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A genuine in-situ water removal at a molecular lever by an enhanced esterification-pervaporation coupling in a catalytically active membrane reactor

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Abstract: A better conversion enhancement of esterification between acetic acid and n-butanol was achieved in a catalytically active membrane reactor (*p*CAMR) when compared to that in a traditional inert membrane reactor (IMR). This enhancement was attributed to a novel composite catalytically active membrane in which a highly porous catalytic layer was introduced. SEM images showed that the membrane consisted of three layers: the top layer was a highly porous catalytic layer with massive macrovoids and "sponge-like" pores, the middle layer was a dense polyvinyl alcohol selective layer, and the bottom layer was a porous polyethersulfone support layer. The preparation of a highly porous catalytic layer instead of a dense one in the composite membrane greatly decreased the overall mass transfer resistance of the reactor from 6.7×10^5 to 5.6×10^5 sec/m, a value which is even comparable to that of IMR (5.1×10^5 sec/m) where the additional catalytic layer was absent. The effects of operational parameters on the esterification-pervaporation coupling performance in *p*CAMR were systematically evaluated. Through a reasonable match between reaction rate and water removal rate, a genuine in-situ water removal at a molecular lever was realized. For comparison, coupling performances in an IMR and a catalytically active membrane reactor with a dense composite membrane (*d*CAMR) were also investigated. Results showed that the coupling performance in *p*CAMR outperformed both IMR and *d*CAMR due to a combination of much lower overall mass transfer resistance and higher mass transfer driving force for water removal in *p*CAMR. After 45 hours at 85 °C, the acid conversion in *p*CAMR reached almost completion, an approximately 43 % of conversion enhancement was achieved when compared to equilibrium conversion.