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Education

Degree	Institute/Board	CPI/%	Year
Ph.D., Chemical Engineering	Indian Institute of Technology, Guwahati	NA	2021
M. Tech - Chemical Engineering (MST)	Indian Institute of Technology, Guwahati	7.6	2015
B. Tech - Chemical Engineering	CVRCE, Bhubaneswar	6.5	2012
Diploma, Chemical Engineering	UGIE, Rourkela	62.8	2009
Secondary	BSE, Odisha	66.5	2003

Experience

- Nuclear Magnetic Resonance Spectroscopy (NMR-600MHz) Operator from July2016 to July 2019

Patent

- A Deep Eutectic solution as heat transfer fluid comprising Diphenyl Ether and Benzophenone, **Pyarimohan Dehury**, and Tamal Banerjee, (*TEMP/E-1/63172/2020-KOL, Patent Appl. No. 202031057115*), Date of Filing, 30th December, 2020.

Publications

- Papu Kumar Naik, **Pyarimohan Dehury**, Sandip Paul and Tamal Banerjee. Evaluation of Deep Eutectic Solvent for the selective extraction of toluene and quinoline at T = 308.15 K and p = 1 bar. *Fluid Phase Equilibria*, 423 (2016),146-155 (**IF: 2.838**). https://doi.org/10.1016/j.fluid.2016.04.018
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- Rupesh Verma, **Pyarimohan Dehury**, Anand Bharti and Tamal Banerjee. Liquid-liquid extraction, COSMO-SAC predictions and process flow sheeting of 1-butanol enhancement using mesitylene and oleyl alcohol. *Journal of Molecular Liquids*, 265 (2018), 824-839 (**IF: 5.065**). https://doi.org/10.1016/j.molliq.2018.06.088
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- **Pyarimohan Dehury**, Upasana Mahanta and Tamal Banerjee. A Comprehensive Assessment on the use of Boron Nitride based Nanofluids Comprising Eutectic mixtures of Diphenyl Ether and Menthol for Enhanced Thermal Media. *ACS Sustainable Chemistry & Engineering* 8 (2020) 14595−14604 (**IF: 7.632**), https://pubs.acs.org/doi/10.1021/acssuschemeng.0c05648

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- **Pyarimohan Dehury** and Tamal Banerjee. Butanol and Ethanol Recovery Using Liquid-Liquid Extraction by Ionic Liquid Solvent [OMIM][Tf2N] at T=298.15 K and p=1 atm. *7th DAE-BRNS Biennial Symposium on Emerging Trends in Separation Science and Technology-SESTEC 2016*, May 17-20, 2016, Indian Institute of Technology, Guwahati.
- **Pyarimohan Dehury** and Tamal Banerjee. Nanoparticles Dispersed Deep Eutectic solvents (NDDES) as Heat Transfer Fluid (HTF) for solar heat collector International *Conference on Nano for Energy and Water (NEW) 2017 and Indo French Workshop on Water Networking*, February 22-24, 2017, UPES, Dehradun.
- Rupesh Verma, Anand Bharti, **Pyarimohan Dehury** and Tamal Banerjee. Liquid-Liquid Extraction and Process Flow sheeting of bio-butanol Enhancement using Mesitylene and Oleyl Alcohol. *BIOPROCESSING INDIA 2017*, December 9-11, 2017, Department of Biosciences and Bioengineering, IIT Guwahati
- **Pyarimohan Dehury** and Tamal Banerjee. Physiochemical Properties of Triphenylphosphonium Bromide based Deep Eutectic Solvent as Novel Thermal Nanofluid. *Materials & Technologies for Energy Conversion and Storage (M-TECS 2018),* September 26-29, 2018, DAE Convention Centre, Mumbai, India.

Projects

- **Nanoparticle Dispersed Deep Eutectic Solvents as Low-Cost Heat Transfer fluid for Concentrated Solar Power (IMPRINT India, MHRD 4077)** 2015-2021
  Prof. Tamal Banerjee
- **Liquid-Liquid Extraction and Conceptual Process Design for the Extraction of Lower Alcohols** 2014-2015
  Prof. Tamal Banerjee
- **Performance Evaluation of Forced Draft Cooling Tower** 2011-2012
  Mr. S Upendra

Project Proposal Writing Experience

I have experience of writing the project proposal **"Nanoparticle Dispersed Deep Eutectic Solvents as Low-Cost Heat Transfer fluid for Concentrated Solar Power"** under **IMPRINT India** an initiative by **MHRD, Govt. of India** vide proposal number: **4077**

Technical Skills

- CHEMCAD
- Aspen Plus
- Aspen Hysis
- Aspen Exchanger Design and Rating
- Matlab

Short Term Courses

- Computer Hardware and Networking, CTTC Bhubaneswar (1month)
- Advanced Diploma in Fire and Safety Engineering, NCFSE, IIE Hyderabad, (6 months)
- Integration of Molecular Design to Process Simulation for Development of Industrial Chemical Products and Processes, GIAN, MHRD, IIT Guwahati (7 days)
- Basic Pneumatic and Hydraulic Control with PLC, Rexroth Bosch Group, CVRCE, Bhubaneswar (20 days)

Positions of Responsibility

- Mess Convenor, Dibang Hostel, 2016-2017
- General Secretary, Dibang Hostel, 2017-2018
- DPPC Student Member, Dept. of Chemical Engineering, 2017-2018
- General Secretary, Dibang Hostel, 2018-2019, 2019-2020

Achievements

- Assisted in Aspen Plus course on State-of-the-art Computational Tools in Science and Engineering conducted by TEQIP, MHRD, IIT Guwahati
- Conducted 1-day Aspen Plus workshop in Reflux-2019, IIT Guwahati

ACS Sustainable Chemistry & Engineering

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Research Article

Comprehensive Assessment on the Use of Boron Nitride-Based Nanofluids Comprising Eutectic Mixtures of Diphenyl Ether and Menthol for Enhanced Thermal Media

Pyarimohan Dehury, Upasana Mahanta, and Tamal Banerjee*

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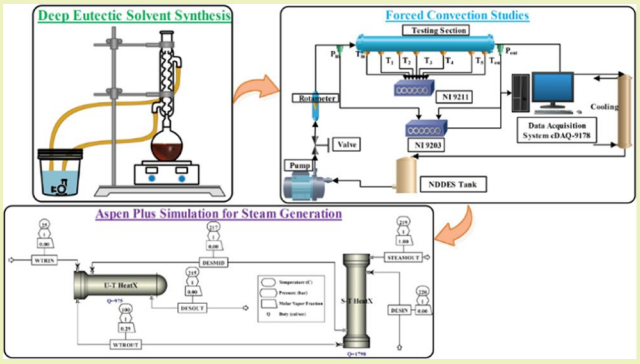
ABSTRACT: The current work explores deep eutectic solvents (DESs) as heat transfer fluids (HTFs) primarily for generating concentrated solar power. The eutectic composition of the DES comprising diphenyl ether and DL-menthol as the hydrogen bond acceptor and hydrogen bond donor was initially computed through the quantum chemical-based COSMO-SAC model. To improve upon the thermal performance and reduce the interfacial resistance, DESs were modified by dispersing hexagonal boron nitride nanoparticles with weight percent ranging from 0.02 to 0.10. Thermophysical properties, namely, density, viscosity, thermal conductivity, and heat capacity, of the HTFs were then measured as a function of temperature. Further, based on these four parameters, the Mouromtseff number (*Mo*) was calculated to rank the nanoparticle-dispersed DESs. The nanofluid consisting of DES-1 with 0.02 wt % of nanoparticles gave the highest *Mo* value, and hence, it was further considered for the experimental forced convection study and process simulation using an Aspen Plus simulator. From the forced convection experiment temperature profiles, the heat transfer coefficient and Nusselt number (*Nu*) were evaluated and compared for nanofluids with the corresponding base fluid. The flow behavior of the thermal fluid along the characteristic length of the test section was investigated for both the laminar and turbulent regimes. The effectiveness of the HTF in terms of steam generation capacity was predicted, and it was observed that the nanofluid with 0.02 wt % was able to successfully convert 100% of the input water (15 kg/h) into superheated steam at the temperature of 494.15 K.



KEYWORDS: *Deep eutectic solvents, Heat transfer fluids, Concentrated solar power, Hexagonal boron nitride*

INTRODUCTION

Solar energy has embarked on its journey in the field of applied energy research as a promising renewable and nonconventional energy resource. It is a clean and abundant source of energy when compared to fossil fuels. The storage of solar radiation in the form of either thermal or electrical energy is an important and key factor for solar energy applications. Solar photovoltaic and concentrated solar power (CSP) are the major industrial level techniques for harvesting solar energy.[1] Several applications of solar energy can be segregated according to temperature levels.[2] Space heating and domestic hot water production are two of the low-temperature applications of solar radiation by direct heating. In most of the commercial CSP plants, solar radiation is collected by a parabolic trough, stored using a heat transfer fluid (HTF), and finally transferred to a steam generator.[1,3] Solar energy can also be stored directly by HTF without the presence of concentrating mirrors.[3] The HTF plays an important role in determining the effectiveness and cost of the process with respect to both CSP and direct storage systems. Examples of commonly used HTFs are molten salts and mineral oils.[4] The melting point of molten salts is above 200 °C, which restricts their application at lower weather conditions.[3,4] Mineral oils need additives in order to enhance the thermal stability. Some of the commercially available HTFs have trade names such as Dowtherm, Syltherm, and Therminol (comprising diphenyl ether and biphenyl).[5] Conventionally, molten salts are primarily used as HTFs in medium- to high-temperature applications. The thermal performance of molten salt-based steam generator technology has been already reported .[6−8] Water was also used in industrial applications such as HTFs.[3,9] However, a narrow liquid range (0−100 °C) and a high vapor pressure of water limit its usability.

Ionic liquids (ILs) have already evolved as a potential solvent for a wide range of industrial applications. The physicochemical

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Evaluation of Thermophysical Properties of Menthol-Based Deep Eutectic Solvent as a Thermal Fluid: Forced Convection and Numerical Studies

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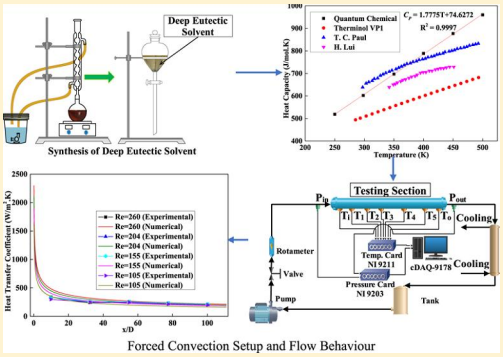
ABSTRACT: Concentrated solar power (CSP) is one of the emerging renewable energy technology, where sunlight is concentrated from a large area and is stored in a collector filled with heat-transfer fluid (HTF). The current work reports the synthesis of novel HTF based on menthol-based deep eutectic solvents (DESs). DES consisting of a hydrogen bond acceptor, namely, DL-menthol and a hydrogen bond donor (oleyl alcohol), has been prepared and explored to evaluate its effectiveness as a thermal fluid. The thermal properties, namely, viscosity, density, thermal conductivity (TC), and heat capacity, are measured and compared with both conventional and commercial solvents within the temperature range T = 298.15−353.15 K. The density of DES was found to decrease with increase in temperature, while the rheological measurements suggest a Newtonian fluid with its shear viscosity decreasing exponentially with increasing temperature. The TC of the DES was found to be ∼0.161 W/m K, which decreases linearly with temperature, while a contrary was observed for heat capacity. Further, the performance of these solvents has been evaluated in a forced convective heat-transfer configuration under laminar flow conditions with N_{Re} = 105, 155, and 260. The convective heat-transfer experiments demonstrated the fact that the thermal entrance length of the DES is very large because of its high viscosity and low TC. The convective heat-transfer data, namely, heat-transfer coefficient and Nusselt number, were compared with the in-house AnuPravaha CFD simulator under laminar conditions. From the obtained thermophysical properties, it is confirmed that the synthesized DES can be used as a next-generation heat storage media in the CSP plant.



Forced Convection Setup and Flow Behaviour

1. INTRODUCTION

The remarkable decrease in the fossil fuels and the simultaneous increase in energy demand has become a challenge for the scientific community. To overcome the ever-expanding energy demand, solar energy can be an alternative source of energy. This is the most copious and readily available sustainable source of energy with zero environmental pollution. The solar energy can be collected and used as potential power sources. In this scenario, heat-transfer fluid (HTF) plays an important role wherein the concentrated solar power (CSP) system[1] is created in terms of parabolic mirrors or solar collectors so as to reflect a higher fraction of sunlight to store energy. Being an important component of any solar thermal system, the solar radiation is absorbed by solar collectors in the form of heat energy and then transfer the heat to a HTF for useful applications. Previously, black liquids have been used as HTF for collecting solar energy.[2] The thermophysical properties for determining the efficiencies for such fluids are thermal conductivity (TC) and specific heat. Additionally, viscosity and density of HTFs also determine the flow behavior of such fluids. Overall, these properties play a vital role in determining the overall efficiency of solar energy utilization.[3,4] However, the restrictions of currently used HTF in CSP are its lower storage capacity and lower thermal stability, resulting in lower cycle efficiency and higher operating cost. Therefore, it is necessary to increase the working efficiency of HTF to achieve a cost-effective efficient CSP system. In general, the CSP is designed based on the thermal fluid. Therefore, CSP is capable of being operated from 473.15 to 1375.15 K.[5−8] Furthermore, for low-to-high-temperature applications, the HTFs deserve superior thermodynamic properties and good thermal stability. In such a scenario, researchers have explored alternative fluids, one of them the conventional eutectic mixtures, comprising of biphenyl derivatives,[9] that is, a combination of diphenyl ether and biphenyl (Therminol VP1). However, these conventional fluids suffer from disadvantages such as high freezing point and lower thermal stability. It is in this scenario, the current work explores alternative solvents, which are also known as deep eutectic solvents (DESs).

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Evaluation and conceptual design of triphenylphosphonium bromide-based deep eutectic solvent as novel thermal nanofluid for concentrated solar power

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Abstract. In a concentrated solar power (CSP) plant, an increase of heat transfer effect of the working fluid is a key deliverable which is usually obtained by enhancing its thermo-physical properties. The current work reports the synthesis of heat transfer fluids (HTF) based on deep eutectic solvents (DESs) consisting of a hydrogen bond donor (HBD), namely, triphenylphosphonium bromide, and a hydrogen bond acceptor (HBA), namely, ethylene glycol. Initially, the thermophysical properties, namely, density, viscosity, thermal conductivity (TC) and specific heat capacity were measured and compared with the conventional solvents. The properties were further enhanced by the dispersion of spherical Al_2O_3 nanoparticles in DESs. The alumina nanoparticles were found to have a negligible effect on the physical properties (density and viscosity) of the base fluid, thereby limiting the pressure drop and also the coefficient of friction. For their potential application as thermal fluids for CSP plants, the thermal properties of DESs and nanoparticle dispersed deep eutectic solvents (NDDESs) were measured within a temperature range of 25–60°C. The TC of 1 wt% Al_2O_3 with the base fluid was around eight times higher than the base DES. It was found that the TCs of DES and NDDES were higher when compared to the commercial HTF, namely, Therminol VP-1. Eventually, the Aspen plus flowsheet was conceptualized to ascertain the steam generation rate and the overall heat transfer coefficient of these novel solvents. A combination of U-shaped for latent heat and shell and tube heat for sensible heat was employed in the flowsheet. The CSP scheme gave a steam generation rate of 1.7 kg h^{-1} at 180°C with a corresponding DES flow rate of 1 m^3 h^{-1}.

Keywords. Deep eutectic solvents; heat transfer fluid; Aspen plus; steam properties.

1. Introduction

Concentrated solar power (CSP) is a valuable source of renewable energy. The solar energy stored in the form of thermal fluid can be exploited in thermodynamic cycles such as Brayton cycle to generate turbine power from gas turbine engines. The advantage of such a system is that the energy stored during the sun hours can be used at night-time primarily due to the reusability of solar energy. One of the main limitations for such a process is its elevated cost owing to parabolic mirrors or collectors and a need for a large land area. This makes the process economically faring poorly when compared to conventional energy sources. It is for this reason that methodology should be developed for utilizing the stored energy in an effective manner. It implies that the scientific community needs to improve the overall efficiency of these solar plants. One of them is to improve the overall heat transfer coefficient of the fluid which usually carries the sensible heat.

In this scenario heat transfer fluids (HTF) play an important role, particularly in CSP, where the solar collectors absorb the solar radiation and convert it into heat energy. This energy is then transferred as heat through a HTF [1]. This makes the evaluation of the thermodynamic properties such as viscosity, density, thermal conductivity (TC) and specific heat capacity (C_p) highly desirable [2,3]. But the limitations of the presently used HTF in CSP are manifested in its lower storage capacity and thermal stability. This ultimately results in a lower cycle efficiency and higher operating cost. Therefore, it is essential to enhance the working efficiency of HTF for achieving a cost-effective CSP system. To meet these requirements, nanoparticle dispersed deep eutectic solvents (NDDESs) have great potential as an alternative to conventional HTF. NDDESs, a class of nanofluids, can be synthesized by dispersing a small amount of nanoparticles in bare deep eutectic solvents (DESs). This synthesis is of one pot in nature and usually occurs within a few hours of the metathesis reaction.

DESs refer to mixtures of two or more compounds in which hydrogen bond donors (HBDs) and hydrogen bond acceptors (HBAs) combine together to form liquids upon mixing. These have melting points below than that of the individual components [4–6]. DESs are now considered as low-cost green solvents having equivalent characteristics compared to ionic liquids (ILs) which are also green in nature but expensive.

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Thermophysical and Forced Convection Studies on (Alumina + Menthol)-Based Deep Eutectic Solvents for Their Use as a Heat Transfer Fluid

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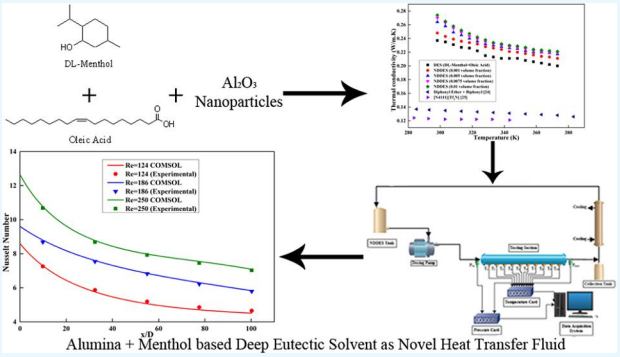
Supporting Information

ABSTRACT: The current work reports the thermophysical and flow measurements of novel thermal solvents based on deep eutectic solvents (DESs) and alumina-based nanoparticle-dispersed deep eutectic solvents (NDDESs) for its use as a potential solar energy storage medium. The DESs were synthesized using a hydrogen bond donor (i.e., oleic acid) and a hydrogen bond acceptor (i.e., DL-menthol) by using the COSMO-SAC-predicted equimolar ratio at a temperature of 350.15 K. Thereafter, NDDESs or nanofluids were formed by dispersing different volume fractions (0.001, 0.005, 0.0075, and 0.01) of Al_2O_3 nanoparticles in the DESs. The optimum volume fraction (0.005) of Al_2O_3 nanoparticles was selected through their thermophysical properties (density, viscosity, thermal conductivity, and specific heat capacity) and its agglomeration or stability behavior. As expected, NDDESs with a 0.005 volume fraction gave a higher enhancement in thermal conductivity, viscosity, heat capacity, and density as compared to DESs. To evaluate the heat transfer coefficient, forced convection experiments were conducted in a circular test section for both DESs and NDDESs under laminar conditions (Re = 124, 186, and 250). The enhancement of the local heat transfer coefficient was found to be higher when compared to their thermophysical properties. This was due to the nanoparticle migration resulting in a non-uniform distribution of both thermal conductivity and viscosity fields, which was inherently found to reduce the thermal boundary layer thickness. In the final section, the heat transfer coefficient and the Nusselt number were also validated with COMSOL Multiphysics simulations.



1. INTRODUCTION

Concentrating solar power (CSP) is currently recognized as a valuable source of renewable energy.[1] The stored thermal energy can be utilized in various thermodynamic cycles such as Brayton cycle to generate turbine power from gas turbine engines. The advantage of CSP is that the energy stored in daylight can be used at nighttime where the thermal fluid can potentially reuse the solar energy. The main drawback includes its elevated cost as compared to conventional energy sources. For this reason, the scientific community aims to improve the overall efficiency of these solar plants. One of them is to improve the efficiency of the heat transfer processes that occur in this application. CSP plants usually adopt a technology involving parabolic cylindrical collectors, which in turn uses a heat transfer fluid for the storage and transport of heat. Keeping the CSP process in mind, increasing the heat transfer effect is a key deliverable usually obtained by enhancing the thermophysical properties of these fluids. The current study is thus meant for generating turbine power using the CSP energy storage.

In CSP, the solar energy is usually concentrated using mirrors and lenses and stored in a thermal fluid. The working fluid used in the CSP plant plays an important role in determining the overall efficiency of the system. The conventional thermal fluids have low-to-moderate thermal stability and heat storage capacity, which results in high operating costs.[1] Researchers have tried ionic liquids (ILs) as one of the alternatives for heat transfer fluid for future generations.[2] However, ILs are highly viscous, costly, and difficult to synthesize. Application of ILs in solar collector applications[3,4] have been recently reported. Wu et al.[3] have focused the applicability of 1-butyl-3-methylimidazolium hexafluorophosphate, 1-octyl-3-methylimidazolium hexafluorophosphate, 1-butyl-3-methylimidazolium *bis*-trifluromethane sulfonamide, 1-butyl-3-methylimidazolium tetrafluoroborate, 1-octyl-3-methylimidazolium tetrafluoroborate, and 1-butyl-3-methylimidazolium *bis*-trifluromethane sulfonamide as a thermal energy storage medium for solar collectors. The storage density of 1-octyl-3-methylimidazolium hexafluorophosphate was found to be 378 MJ/m^3. Moens and Blake[4] have performed an overall assessment of ILs for its use as a heat transfer fluid in solar parabolic trough systems.

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Partitioning of butanol between a hydrophobic ionic liquid and aqueous phase: Insights from Liquid Liquid Equilibria measurements and Molecular Dynamics simulations

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ABSTRACT

This work investigates the effectiveness of 1-methyl-3-octylimidazolium *bis* (trifluoromethylsulfonyl) imide, [OMIM] [Tf_2N] as a solvent to recover 1-butanol from aqueous stream. The solvent [OMIM] [Tf_2N] (1.320 g/cm^3) possessed a higher density and formed two clear and distinct phases after extraction. Both Liquid-Liquid Equilibrium (LLE) experimental studies and Molecular Dynamic (MD) simulation were carried out for [OMIM] [Tf_2N]-1-butanol-water system to explain the effectiveness of the solvent. A type II phase behavior with a large immiscible region was observed for the system at $T = 298.15$ K and $p = 1$ atm. High values of selectivity ranging from 555 to 3583 have been observed for 1-butanol extraction. The distribution coefficients were also found to be greater than unity. The experiments indicated an easier separation of solute from aqueous phase to extract phase. The NMR spectra confirmed the absence of solvent in the water rich phase. NRTL and UNIQUAC models gave root mean square deviation (RMSD) in the range of 0.1%–0.5% for the ternary system. The MD simulations were then performed in an NVT ensemble for a time period of 40 ns using OPLS-AA force field. The first solvation shell for 1-butanol was obtained within 0–4.35 Å and 0–5.75 Å with [OMIM] and [Tf_2N] ions respectively. This highlights the fact that butanol molecules are highly solvated by the presence of both ions.

1. Introduction

The reserves of hydrocarbon based fossil fuels being available in few countries are not sufficient for prolonged use. The combustion of these fossil fuels further emits greenhouse gases and threatens the balance of the ecosystem. It invariably becomes a challenge for governments, engineers, scientists and economists to reduce dependence on the conventional fuels. The gradual decrease of fossil fuel resources and ever increasing environmental pollution has thus led us to focus on alternative energy resources such as biomass. According to BP statistical review, the production of biofuels has increased by 7.4% in 2014 [1]. To overcome the drawbacks of the conventional fossil fuels, biomass derived 1-butanol as an alternative fuel is gaining importance recently.

In the Acetone-Butanol-Ethanol (ABE) fermentation [2–4] process, bacteria like *Clostridium acetobutylicum* [2,3] and *Clostridium bjerinkci* [3,4] ferment biomass under anaerobic conditions and hence Acetone, Butanol, and Ethanol are being produced with a proportion of 3:6:1. Hence butanol produced from this fermentation process has potential to be used as a fuel. Further the calorific value [2] of butanol (29.2×10^6 kJ/m^3) is much higher than that of Ethanol (19.6×10^6 kJ/m^3). Butanol also shows lesser flammability and hydrophilicity than ethanol. Furthermore, it is easily miscible with gasoline in any proportion and has industrial applications [5]. However, in the conventional process, butanol concentration inside the broth greater than 10 g/L prevents the growth of the microbial cells during fermentation process [6]. Therefore, to overcome this and to enhance the use of 1-butanol, its separation from water present in the broth is essential.

Methods like pervaporation, extraction, adsorption and gas stripping have been investigated earlier [7–12]. The main disadvantage for the recovery of 1-butanol from fermentation broth through adsorption is that it can only be used in laboratory scale. This is due to the small-capacity of adsorbents which is not economically acceptable on an industrial or semi-industrial scale. Separation by distillation is further complicated since the lower chain alcohol such as butanol forms an azeotropic mixture with water [13]. Membrane separation and pervaporation are not cost

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Liquid-liquid extraction, COSMO-SAC predictions and process flow sheeting of 1-butanol enhancement using mesitylene and oleyl alcohol

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Aspen Plus

ABSTRACT

The current work reports the extraction of 1-butanol from aqueous streams using low density solvents namely, mesitylene ($\rho = 0.864$ g/cm^3) and oleyl alcohol ($\rho = 0.849$ g/cm^3). The ternary Liquid-Liquid Equilibrium (LLE) studies for mesitylene (1) + 1-butanol (2) + water (3) and oleyl alcohol (1) + 1-butanol (2) + water (3) were conducted to explain the effectiveness of the two solvents. A type-I phase behavior with a large immiscible region was observed at $T = 298.15$ K and $p = 0.1$ MPa. High values of selectivity ranging from 400 to 2500 for mesitylene and 750–6500 oleyl alcohol were observed. Distribution coefficient values higher than unity indicated an easier diffusion of 1-butanol from aqueous phase to extract phase. It also confirmed a lower solvent to feed ratio for separation of 1-butanol from water. ^{1}H NMR spectra indicated an aqueous rich phase free of solvent and while the contrary was observed in the solvent rich phase. Non-random two liquid (NRTL) and UNIversal QUAsichemical (UNIQUAC) models gave root mean square deviation (RMSD) in the range of 0.1–0.5% for both the systems. Further the predictions of the tie lines were also confirmed though the quantum chemical based COnductor like Screening MOdel Segment Activity Coefficients (COSMO-SAC) which gave RMSD in the range of 5%. Based on the selectivity values of 1-butanol at lower concentration, mesitylene was chosen as the recommended solvent for extraction. Thereafter a hybrid extraction process using Aspen Plus V8.8® was designed to carry out an optimized flowsheet concerning the recovery and recycle of butanol and mesitylene respectively.

1. Introduction

The increasing demand of energy in the developing countries has led to the depletion of fossil fuels at a high rate. The primary energy consumption has increased worldwide by 1% in 2016 following a growth of 0.9% in 2015 as well as 1% in 2014 [1]. In the present scenario fossil fuels such as oil, natural gas and coal are the world's leading energy sources. The excess consumption of these fossil fuels further creates greenhouse gas emission and poses threat to human life. Thus it becomes a challenge for governments, engineers, scientists and economists so as to mitigate the ill effects of these gases. To overcome these challenges lower alcohols such as 1-butanol as an alternative fuel is gaining importance [2].

Butanol is conventionally produced through the ABE (Acetone-Butanol-Ethanol) fermentation where bacteria like clostridium acetobutylicum and clostridium bjerinkci ferment biomass under anaerobic conditions thereby producing acetone, butanol, and ethanol with a proportion of 3:6:1 [3–5]. Bio-butanol obtained by ABE fermentation process is now considered as a potential biofuel. Bio-butanol like 1-butanol have similar properties as 1-butanol obtained from petroleum products. It has a higher calorific value (29.2 MJ/dm^3) as compared to ethanol (19.6 MJ/dm^3) and has a lesser flammability and lower hydrophilicity values. The RON and MON numbers of butanol are also close to petrol while at the same time less corrosive than ethanol. All these features make 1-butanol as a useful additive to gasoline and as biofuels [3, 5–7]. However the separation of lower chain alcohols such as 1-butanol is difficult as it forms azeotropic mixtures with water [8–10]. Hence it becomes essential to separate 1-butanol from water, so as to lessen the effect of azeotrope formation.

It should be noted that a high concentration of 1-butanol inhibits the growth of microbes and bacterial cell in the fermentation broth. Hence a systematic removal of this compound is essential [3, 11]. Methods such as extraction, adsorption, pervaporation, gas striping and membrane separation have been conventionally used for the separation of 1-butanol during fermentation broth [3, 12–18]. Membrane separation and pervaporation are expensive due to its low mass transfer rates and requirement of low pressure. Adsorbents for butanol have low capacity which discourages its use in industrial or semi-industrial plant. On the other hand membrane reactors immobilizes the microorganisms, but in industrial scale the cell immobilized technique possess more disadvantages due to poor mechanical strength and an increase in mass

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Evaluation of Deep Eutectic Solvent for the selective extraction of toluene and quinoline at $T = 308.15$ K and $p = 1$ bar

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ABSTRACT

The current work reports the selective separation of aromatic and poly aromatic hydrocarbon (PAH) with Deep Eutectic Solvents (DES). The low cost DES are based on a mixture of a hydrogen bond donor and organic salt. The organic salt namely Methyltriphenylphosphonium bromide(MTBP) along with the hydrogen bond donor (HBD) were taken in a ratio of 1:4 to synthesize potential DES. DES were then varied based on the selection of two hydrogen bond donor namely ethylene glycol(DES1) and glycerol(DES2). In order to study their effectiveness, Liquid-liquid Equilibrium experiments were performed for the removal of toluene and quinoline respectively. LLE data corresponding to the ternary systems:[DES1(1) + Toluene(2) + Heptane(3)],[DES2(1) + Toluene(2) + Heptane(3)], [DES1(1) + Quinoline(2) + Heptane(3)] and [DES2(1) + Quinoline(2) + Heptane(3)] were generated at 308.15 K and atmospheric pressure. ^{1}H NMR analysis were then used for the quantification of both extract and raffinate phases. Distribution coefficient (β) and selectivity (S) were subsequently obtained and it was found that toluene had a poor selectivity than quinoline. The cross contamination of DES and heptane across either phases were found to be nearly zero. Further the Non-random two liquid (NRTL) and UNiversal QUAsi Chemical (UNIQUAC) thermodynamic model were used to compare the experimental tie line data. This gave an excellent fit with a root mean square deviation (RMSD) values for both models ranging from (0.28–0.31%) and (0.22–0.73%) respectively. DES1, namely Methyltriphenylphosphonium bromide + ethylene glycol was thus recommended as a potential solvent for the separation of aromatic and PAH component.

1. Introduction

Desulphurization and denitrification are an essential part of a refinery set up. It is invariably necessary to remove the sulphur and nitrogen containing aromatic species from fuel oil. Fuel oil consists of 25% aromatics, 15% paraffin, 45% naphthalene and 15% non-hydrocarbon compound. The aromatic nitrogen compounds exist in two different types namely non basic and basic nitrogen compounds. The former includes compounds such as pyrrole, indole, indoline, carbazole and benzocarbazole. The basic nitrogen compounds known are pyridine, quinoline and benzoquinoline. Nitrogen compounds having non-heteroaromatic or heteroaromatic structure with multiple ring adversely affect the stability of diesel oil during its storage [1]. This reduces the efficiency of hydrodenitrification (HDN) process due to the poisoning of the catalyst. Hence, it is important to reduce the nitrogen level of the diesel oil both due to its potential pollution threat and its storage requirements. Nowadays the maximum nitrogen content is also limited to <0.1 ppm. Further the nitrogen based compounds are known to have low reactivity and high refractoriness as compared to the conventional sulphur compounds in diesel oil. The nitrogen molecules are also known to influence the formation of coke at specified and/or moderate operating conditions [1]. This makes the removal of aromatic and PAHs from the fuel oil an essential step before utilization.

Thus in summary PAH of both nitrogen and sulphur points out to a hazardous threat due to its emission into the atmosphere. The toxic effects are mainly due to the carcinogenic products released in the environment as a result of combustion [2]. There are various methods adopted for the removal of these aromatics from fuel oil. PAH are usually removed in a hydrotreater where hydrogen concentration in terms of partial pressure is increased to an extent in

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