Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas - DTU Orbit (09/11/2017)

Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas

Ionic liquids (Ms) have been receiving increasing attention as a potential decarbonization solvent. However, the enormous number of potential ILs that can be synthesized makes it a challenging task to search for the best IL for CO_2 removal from methane. In this work, a method was proposed to screen suitable ILs based on the COSMO-RS (conductor-like screening model for real solvents) model, an absorption mechanism, and experimental data. Besides the Henry's constant, the viscosity and toxicity of ILs should also be taken into consideration for an industrial decarbonization process. Furthermore, process simulation was performed to evaluate the new IL-based decarbonization technology. Considering CO_2 solubility, CO_2/CH_4 selectivity and toxicity and viscosity of ILs, [bmim][NTf_2] has been screened to be the potential solvent among 90 classes of ILs. Based on reliable experimental data, a rigorous thermodynamic model was established. The simulation results have been found to agree well with the available experimental results. Two process flow sheet options, use of two single-stage flash operations or a multistage flash operation following the absorber, have been simulated and assessed. Compared with the well-known MDEA (methyldiethanolamine) process for CO_2 capture, the single-stage and multistage process alternatives would reduce the total energy consumption by 42.8% and 66.04%, respectively.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Chinese Academy of Sciences, Technical University of Denmark
Authors: Liu, X. (Ekstern), Huang, Y. (Ekstern), Zhao, Y. (Ekstern), Gani, R. (Intern), Zhang, X. (Ekstern), Zhang, S. (Ekstern)
Pages: 5931-5944
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Industrial and Engineering Chemistry Research
Volume: 55
Issue number: 20
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2

Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398
Original language: English
DOIs:
10.1021/acs.iecr.6b00029
Source: FindIt
Source-ID: 2304243931
Publication: Research - peer-review › Journal article – Annual report year: 2016