# Energy-efficient recovery of tetrahydrofuran and ethyl acetate by triple-column extractive distillation: entrainer design and process optimization

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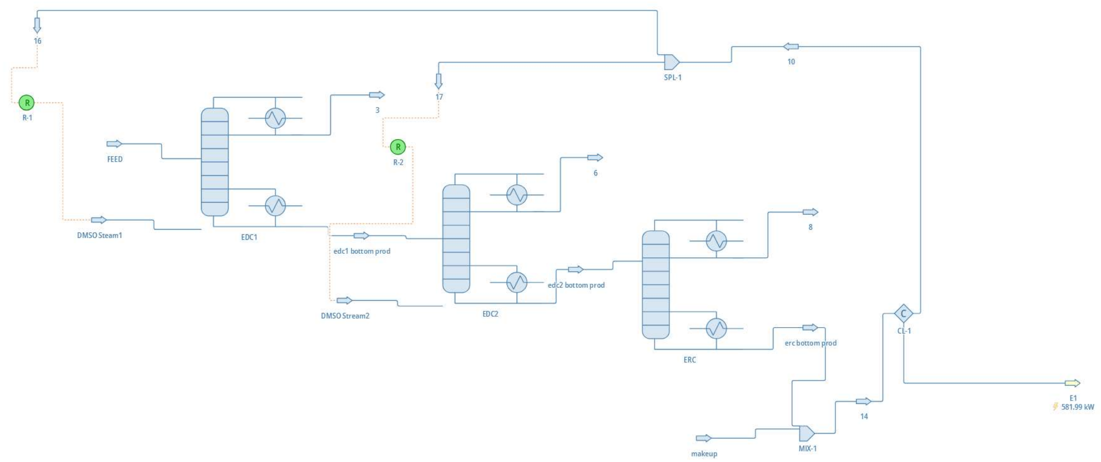
## ABSTRACT

This work presents an energy-efficient process for recovering tetrahydrofuran (THF) and ethyl acetate (EtAC) from industrial effluent using a triple-column extractive distillation system. Thermodynamic analysis and Computer-Aided Molecular Design (CAMD) identified dimethyl sulfoxide (DMSO) as the optimal entrainer. The flowsheet employs a direct separation approach in which the feed stream, composed of water, EtAC, and THF, is introduced into the first extractive distillation column (EDC1) along with a pure DMSO stream. The distillate from EDC1 yields a high-purity THF product (99%), while the bottoms, containing DMSO, EtAC, water, and trace THF, are fed to the second extractive distillation column (EDC2). A supplementary DMSO stream enhances separation in EDC2, producing a 99% pure EtAC distillate and a bottoms stream consisting primarily of water and DMSO. The bottoms from EDC2 undergo further processing in an entrainer recovery column (ERC), where DMSO is separated from water. The ERC distillate is a purified water stream, while the bottoms consist of 99.99% pure DMSO. This recovered DMSO is cooled, combined with a makeup stream, and split into two recycle streams, which are reintroduced into EDC1 and EDC2 to optimize entrainer reuse. The process demonstrates efficient recovery of high-purity THF and EtAC from industrial wastewater, validating extractive distillation with DMSO as an effective separation method.

# Flow Sheet




# Result

| Property / Streams | Units | 10 | 14 | 16 | 17 |
|---|---|---|---|---|---|
| Temperature | K | 308.15 | 436.3375979 | 308.15 | 308.15 |
| Pressure | bar | 0.5 | 0.5 | 0.5 | 0.5 |
| Molar Flow | kmol/h | 103.68592 | 103.68592 | 75.01676312 | 28.66915688 |
| Molar Fraction (Overall Liquid) / Ethyl acetate | | 0.00003857804415 | 0.00003789884308 | 0.00003857804415 | 0.00003857804415 |
| Molar Fraction (Overall Liquid) / Dimethyl sulfoxide | | 0.9990842856 | 0.9990871751 | 0.9990842856 | 0.9990842856 |
| Molar Fraction (Overall Liquid) / Tetrahydrofuran | | 0.00003857804415 | 0.00003781368936 | 0.00003857804415 | 0.00003857804415 |
| Molar Fraction (Overall Liquid) / Water | | 0.0008385583004 | 0.000837112384 | 0.0008385583004 | 0.0008385583004 |

| Property / Streams | Units | 3 | 6 | 8 | DMSO Steam1 | DMSO Stream2 |
|---|---|---|---|---|---|---|
| Temperature | K | 318.8397297 | 330.2628831 | 354.376781 | 308.15 | 308.15 |
| Pressure | bar | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| Molar Flow | kmol/h | 32.98560312 | 33.04027688 | 33.99012 | 75.01676312 | 28.66915688 |
| Molar Fraction (Overall Liquid) / Ethyl acetate | | 0.003995956492 | 0.9948260562 | 0.00008423492037 | 0.00003857804415 | 0.00003857804415 |
| Molar Fraction (Overall Liquid) / Dimethyl sulfoxide | | 0 | 0.00009478633107 | 0.000555317854 | 0.9990842856 | 0.9990842856 |
| Molar Fraction (Overall Liquid) / Tetrahydrofuran | | 0.9957061978 | 0.004843452758 | 0.000000044667796 26 | 0.00003857804415 | 0.00003857804415 |
| Molar Fraction (Overall Liquid) / Water | | 0.0002978456629 | 0.0002357047216 | 0.9993604026 | 0.0008385583004 | 0.0008385583004 |

| Property / Streams | Units | edc1 bottom prod | edc2 bottom prod | erc bottom prod | FEED | makeup |
|---|---|---|---|---|---|---|
| Temperature | K | 345.1285041 | 407.0403806 | 436.4633149 | 313.15 | 298.15 |
| Pressure | bar | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 |
| Molar Flow | kmol/h | 142.03116 | 137.66004 | 103.66992 | 100 | 0.016 |
| Molar Fraction (Overall Liquid) / Ethyl acetate | | 0.2314357284 | 0.0000207987349 | 0 | 0.33 | 0.25 |
| Molar Fraction (Overall Liquid) / Dimethyl sulfoxide | | 0.5278064533 | 0.7526210869 | 0.9991998963 | 0 | 0.25 |
| Molar Fraction (Overall | | 0.001118941325 | 0.00000001102907937 | 0 | 0.33 | 0.25 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **Liquid) / Tetrahydrofuran** | | | | | | |
| **Molar Fraction (Overall Liquid) / Water** | | 0.239638877 | 0.2473581034 | 0.000800103722 | 0.34 | 0.25 |

## References


Yang, A., Su, Y., Shi, T., Ren, J., Shen, W., & Zhou, T. (2022). Energy-efficient recovery of tetrahydrofuran and ethyl acetate by triple-column extractive distillation: Entrainer design and process optimization. *Frontiers of Chemical Science and Engineering, 16*(2), 303–315. https://doi.org/10.1007/s11705-021-2044-z