar ability to intermolecular interactions. In the case of, e.g. polymer and solvent such it may indicate solubility of polymer in the solvent [1, 2].

The principle aim of this work was an application of Inverse Gas Chromatography (IGC) for the estimation of solubility parameter for a number of compounds used at Pharmacy. The retention data of number of solvents (test solutes) were used to calculate Flory-Huggins interaction parameter (χ_{12}^{∞}) and solubility parameter (δ_2) [3]. The Hansen's three dimensional solubility parameter concept was used to estimate corrected solubility parameter (δ_T) and and its components (δ_d, δ_p, δ_h). This use of such assumption allows the more sophisticated characterization of examined systems [4].

Estimation of solubility parameter is connected with some restrictions and/or drawbacks.

Values of solubility parameter of test solutes (δ_1) most often differ depending on the method (experimental or computational, additive) used for their estimation. It significantly affects further calculations of solubility parameter (δ_2) total solubility parameter (δ_T). Proper selection of test solutes is also important and influences the precision and accuracy of the estimation of dispersive, polar and hydrogen bonding components of solubility parameters.

Exemplary our results of calculation of Hansen's solubility parameters foe the series of different solvents, the influence of the data selection (test solutes, data source, method of calculations) will be presented and discussed.

References

1. Barton, A. F. M., Handbook of Solubility Parameter and Other Cohesion Parameters, CRC Press, (1983).
2. Hansen, C. M., J. Paint Technol., 39 (1967) 104.
3. Lloyd, D. R., Ward, T. C., Schreiber, H. P., Inverse Gas Chromatography – Characterization of Polymers and Other Materials, American Chemical Society, Washington, DC 1989.
4. Hansen, C. M., Hansen Solubility Parameters: A User's Handbook, CRC Press, (1999).