Comparison of activity coefficient models for electrolyte systems

Comparison of activity coefficient models for electrolyte systems

Three activity coefficient models for electrolyte solutions were evaluated and compared. The activity coefficient models are: The electrolyte NRTL model (ElecNRTL) by Aspentech, the mixed solvent electrolyte model (MSE) by OLI Systems Inc., and the Extended UNIQUAC model from the Technical University of Denmark (DTU). Test systems containing a single salt (NaCl), multiple salts, and mixed solvent aqueous electrolyte solutions were chosen. The performance of the activity coefficient models were compared regarding the accuracy of solid-liquid and vapor-liquid equilibrium calculations for the test systems.

General information
Publication status: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Haldor Topsoe AS, Akzo Nobel Functional Chemicals AB, Shell Global Solutions (Malaysia) Sdn Bhd, SQM Salar S.A.
Contributors: Lin, Y., ten Kate, A., Mooijer, M., Delgado, J., Fosbøl, P. L., Thomsen, K.
Pages: 1334-1351
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: A I Ch E Journal
Volume: 56
Issue number: 5
ISSN (Print): 0001-1541
Ratings:
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.085 SNIP 1.423
Web of Science (2010): Impact factor 2.03
Web of Science (2010): Indexed yes
Original language: English
Keywords: process, thermodynamics/classical, crystallization, simulation
DOIs:
10.1002/aic.12040
Source: orbit
Source ID: 259878
Research output: Contribution to journal › Journal article – Annual report year: 2010 › Research › peer-review