Scopus

Documents

Khan, H.W.[a] , Elgharbawy, A.A.[b] , Shah, M.U.H.[c] , Negash, B.M.[d] , Khan, M.K.[e] , Khan, K.[f] , Kamyab, H.[g h i] , Yusuf, M.[j]

Exploring ionic liquids for formaldehyde separation via computational COSMO-RS screening
(2023) *Chemical Engineering Research and Design*, 196, pp. 588-598.

DOI: 10.1016/j.cherd.2023.06.055

[a] Department of Chemical Engineering, Universiti Teknologi Petronas, Seri Iskandar, Perak, 32610, Malaysia
[b] International Institute for Halal Research and Training (INHART), International Islamic University Malaysia, Kuala Lumpur53100, Malaysia
[c] University of Engineering and Technology, Peshawar, Pakistan
[d] Department of Petroleum Engineering, Universiti Teknologi Petronas, Seri Iskandar, Perak, 32610, Malaysia
[e] Aligarh Muslim University, Aligarh, 202002, India
[f] Interdisciplinary Research Centre for Renewable Energy and Power Systems (IRC-REPS) Research Institute, King Fahd University of Petroleum & Minerals, Dhahran, 31261, Saudi Arabia
[g] Faculty of Architecture and Urbanism, UTE University, Calle Rumipamba S/N and Bourgeois, Quito, Ecuador
[h] Department of Biomaterials, Saveetha Dental College and Hospital, Saveetha Institute of Medical and Technical Sciences, Chennai600 077, India
[i] Process Systems Engineering Centre (PROSPECT), Faculty of Chemical and Energy Engineering, Faculty of Engineering, Universiti Teknologi Malaysia, Johor, Skudai, Malaysia
[j] Institute of Hydrocarbon Recovery, Universiti Teknologi PETRONAS, Bandar, Seri Iskandar, Perak, 32610, Malaysia

Abstract
Formaldehyde is an emerging human carcinogen from gaseous spark ignition engines and in aqueous stream. In addition to causing leukaemia and nasal cancer, the emissions harm the environment. The present study examined ionic liquids (ILs) as greener alternatives for removing formaldehyde from different sources. Because of its reliability and excellent predicting ability a conductor-like screening model for real solvents (COSMO-RS) were employed as a simulation means to evaluate potential ILs for formaldehyde. Screened IL can be used as an extracting agent, an adsorbent, a carrier, or an absorbent in formaldehyde separation. 392 different cation-anion combinations were screened. To measure the efficacy of IL, the activity coefficient at infinite dilution, capacity, selectivity, and interaction energies were predicted for all 1600 ILs combinations. Short-chain quaternary ammonium cations were found to be potentially effective compared to long-chain and aromatic cations. Moreover, halogenated and food-grade anions such as fluoride, acetate, and lysinate showed higher capacity and selectivity. Whereas than weakly coordinating anions such as [AsF6] and [BCl4] were observed to be least effective for formaldehyde separation. ILs tetramethylammonium hydroxide [TMAmm][OH], tetramethylammonium fluoride [TMAmm][F], tetramethylammonium acetate [TMAmm][Ac], and [TMAmm][Lys] were found to be the most effective separating agents for formaldehyde. This study will facilitate the selection and design of biobased ILs for the separation of formaldehyde. © 2023 Institution of Chemical Engineers

Author Keywords
COSMO-RS; Formaldehyde; Green solvents; Ionic Liquids; Separation processes

Index Keywords
Fluorine compounds, Formaldehyde, Negative ions, Positive ions; Cation-anions, Conductor-like screening model for real solvents, Extracting agents, Greener solvents, Human carcinogen, Nasal cancer, Separation process, Spark-ignition engine, Tetramethyl ammonium hydroxide, Tetramethylammonium; Ionic liquids

References

- Bellat, J.P., Bezverkhyy, I., Weber, G., Royer, S., Averlant, R., Giraudon, J.M., Lamonier, J.F.
  Capture of formaldehyde by adsorption on nanoporous materials
  (2015) *J. Hazard. Mat.*, 300, pp. 711-717.
- Bhattacharya, M., Mandal, M.K.
  Synthesis and characterization of ionic liquid based mixed matrix membrane for acid gas separation
  (2017) *J. Clean. Prod.*, 156, pp. 174-183.
- Chen, L., Liu, X., Sun, Y., Zhou, L., Nie, Y., Song, K.
  Screening ionic liquids for dissolving a melamine formaldehyde resin prepolymer to

fabricate flame-retardant fibers
(2020) *ACS Sust. Chem. Eng.*, 8, pp. 18314-18323.

- Claus, J., Sommer, F.O., Kragl, U.
Ionic liquids in biotechnology and beyond
(2018) *Solid State Ion.-.*, 314, pp. 119-128.

- Diedenhofen, M., Klamt, A.
COSMO-RS as a tool for property prediction of IL mixtures—A review
(2010) *Fluid Phase Equilib.*, 294, pp. 31-38.

- Ekeoma, B.C., Ekeoma, L.N., Yusuf, M., Haruna, A., Ikeogu, C.K., Merican, Z.M.A., Kamyab, H., Chelliapan, S.
Recent advances in the biocatalytic mitigation of emerging pollutants: A comprehensive review
(2023) *J. Biotechnol.*, 369, pp. 14-34.

- Elgharbawy, A.A.M., Putra, S.S.S., Khan, H.W., Azmi, N.A.D., Sani, M.S.A., Ab Llah, N., Hayyan, A., Basirun, W.J.
Menthol and fatty acid-based hydrophobic deep eutectic solvents as media for enzyme activation
(2023) *Processes*, 11, p. 547.

- Fan, Y., Li, Y., Dong, X., Hu, G., Hua, S., Miao, J., Zhou, D.
Extraction of phenols from water with functionalized ionic liquids
(2014) *Indus. Eng. Chem. Res.*, 53, pp. 20024-20031.

- Garcia-Chavez, L.Y., Hermans, A.J., Schuur, B., de Haan, A.B.
COSMO-RS assisted solvent screening for liquid–liquid extraction of mono ethylene glycol from aqueous streams
(2012) *Sep. Purify. Technol.*, 97, pp. 2-10.

- Geng, P., Zhang, H., Yang, S., Yao, C.
Comparative study on measurements of formaldehyde emission of methanol/gasoline fueled SI engine
(2015) *Fuel*, 148, pp. 9-15.

- Gonfa, G., Bustam, M.A., Murugesan, T., Man, Z., Mutalib, M.
Thiocyanate based task-specific ionic liquids for separation of benzene and cyclohexane
(2013) *Chem. Eng.*, 32, pp. 1939-1944.

- Gonfa, G., Muhammad, N., Bustam, M.A.
Probing the interactions between DNA nucleotides and biocompatible liquids: COSMO-RS and molecular simulation study
(2018) *Sep. Purif. Technol.*, 196, pp. 237-243.

- Gong, C., Huang, W., Liu, J., Wei, F., Yu, J., Si, X., Liu, F., Li, Y.
Detection and analysis of formaldehyde and unburned methanol emissions from a direct-injection spark-ignition methanol engine
(2018) *Fuel*, 221, pp. 188-195.

- Guimarães, J.R., Farah, C.R.T., Maniero, M.G., Fadini, P.S.
Degradation of formaldehyde by advanced oxidation processes
(2012) *J. Environ. Manag.*, 107, pp. 96-101.

- Guo, X., Ren, C.X., Jiang, S., Li, J., Zhang, S., Wang, Y., Ma, W.
Study on functionalized acidic imidazolium-based ionic liquids as effective adsorbents for HCHO storage
(2023) *J. Chem. Technol. Biotechnol.*, 98, pp. 204-212.

- Haron, G.A.S., Mahmood, H., Noh, M.H.B., Moniruzzaman, M.
Ionic liquid assisted nanocellulose production from microcrystalline cellulose: correlation between cellulose solubility and nanocellulose yield via COSMO-RS prediction
(2022) *J. Mol. Liq.*, 368.

- Huang, Y., Ouyang, D., Ji, Y.
The role of hydrogen-bond in solubilizing drugs by ionic liquids: A molecular dynamics and density functional theory study
(2022) *AIChE J.*, 68.

- Islam, N., Khan, H.W., Gari, A.A., Yusuf, M., Irshad, K.
Screening of ionic liquids as sustainable greener solvents for the capture of greenhouse gases using COSMO-RS approach: computational study
(2022) *Fuel*, 330.

- Jarusutthirak, C., Sangsawang, K., Mattaraj, S., Jiraratananon, R.
Treatment of formaldehyde-containing wastewater using membrane bioreactor
(2012) *J. Environ. Eng.*, 138, pp. 265-271.

- Kang, B., Tang, H., Zhao, Z.
S. Song. Hofmeister series: Insights of ion specificity from amphiphilic assembly and interface property
(2020) *ACS Omega*, 5, pp. 6229-6239.

- Karpińska, M., Wlazło, M., Ramjugernath, D., Naidoo, P., Domańska, U.
Assessment of certain ionic liquids for separation of binary mixtures based on gamma infinity data measurements
(2017) *RSC Adv.*, 7, pp. 7092-7107.

- Khan, H.W., Elgharbawy, A.A.M., Bustam, M.A., Goto, M., Moniruzzaman, M.
Vegetable oil–ionic liquid-based emulsion liquid membrane for the removal of lactic acid from aqueous streams: emulsion size, membrane breakage, and stability study
(2022) *ACS Omega*, 7, pp. 32176-32183.

- Khan, H.W., Elgharbawy, A.A.M., Bustam, M.A., Goto, M., Moniruzzaman, M.
Ionic liquid-based green emulsion liquid membrane for the extraction of the poorly soluble drug ibuprofen
(2023) *Molecules*, 28, p. 2345.

- Khan, H.W., Elgharbawy, A.A.M., Bustam, M.A., Goto, M., Moniruzzaman, M.
Ionic liquid-based green emulsion liquid membrane for the extraction of the poorly soluble drug ibuprofen
(2023) *Molecules*, 28, p. 2345.

- Khan, H.W., Elgharbawy, A.A.M., Bustam, A., Moniruzzaman, M.
Design and selection of ionic liquids via COSMO for pharmaceuticals and medicine
(2021) *Application of Ionic Liquids in Drug Delivery*, pp. 137-164.
Springer Singapore Singapore

- Khan, P.A., Johl, S.K., Akhtar, S., Asif, M., Salameh, A.A., Kanesan, T.
Open innovation of institutional investors and higher education system in creating open approach for SDG-4 quality education: a conceptual review
(2022) *J. Open Innov.: Technol., Mark. Compl.*, 8, p. 49.

- Khan, P.A., Johl, S.K., Akhtar, S.
Vinculum of sustainable development goal practices and firms' financial performance: a moderation role of green innovation
(2022) *J. Risk Finan. Manag.*, 15, p. 96.

- Khan, P.A., Johl, S.K., Johl, S.K.
  Does adoption of ISO 56002–2019 and green innovation reporting enhance the firm sustainable development goal performance? An emerging paradigm
  (2021) *Bus. Strategy Environ.*, 30, pp. 2922-2936.

- Khan, P.A., Johl, S.K., Singh, P., Johl, S.K., Shamim, A., Nurhayadi, Y., Wijiharjono, N. U.S. Al-Azizah. Injecting Green Innovation Reporting into Sustainability Reporting." In SHS Web of Conferences, 124({C}2021a{C}): 05003. EDP Sciences.

- Khan, H.W., Khan, M.K., Moniruzzaman, M., Al Mesfer, M.K., Danish, M., Irshad, K., Yusuf, M., Chelliapan, S.
  Evaluating ionic liquids for its potential as eco-friendly solvents for naproxen removal from water sources using COSMO-RS: computational and experimental validation
  (2023) *Environ. Res.*, 231.

- Khan, I., Kurnia, K.A., Mutelet, F., Pinho, S.P., Coutinho, J.A.P.
  Probing the interactions between ionic liquids and water: experimental and quantum chemical approach
  (2014) *J. Phys. Chem. B.*, 118, pp. 1848-1860.

- Khan, H.W., Moniruzzaman, M., Nasef, M.M.E., Bustam, M.A.
  Ionic liquid assisted cellulose aerogels for cleaning an oil spill
  (2020) *Maters Today.: Proceed*, 31, pp. 217-220.

- Khan, H.W., Reddy, A.V.B., Bustam, M.A., Goto, M., Moniruzzaman, M.
  Development and optimization of ionic liquid-based emulsion liquid membrane process for efficient recovery of lactic acid from aqueous streams
  (2021) *Biochem. Eng. J.*, 176.

- Khan, H.W., Reddy, A.V.B., Nasef, M.M.E., Bustam, M.A., Goto, M., Moniruzzaman, M.
  Screening of ionic liquids for the extraction of biologically active compounds using emulsion liquid membrane: COSMO-RS prediction and experiments
  (2020) *J. Mol. Liq.*, 309.

- Khan, H.W., Yusuf, M., Elgharbawy, A.A.M., Makarem, M.A., Mysore, K.
  Carbon capture by ionic liquids
  (2023) *Reference Module in Earth Systems and Environmental Scences*, Elsevier

- Klamt, A.
  COSMO-RS: from quantum chemistry to fluid phase thermodynamics
  (2018) *Computer Aided Chemical Engineering*, 43, p. 9.
  Elsevier

- Kordkheili, Y., Hamed, Pizzi, A.
  A comparison between lignin modified by ionic liquids and glyoxalated lignin as modifiers of urea-formaldehyde resin
  (2017) *J. Adhes.*, 93, pp. 1120-1130.

- Kumar, L., Banerjee, T., Mohanty, K.
  Prediction of selective extraction of cresols from aqueous solutions by ionic liquids using theoretical approach
  (2011) *Sep. Sci. Technol.*, 46, pp. 2075-2087.

- Lv, B., Xia, Y., Shi, Y., Liu, N., Li, W., Li, S.
  A novel hydrophilic amino acid ionic liquid [C₂OHmim][Gly] as aqueous sorbent for CO₂ capture
  (2016) *Int. J. Greenh. Gas. Con.*, 46, pp. 1-6.

- Malik, H., Khan, H.W., Shah, M.U.H., Ahmad, M.I., Khan, I., Al-Kahtani, A.A., Sillanpaa, M.
Screening of ionic liquids as green entrainers for ethanol water separation by extractive distillation: COSMO-RS prediction and aspen plus simulation
(2023) *Chemos*, 311.

- Martín, C.F., Plaza, M.G., Garcia, S., Pis, J.J., Rubiera, F.
C. Pevida. Microporous phenol–formaldehyde resin-based adsorbents for pre-combustion CO₂ capture
(2011) *Fuel*, 90, pp. 2064-2072.

- Mohammed, S.A.S., Yahya, W.Z.N., Bustam, M.A., Kibria, M.G., Masri, A.N., Kamonwel, N.D.M.
Study of the ionic liquids' electrochemical reduction using experimental and computational methods
(2022) *J. Mol. Liq.*, 359.

- Mohammed, S.A.S., Yahya, W.Z.N.
(2021), M.A. Bustam. Computational studies of ionic liquids as co-catalyst for CO2 electrochemical reduction to produce syngas using COSMO-RS. In E3S Web of Conferences, 287(2021):02016. EDP Sciences.

- Mohan, M., Keasling, J.D., Simmons, B.A., Singh, S.
In silico COSMO-RS predictive screening of ionic liquids for the dissolution of plastic
(2022) *Green. Chem.*, 24, pp. 4140-4152.

- Motlagh, S.R., Elgharbawy, A.A., Khezri, R., Harun, R., Omar, R.
Ionic liquid-based microwave-assisted extraction of protein from Nannochloropsis sp. biomass
(2021) *Biomass-.-. Conver. Bioref.*, pp. 1-12.

- Nagy, B., Geissler, E., Laszlo, K.
Room temperature ionic liquids to tailor resorcinol–formaldehyde polymer gels
(2020) *Micro Mesop. Mater.*, 294.

- Nakaya, N., Hosoya, T., Miyafuji, H.
Ionic liquids as formaldehyde-free wood adhesives
(2018) *J. Wood Sci.*, 64, pp. 794-801.

- Paduszyński, K.
An overview of the performance of the COSMO-RS approach in predicting the activity coefficients of molecular solutes in ionic liquids and derived properties at infinite dilution
(2017) *Phys. Chem. Chem. Phys.*, 19, pp. 11835-11850.

- Paliulis, D.
Removal of formaldehyde from synthetic wastewater using natural and modified zeolites
(2016) *Pol. J. Environ. Stud.*, 25, pp. 251-257.

- Pike, S., Hutchinson, J.J., Hunter, C.A.
H-bond acceptor parameters for anions
(2017) *J. Am. Chem. Soc.*, 139, pp. 6700-6706.

- Quijano, G., Couvert, A., Amrane, A., Darracq, G., Couriol, C., Cloirec, P.L., Paquin, L., Carrié, D.
Toxicity and biodegradability of ionic liquids: new perspectives towards whole-cell biotechnological applications
(2011) *Chem. l Eng. J.*, 174, pp. 27-32.

- Qureshi, F., Yusuf, M., Ibrahim, H., Kamyab, H., Chelliapan, S., Pham, C.Q., Vo, D.-V.N.
Contemporary avenues of the Hydrogen industry: Opportunities and challenges in the eco-friendly approach
(2023) *Environ. Res.*, 229, p. 115963.

- Rashid, Z., Wilfred, C.D., Gnanasundaram, N., Arunagiri, A., Murugesan, T.
Screening of ionic liquids as green oilfield solvents for the potential removal of asphaltene from simulated oil: COSMO-RS model approach
(2018) *J. Mol. Liq.*, 255, pp. 492-503.

- Rezaei Motlagh, S., Harun, R., Awang Biak, D.R., Hussain, S.A., Wan Ab Karim Ghani, W.A., Khezri, R., Wilfred, C.D., Elgharbawy, A.A.M.
Screening of suitable ionic liquids as green solvents for extraction of eicosapentaenoic acid (EPA) from microalgae biomass using COSMO-RS model
(2019) *Molecules*, 24, p. 713.

- Rezaei, S.M., Harun, R., Biak, D.R.A., Hussain, S.A., Elgharbawy, A.A., Khezri, R., Wilfred, C.D.
Prediction of potential ionic liquids (ILs) for the solid–liquid extraction of docosahexaenoic acid (DHA) from microalgae using COSMO-RS screening model
(2020) *Biomol*, 10, p. 1149.

- Romero, A., Santos, A., Tojo, J., Rodríguez, A.J.J.O.H.M.
Toxicity and biodegradability of imidazolium ionic liquids
(2008) *J. Hazard. Mat.*, 151, pp. 268-273.

- Safari, M., Yamini, Y., Tahmasebi, E., Latifeh, F.
Extraction and preconcentration of formaldehyde in water by polypyrrole-coated magnetic nanoparticles and determination by high-performance liquid chromatography
(2015) *J. Sep. Sci.*, 38, pp. 3421-3427.

- Sajjad, Z., Gilani, M.A., Nizami, A.S., Bilad, M.R., Khan, A.L.
Development of novel hydrophilic ionic liquid membranes for the recovery of biobutanol through pervaporation
(2019) *J. Env. Manag.*, 251.

- Schlosser, S., Martak, J., Blahusiak, M.
Specific phenomena in carboxylic acids extraction by selected types of hydrophobic ionic liquids
(2018) *Chem. Pap.*, 72, pp. 567-584.

- Song, H., Li, Z., Chen, J., Xia, C.
Brönsted acidic ionic liquids as efficient and recyclable catalysts for the carbonylation of formaldehyde
(2012) *Catal. Lett.*, 142, pp. 81-86.

- Tawalbeh, M., Mohammed, S., Al-Othman, A., Yusuf, M., Mofijur, M., Kamyab, H.
MXenes and MXene-based materials for removal of pharmaceutical compounds from wastewater: Critical review
(2023) *Environ. Res.*, 228, p. 115919.

- Ting, H.C., Khan, H.W., Reddy, A.V.B., Goto, M., Moniruzzaman, M.
Extraction of salicylic acid from wastewater using ionic liquid-based green emulsion liquid membrane: COSMO-RS prediction and experimental verification
(2022) *J. Mol. Liq.*, 347.

- Toha, M.A., Johl, S.K., Khan, P.A.
Firm's sustainability and societal development from the lens of fishbone eco-innovation: a moderating role of ISO 14001-2015 environmental management

system
(2020) *Processes*, 8, p. 1152.

- Wang, W., Ma, X., Grimes, S., Cai, H., Zhang, M.
Study on the absorbability, regeneration characteristics and thermal stability of ionic liquids for VOCs removal
(2017) *Chem. Eng. J.*, 328, pp. 353-359.

- Wang, Q., Wang, J., Rui, W., Yang, D., Wan, X., Zhou, C., Li, R., Yang, Y.
Metal-carbonate interface promoted activity of Ag/MgCO₃ catalyst for aqueous-phase formaldehyde reforming into hydrogen
(2023) *Fuel*, 337.

- Wichmann, K., Loschen, C., Klamt, A.
Drug solubility, reaction thermodynamics, and co-crystal screening
(2019) *Chem. Eng. Pharm. Ind.: Act. Pharm. Ingred.*, pp. 467-491.

- Yasmeen, I., Ilyas, A., Shamair, Z., Gilani, M.A., Rafiq, S., Bilad, M.R., Laeeq Khan, A.
Synergistic effects of highly selective ionic liquid confined in nanocages: Exploiting the three component mixed matrix membranes for CO₂ capture
(2020) *Chem. Eng. Res. Des.*, 155, pp. 123-132.

- Yuan, D., Tian, L., Gu, D., Shen, X., Zhu, L., Wu, H., Wang, B.
Fast and efficient oxidation of formaldehyde in wastewater via the solar thermal electrochemical process tuned by thermo-electrochemistry
(2017) *J. Clean. Prod.*, 156, pp. 310-316.

- Yusuf, M., Farooqi, A.S., Alam, M.A., Keong, L.K., Hellgardt, K., Abdullah, B.
Latest trends in Syngas production employing compound catalysts for methane dry reforming
(2020) *IOP Conf. Ser. Mater. Sci.*, 991, p. 12071.

- Zhang, K., Liu, C., Li, S., Fan, J.
A hydrophobic deep eutectic solvent based vortex-assisted liquid-liquid microextraction for the determination of formaldehyde from biological and indoor air samples by high performance liquid chromatography
(2019) *J. Chromatogr., A*, 1589, pp. 39-46.

- Zhang, C., Song, Z., Jin, C., Nijhuis, J., Zhou, T., Noël, T., Gröger, H., Hessel, V.
Screening of functional solvent system for automatic aldehyde and ketone separation in aldol reaction: a combined COSMO-RS and experimental approach
(2020) *Chem. Eng. J.*, 385.

- Zvulunov, Y., Ben-Barak-Zelas, Z., Fishman, A., Radian, A.
A self-regenerating clay-polymer-bacteria composite for formaldehyde removal from water
(2019) *Chem. Eng. J.*, 374, pp. 1275-1285.

Correspondence Address
Khan H.W.; Department of Chemical Engineering, Seri Iskandar, Malaysia; email: humawarsi27@gmail.com

Publisher: Institution of Chemical Engineers

ISSN: 02638762
CODEN: CERDE
Language of Original Document: English
Abbreviated Source Title: Chem. Eng. Res. Des.
2-s2.0-85165244964
Document Type: Article
Publication Stage: Final
Source: Scopus