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Virtual Group Theory: A New Method to Predict the Adsorption Equilibrium of Organic Mixtures at Various Site Conditions

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A new method (virtual group theory or VGT) is developed to predict multi-component adsorption equilibrium of organic vapors, and hence the service life time of filter cartridges. The method is developed based on the theory that adsorbed organic contaminants can be treated as a virtual liquid mixture, while the adsorption effect is taken as a virtual group that dilutes the mixture, hence reducing the saturated vapor pressure of each component. The resulting virtual vapor-liquid equilibrium (VLE) is then solved by traditional group contribution models such as the UNIFAC model.

Test calculation of a number of organic vapors has demonstrated that the VGT method can accurately predict adsorption equilibrium of organic vapors and their mixture. Also, the VGT can predict adsorption equilibrium of the organic mixture at different humidity levels.