Plausible Implications of reactive chromatography for continuous production of ethyl chloroacetate

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Abstract: Reactive separations which entails reactions and separation occurring in single unit provides opportunity to explore greener and sustainable technology for industrial production by offering benefits such as compact equipment designs, smaller inventories, energy optimisation and selective synthesis (Moulijn et al.,2017). Such a coupling is the ingrained feature of reactive chromatography where the solid media acts as catalyst for reaction and as an adsorbent for separations (Kiss,2014).This integration is useful for simultaneous production and product removal which is highly desirable in reactions limited by chemical equilibrium such as esterification, transesterification, etherification and some oxidative coupling (Bhaskar Bhandare, 2019).
Esterification of Ethanol (EtOH) and Mono chloro acetic acid (MCA) is one such esterification process where the yield of the desired ester – Ethyl chloro acetate (ECA) is limited by chemical equilibrium (Figure 1). ECA is a widely used organic solvent used in pharmaceuticals, plant protection chemicals and heterocyclic compounds production. The reaction could be furthered in forward direction by continuous removal of the undesired product.

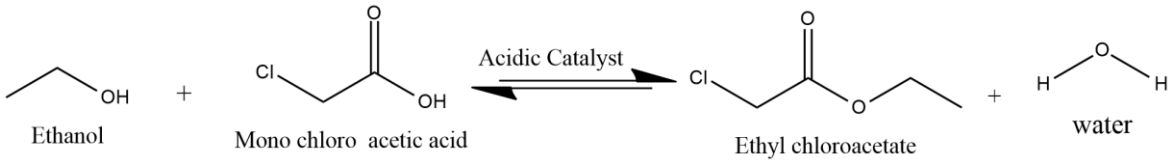

Figure 1: Esterification of Ethanol and Mono chloroacetic acid

In this work, we study this reaction in batch RC i.e., Fixed bed chromatographic reactor (FBCR) to determine ECA production feasibility. It was observed that water continuously gets adsorbed in the adsorbent leading the reaction in forward direction. Also, for a proximate time, mixture of ECA and ethanol is eluted out indicating reaction feasibility of RC for continuous production. The catalyst/adsorbent used for the bed was Amberlyst-15 (acidic ion exchange resin), which being a heterogeneous catalyst offers ease of separation and benefits of reusability. Reactions were performed for mixture of EtOH and MCA at different temperatures and molar concentrations to understand the impact on the reactive breakthrough profile.
Further, to get the glimpse of the relative affinity of each component during adsorption, experiments were performed for non-reactive binary pairs in the same FBCR setup and binary adsorption parameters were determined.
Reaction kinetics was obtained by varying different parameters and fitted to a suitable model equation. These parameters could be used further to develop FBCR model equation coupled with reaction term which subsequently can be employed for designing a continuous production process i.e., simulated moving bed reactor (SMBR).

References

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