J Pet Environ Biotechnol 2016, 7:6 (Suppl)
http://dx.doi.org/10.4172/2157-7463.C1.026

Modeling of phase equilibria at high pressure using different cubic equations of state-mixing rule combinations

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Generally the experimental measurement of phase equilibria data at high pressure is complex, difficult, expensive and time consuming; hence there is need for reliable equations of state. A great number of equation of states are known but the other major difficulty is the choice of the most adequate combination of an equation of state (EOS) and a mixing rule (MR), for a given system at defined operating conditions. Consequently, to illustrate this crucial point, the present work considered the modeling of the solubility of chosen pharmaceutical compounds in supercritical carbon dioxide using known cubic equations of state in combination with four different mixing rules, namely, that of van der Waals, Panagiotopoulos and Reid, Wong-Sandler and Kwak and Mansoori mixing rules. A priori of the required physicochemical and critical properties of the considered compounds were predicted using well known methods based on the group contribution concept. The interaction parameters kij was obtained from experimental data available in the literature and involving the chosen pharmaceutical compounds, by the optimization of a well-defined objective function using the Nelder-Mead version of the simplex technique. For most systems, a quite good agreement between the calculated and experimental data was obtained for few EOS-MR combinations only, confirming that the accuracy of the results depends upon the choice of the combination. Finally the model of the best EOS-MR combination can be used to perform computer experiments according to various specific applications like for instance crystallization process using supercritical fluid where thermodynamics and phase equilibrium are the key matters.

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Natural nanotechnologies

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Some of the processes occurring in the environment and associated with migration of nanoparticles of metals can be considered as the natural nanotechnologies. Their detailed study will contribute to the future development of the industrial technologies, which are especially important for scarce and precious metals. As a priority it should highlight the problems of development of objects with nano gold. The discovery in Russia of a number of major gold deposits with so-called refractory ores (Olimpiadinskoe, Maiskoe, and Nezhdaninskoe) requires significant improvement in the technology of their development. Presumably, some of the gold in them is represented by nanometer-sized forms of occurrence. One of directions of solving this problem is the study of natural processes of nano gold concentration. It turned out that it is directly connected with the problem of "new" gold origin. We have shown growths of the newly formed metal on placer gold surface represent aggregates of nanoparticles deposited from ionic or colloidal solutions. Conditions required for mass deposition of "new" gold are favorable geological environment (weathering rocks of sulfide ore bodies with an abundance of nano-gold minerals-concentrators: Aspyrite, arsenopyrite, etc., tailings of the excavation of alluvial deposits, buried placers, etc.), uneven gold surface with numerous micro- and nano-defects, etc. As another option we can consider the natural process of amalgamation, which leads to the formation of aggregate grains composed of nanoparticles of mercury-bearing gold and cementing their amalgams. Finally, the natural processes of nano gold concentration can be implemented in environments where gold-bearing solutions migrate in the rocks containing natural sorbents of metal (carbonaceous substance, chlorides, ferriferous compounds, etc.). Natural nanotechnologies can be the basis for the creation of industrial technologies of development of deposits with nanoscale gold or recycling their wastes. Besides, the experimental studies play an important role. They confirm the high sorption capacity of gold nanoparticles and their tendency to aggregate.

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