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Efficient separation of allyl chloride from 1-chloropropane by one-dimensional zeolites

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Zeolites have great potential in adsorption and separation of alkanes-olefins mixtures with similar properties due to its shape selectivity and huge specific surface area1. In our work, a series of zeolites were quickly screened to separate 1-chloropropane from 1-chloropropane/allyl chloride gas mixtures by the molecular simulation. The adsorption isotherm curves of simple component were obtained on the basis of the Grand Canonical Monte Carlo method, and the gas mixture fluxes were calculated by the non-equilibrium molecular dynamics method. The results show that zeolites with special configurations (e.g., AHT type) only absorbed allyl chloride so that allyl chloride was selectively separated from 1-chloropropane under the pressure range of 0.001-100 kPa. These zeolites have one-dimensional and elliptical channels with the length of about 6.8 Å and the width of about 3.3 Å, which mostly matched with the low energy configuration of allyl chloride2. Based on the single selective adsorption of these zeolites, the fluxes of zeolite membranes under different thicknesses and pressures were investigated to analyze the separation efficiency of the mixture. The preliminary conclusions provide a new avenue to explore for the purification of allyl chloride in the membrane industry.

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Primary authors: ZHANG, Yujia; XU, Yinxiang; XU, Junbo; YANG, Chao

Presenter: ZHANG, Yujia

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