Study of high-pressure adsorption from supercritical fluids by the potential theory

The multicomponent potential theory of adsorption (MPTA), which has been previously used to study low-pressure adsorption of subcritical fluids, is extended to adsorption equilibria from supercritical fluids up to high pressures. The MPTA describes an adsorbed phase as an inhomogeneous fluid with thermodynamic properties that depend on the distance from the solid surface (or position in the porous space). The description involves the two kinds of interactions present in the adsorbed fluid, i.e. the fluid-fluid and fluid-solid interactions, accounted for by means of an equation of state (EoS) and interaction potential functions, respectively. This makes it possible to generate the different MPTA models by combination of the relevant EoS/potentials. In the present work, the simplified perturbed-chain statistical associating fluid theory (sPC-SAFT) EoS is used for the thermodynamic description of both the adsorbed and the gas phases. We have also evaluated the performance of the classical Soave-Redlich-Kwong (SRK) EoS. The fluid-solid interactions are described by simple Dubinin-Radushkevich-Astakhov (DRA) potentials. In addition, we test the performance of the 10-4-3 Steele potential. It is shown that application of sPC-SAFT slightly improves the performance of the MPTA and that in spite of its simplicity, the DRA model can be considered as an accurate potential, especially, for mixture adsorption. We show that, for the sets of experimental data considered in this work, the MPTA is capable of predicting adsorption of pure components and binary mixtures in wide ranges of pressure and temperature. A good agreement with the theoretical predictions is achieved in most of the cases. The MPTA is capable to correctly describe complex physical behavior observed at supercritical/high-pressure conditions. Some limitations of the model are also discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Contributors: Monsalvo, M. A., Shapiro, A.
Pages: 56-64
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Fluid Phase Equilibria
Volume: 283
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.22 SJR 0.95 SNIP 1.033
Web of Science (2017): Impact factor 2.197
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.85 SNIP 1.187
Web of Science (2016): Impact factor 2.473
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 1.99 SJR 0.866 SNIP 0.998
Web of Science (2015): Impact factor 1.846
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.28 SJR 0.981 SNIP 1.232
Web of Science (2014): Impact factor 2.2
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.31 SJR 1.001 SNIP 1.277
Web of Science (2013): Impact factor 2.241
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2