Accepted Manuscript

Title: Development of Alternative Methanol/Dimethyl Carbonate Separation Systems by Extractive Distillation – A Holistic Approach

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PII: S0263-8762(17)30469-0

DOI: http://dx.doi.org/10.1016/j.cherd.2017.09.016

Reference: CHERD 2820

To appear in:

Received date: 27-3-2017 Revised date: 15-8-2017 Accepted date: 12-9-2017

Please cite this article as: Hu, Chi-Chih, Cheng, Shueh-Hen, Development of Alternative Methanol/Dimethyl Carbonate Separation Systems by Extractive Distillation — A Holistic Approach.Chemical Engineering Research and Design http://dx.doi.org/10.1016/j.cherd.2017.09.016

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ACCEPTED MANUSCRIPT

Development of Alternative Methanol/Dimethyl Carbonate Separation Systems by Extractive Distillation - A Holistic Approach

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Graphical abstract

Three-tiered holistic approach **Activities Outcomes** Tier 3: (i) MSA effectiveness (conventional systems): (i) Carry out separation system optimization via Methyl salicylate > phenol* ≈ an iterative optimization algorithm. 4-methyl-2-pentanone* > dimethyl oxalate* Attribute: TAC (total annual cost). > ethyl benzoate > 2-ethoxyethanol* (ii) Compare the effectiveness of chosen MSA's Flowsheet (ii) MSA effectiveness (heat-integrated systems) : with that of others. Simulation Methyl salicylate > phenol* dimethyl oxalate* ≈ 4-methyl-2-pentanone* Optimization > ethyl benzoate > 2-ethoxyethanol* *: MSA taken from literature. Tier 2: Tier 2: (i) Isobaric VLE data: binary methanol/ethyl (i) Collect and/or measure necessary VLE benzoate, methanol/methyl salicylate, data. dimethyl carbonate/ethyl benzaote, and (ii) Perform VLE data reduction. Filling the VLE Data Gap dimethyl carbonate/methyl salicylate systems (ii) NRTL parameters for the systems. Tier 1: (i) Perform model-based prescreening (i) Prescreening: UNIFAC-DMD and COSMO-SAC models 12 potentially promising MSA's (S_{ii} >1.96) MSA's Screening were chosen from 35 candidates. Attribute : S_{ij}^{∞} from the predicative models. (ii) Experimental screening: (ii) Conduct experimental screening - r_{iE} measurement via headspace gas Top 2 MSA's with large Z-scores were chromatography. preserved for tier 2. Attribute : Composite Z-score

Highlights

- A holistic, three-tier approach is employed to develop MeOH/DMC separation systems.
- A two-level screening strategy is deployed in the search of good entrainers.
- A composite Z-score is incorporated to aid in the entrainer search.
- Effectiveness of the entrainers is assessed via process simulation and optimization.
- One of the proposed entrainers (methyl salicylate) outperforms all other entrainers.

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