

Numerical modelling of mass transfer for solvent-carbon dioxide system at supercritical (miscible) conditions

ABSTRACT

A numerical procedure of mathematical model for mass transfer between a droplet of organic solvent and a compressed antisolvent is presented for conditions such that the two phases are fully miscible. The model is applicable to the supercritical antisolvent (SAS) method of particle formation. In this process, solute particles precipitate from an organic solution when sprayed into a compressed antisolvent continuum. Effects of operating temperature and pressure on droplet behavior were examined. The CO₂ critical locus and the conditions for which the densities of solvent and carbon dioxide are equal are identified. Calculations were performed using Peng-Robinson equation of state. The model equations were put into the form that allowed the application of the Matlab standard solver pdepe. Calculations with toluene, ethanol, acetone (solvents) and carbon dioxide (antisolvent) demonstrated that droplets swell upon interdiffusion when the solvent is denser than the antisolvent and shrink when the antisolvent is denser. Diffusion modeling results might be used for data interpretation or experiments planning of the more complex real SAS process.

Keyword: Diffusion; Supercritical antisolvent method; Droplets swell; Droplets shrink