Modeling of a fixed bed adsorptive drying of chlorine

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Abstract title	MODELING OF A FIXED BED ADSORPTIVE DRYING OF CHLORINE
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Background

Chlorine is an important reagent in many industrial processes. Annually more than 45 million tons of chlorine are produced worldwide [1]. Wet chlorine is extremely corrosive [2], therefore, industrial chlorine is dried below 50ppm water content with sulfuric acid before liquefaction and transport [3]. As a polishing step for liquid chlorine or as an alternative for sulphuric acid drying, molecular sieves can be used to remove water in a temperature swing adsorption process [4]. The molecular sieves are regenerated with hot air. The adsorption equilibrium for this system is not reported in literature and information on liquid phase adsorption is scarce.

Aim

An experimental study is performed of the adsorption of water on molecular sieve 3A in a lab-scale packed bed. Dichloromethane (DCM) is chosen as a model molecule for chlorine because of its similar physical properties. The experimental data is used to validate an engineering model. This model is used for design, optimization, and economic evaluation of a 10 000 tons of chlorine per year process.

Method

The drying of liquid and gaseous DCM containing water in a packed bed of molecular sieves is modeled. The fluid phase is modeled as CSTRs in series. The number of CSTRs is determined by the Peclet number. The molecular sieve packing is present in batch mode. In the mass balances, the mass transfer is approximated with the linear driving force model. The adsorption isotherms of water from DCM on molecular sieves 3A are implemented in the model. The input parameters are given in Table 1. The parameters used in the simulation represent the lab-scale setup.

Results

The influence of different parameters on the adsorption curves has been analyzed. For a liquid DCM flow rate of 5 g/s and 300 g of molecular sieves, breakthrough is reached after 5,4 hours, see Figure 1. Increasing residence time, decreasing particle size, or decreasing mass transfer coefficient reduce the time to reach breakthrough, as expected. The breakthrough curves become steeper near the breakthrough point. Including internal mass transfer resistance in the particle should improve the model accuracy in that region. The model is sufficiently accurate for the design of the industrial process. Two packed beds with 32000 kg molecular sieve are required for replacement of the sulphuric acid drying, with an adsorption time of 23 hr.

References

[1] Schmittinger P. et al, 2012, "Chlorine," Ullmann's Encyclopedia of Industrial Chemistry.

[2] Ketelaar A. A., 1960, "The Drying and Liquefaction of Chlorine and the Phase Diagram Cl2-H2O," 5(3), pp. 1-5.

[3] Brien T. F. O., 2005, Handbook of Chlor-Alkali Technology Volume I, Springer.

[4] Ruthven D. M., 1984, "Principles of adsorption and adsorption processes," Chemical Engineering and Processing: Process Intensification, p. 433.

Images

Parameter	Unit	Value
Inlet concentration	ppm	2000
Flow rate	g/s	5
Temperature	°C	30
Particle size	mm	2
Bed porosity	-	0,41

Table 1. Parameters used for simulation

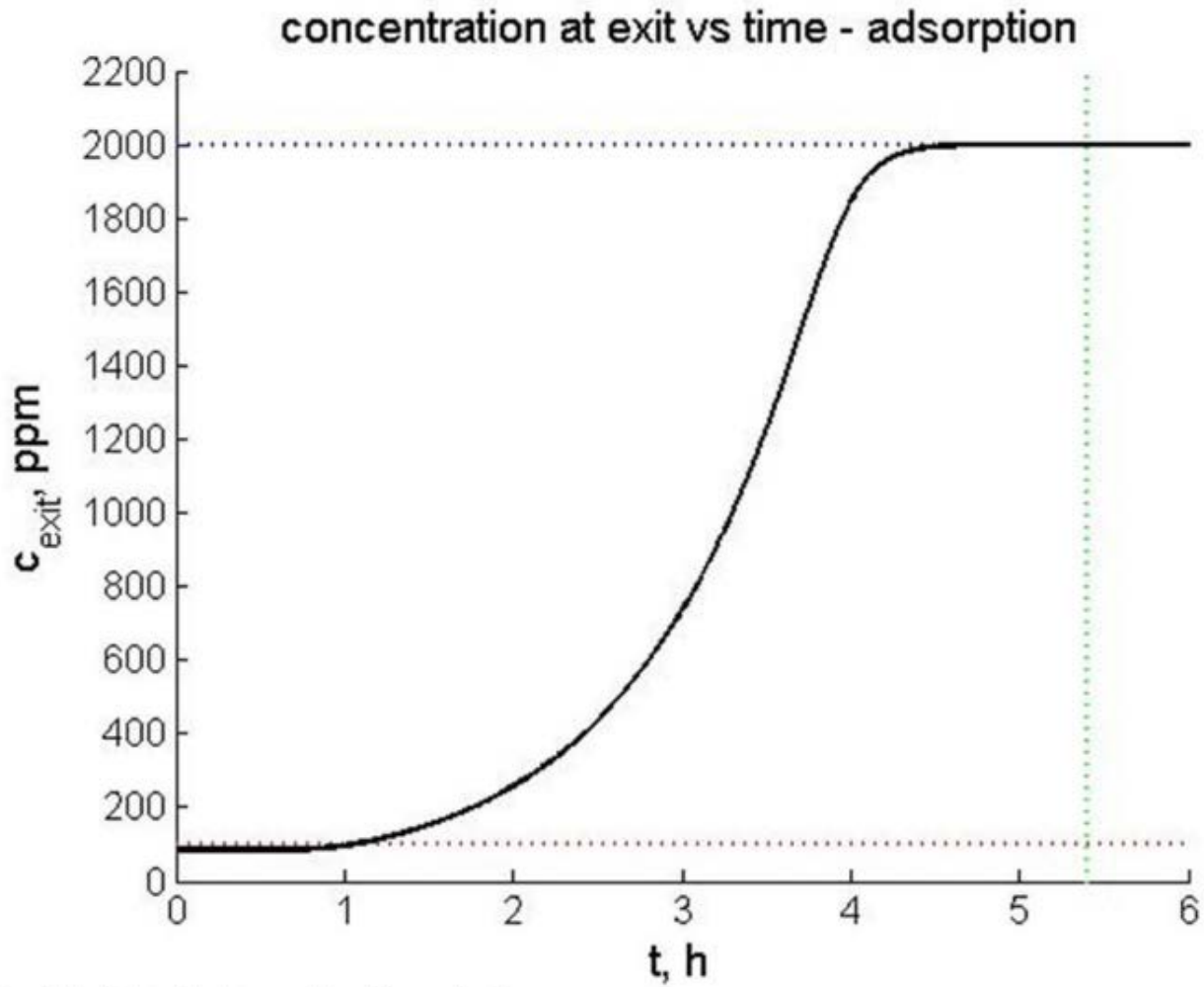

Figure 1. Adsorption breakthrough curve model result for parameters in Table 1.