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Determination of dapagliflozin propanediol monohydrate solubility in supercritical carbon-dioxide: Presenting a new model

Abstract:

Enhancing the solubility of pharmaceuticals with low water solubility has emerged as an effective approach for generating more efficient nanoparticles. To attain this objective, having knowledge about drug solubility in supercritical conditions is essential. Hence, this study sought to explore the solubility of dapagliflozin propanediol monohydrate (DPM) in supercritical carbon dioxide (SC-CO2) across a temperature range of 308-338 K and a pressure range of 120 to 270 bar. This research represents the first examination of DPM solubility under these conditions. The mole fraction of DPM dissolved in SC-CO2 ranged from 1.517×10-5 to 7.933 ×10-5, corresponding to a solubility range of 0.234 to 1.247 g/L. The highest solubility was observed at a temperature of 338 K and a pressure of 270 bar, with a mole fraction of 7.933×10-5. Two different groups of models were employed to correlate the experimental data: PR-EoS based model and empirical and semi-empirical models (including Bartle, Sodeifian, Chrastil, Sparks, Galapati-Madras). Moreover, a novel empirical model featuring four adjustable parameters was created to ascertain solute solubility in SC-CO2. The effectiveness of the proposed model surpassed that of existing empirical models found in the literature (Sparks et al., Jouyban et al., and Bian et al.). Experimental solubility data of DPM and 27 solubility datasets sourced from published literature were employed to validate the accuracy of this model. The proposed model successfully correlated the experimental solubility of dapagliflozin propanediol monohydrate with a satisfactory level of accuracy (AARD% = 14.41, Radj = 0.9731 and F-value = 137.84).

Biography

Gholamhossein Sodeifian (1971) graduated in chemical engineering (M.S) from University of Tehran, in 1997 and received his doctorate (Ph.D), in polymer Engineering from Tarbiat Modares University, Tehran, in 2002. After that, he has worked till now as a chemical engineering professor, at University of Kashan, and teaches many courses such as advanced mass transfer, supercritical fluid technology, optimization and modeling, advanced rheology of non-Newtonian fluids and polymer melts, mechanical and physical properties of polymers, experimental design, especial methods in separation processes and drug delivery in pharmaceutical systems. His researches focused on extraction of essential and seed oils, solubility measurement of solid drugs, micro and nano-particle formation of pharmaceutical materials in supercritical carbon dioxide (SC-CO2), and other new techniques. He has developed for the first time in the world a new and efficient technique for nanoparticle formation, i.e., US-RESOLV. He has published more than 98 ISI scientific paper with 5 inventions and 9 books in Persian language. Also, professor Sodeifian is named in the world's top 2% of scientists list in 2020, 2021, 2022 and 2023.