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Purification of Nitrogen Trifluoride via Physical Absorption

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Abstract

Nitrogen trifluoride (NF_3) is an important gas used in the electronics industry, where it is required at high purity (>99.999%). CF_4 is a significant impurity in the commercial production of NF_3. These two chemicals have very similar physical properties making it very difficult to separate them. Membrane technology, cryogenic distillation, and zeolite absorption have been studied as potential purification techniques. Currently, cryogenic distillation is commercially used for purification. The high energy requirements for cryogenic distillation is the motivation to investigate alternate methods for purifying NF_3.

In this study, physical separation was investigated using several solvents identified via a solvent screening process. Screening processes included the use of Robbin's chart, thermodynamic predictive methods, such as the PSRK, UNIQUAC, UNIFAC, and COSMO-SAC. The final list of solvents was based on the physical properties and trends observed from the literature. Other aspects such as toxicity, price and availability of the solvents were also considered.

Phase equilibrium measurements were performed using two different high-pressure apparatus for various binary combinations of the NF_3 and CF_4 with the shortlisted solvents. The feasibility of separating the CF_4 impurity from NF_3 using physical separation technologies, viz. absorption and extractive distillation was also investigated.

The phase equilibria results show a tendency for either polar or nonpolar compounds to selectively absorb NF_3. The results into the screening of new solvents for these components show promising trends. While absorption was not capable of purifying NF_3 to the desired purity, results obtained from extractive distillation simulations show that a product purity of 99.9999 % of NF_3 is possible from an equimolar mixture of NF_3 and CF_4.

HIGH PRESSURE DENSITIES OF ETHYLENE GLYCOL AND CAFFEINE MIXTURES

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Ethylene glycol is a well-known fluid that is recognized for its application in heat transfer processes [1]. In order to improve its characteristics and performances, adding other particles in the mixture of ethylene glycol and water, such as nanoparticles has been investigated [2]. A substance widespread available, easily distributed and cost effective is caffeine. Caffeine can be recycled from coffee or tea waste, which makes it profitable and sustainable. Literature data state that caffeine addition to ethylene glycol improves its properties as a heat transfer fluid, primarily due to higher heat capacities, higher system fluidity and lower viscosity [3]. This work investigates different thermodynamic properties of caffeine + ethylene glycol mixtures. Densities have been measured at high pressures from (0,1 – 60) MP and at the temperature range (20 - 140) ºC. All measurements were performed using an Anton Paar DMA 5000 HP density meter with a vibrating tube [4]. The obtained results were fitted by the modified Tammann-Tait equation and parameters were used to determine the isothermal compressibility coefficient, the coefficient of isobaric expansion, the internal pressure and the difference of specific heat capacity at constant pressure and constant volume. Experimental values and calculated thermodynamic parameters reported in this work will help in concluding whether the caffeine + ethylene glycol mixtures are good candidates as heat transfer fluids.

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