

Modeling and Adsorption Tests for an Atmospheric Detritiation Dryer

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1. Introduction

The recovery of tritium from waste gas stream is important with respect to reduction of tritium emission to environment. The fusion research facility and power plant will require large atmospheric detritiation system to mitigate tritium releases and to recover heavy water vapor. The best available technology for these systems is the oxidized-and-adsorb process, where tritiated species are converted to tritium oxide (HTO) and adsorbed on an atmospheric detritiation dryer [1,2,3,4].

Conventional atmospheric detritiation dryers use synthetic zeolites as the adsorbent and rely on a thermal-swing cycle. This permits continuous detritiation of a gas by using multiple desiccant beds, each beds being regenerated following a periods of moisture removal (adsorption).

In designing a fixed bed dryer and preparing an advanced dryer control, it is necessary to quantify the bed utilization and dynamic behavior against inlet humidity and flow rate. This study is aimed at obtaining an insight into the breakthrough behavior in small column experiments and dynamic modeling for the operating performance of the atmospheric detritiation dryer.

2. Mathematical Model

An adsorber is considered as an isothermal fixed bed column with constant void fraction. The fixed bed is composed of cylindrical pellets of adsorbent with the uniform diameter. The adsorbent is a porous solid with constant porosity. The governing equation for the bulk-fluid phase of the adsorption column can be written as follows:

$$\frac{\partial C}{\partial t} = \frac{1}{Pe} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - \gamma(C - c|_{r=R}) \quad (1)$$

The boundary conditions for the inlet and the outlet of the column, and the initial condition are of the following form.

$$\left. \frac{\partial C}{\partial z} \right|_{z=0} = Pe(C|_{z=0} - 1), \quad \left. \frac{\partial C}{\partial z} \right|_{z=L} = 0, \quad C(z,0) = 0$$

Accumulation in the pores as well as in the solid phase and radial diffusion in the cylindrical particle is described by equation.

$$\left(1 + K \frac{\partial q}{\partial c}\right) \frac{\partial c}{\partial t} = \delta \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \quad (2)$$

The Langmuir type of adsorption isotherm has been considered in this study:

$$q = \frac{ABc}{1 + Bc} \quad (3)$$

We obtain the following equation for the particle:

$$\left\{1 + \frac{KB}{(1 + ABc)^2}\right\} \frac{\partial c}{\partial t} = \delta \left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \quad (4)$$

The following boundary conditions and initial condition are considered.

$$\left. \frac{\partial c}{\partial r} \right|_{r=0} = 0, \quad \left. \frac{\partial c}{\partial r} \right|_{r=R} = Bi(C - c|_{r=R}), \quad c(r,0) = 0$$

The equations are written in dimensionless form as reported in literature [5].

We obtain a system of ordinary differential equation for both the bulk-fluid and particle phase by applying the method of lines

3. Experimental

Molecular sieve and Mordenite are the synthetic zeolite adsorbent with a constant pores size as described in Table 1. The pores size influences the adsorption qualities. A series of regeneration/adsorption cycles was performed using a bench-scale dryer. The dryer was loaded with cylindrical pellets of 1.6mm (nominal). Each test consisted of regenerating a 10cm long by 1.1cm diameter bed to a known condition, followed by an adsorption using moisture stream with constant humidity. The bed was vertical and gas flowed downward during adsorption and regeneration.

Table. 1 Typical properties of synthetic zeolites

Typical properties	Synthetic zeolites, (Molecular sieve, 1/16")			Morde- nite, 1/16"
	4A	5A	13X	
Type	4A	5A	13X	-
Nominal pore diameter (Å)	4	5	10	-
Bulk density (kg/m ³)	740	720	670	-
Particle diameter (mm)	1.6	1.6	1.6	1.6
Heat of adsorption (kcal/kgH ₂ O)	1000	1000	1000	-

Constant humidity was used during each adsorption test. CEM (Control-Evaporation-Mixing, Bronkhorst Hi-Tec. Co.) system was applied to supply the carrier gas adjusted with constant humid condition. The defined quantity of the liquid can be mixed with the carrier gas and vaporized in the CEM system. Capacitance-type hygrometers from Michell Instruments with Cermet sensors monitored the inlet and outlet stream of the dryer bed.

The outlet humidity expressed as dew-point temperature was automatically recorded through the interface with a computer.

4. Results and Discussion

4.1 Numerical Simulation

The model equations are solved using explicit method of finite difference technique with the appropriate initial and boundary conditions. 30 interior grid points for the axial domain in the fluid phase and 5 interior points for the radial domain in the adsorbent phase were selected, respectively, to solve the mathematical model in this study. The built-in function 'ode15s.m' of MATLAB software was used as the ODE solver to have the solutions from a set of ordinary differential equations. The outlet concentration at different time is determined and breakthrough patterns are generated as shown in Figure 1. The model parameters of particle diffusion coefficient and axial dispersion coefficient could be adjusted to give the best-fit curve.

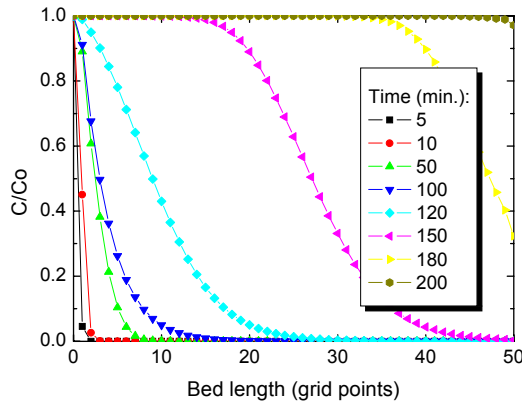


Figure 1. Concentration profiles at different time..

4.2 Breakthrough Tests of Synthetic Zeolites

Figure 2 shows that the breakthrough for the Molecular sieve 13X appears later than others at constant humidity. Among the synthetic zeolites tested in this study, Molecular sieve 13X has a higher capacity. The breakthrough appears earlier and the breakthrough curves are steeper at higher humid condition. Those are to say that breakthrough zone occurring mass transfer from fluid to adsorbent becomes narrower due to higher driving force.

The driving force for adsorption, as well as regeneration, is the difference in water vapor pressures in air and at the desiccant surface. The amounts of water vapor passed during each adsorption step to reach breakthrough were estimated to be about 0.1–2.5 gH₂O/g adsorbent by time-integrating the outlet water vapor content and multiplying by the air flow-rate.

The breakthrough appears earlier at higher temperature condition. This tendency is thought that increasing adsorption temperature increases the

temperature difference of the air stream through the adsorption column.

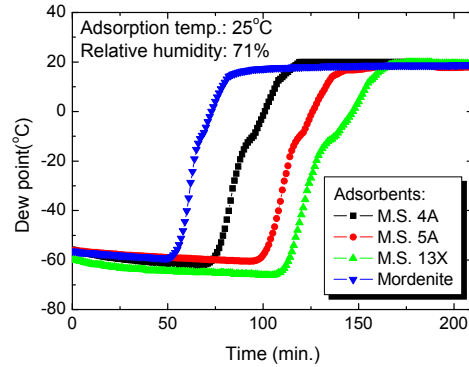


Figure 2. Breakthrough curves for water vapor adsorption on Molecular sieves and Mordenite at constant humidity.

5. Conclusion

The mathematical model of isothermal adsorption in a fixed bed has been solved using method of lines. In an isothermal fixed bed adsorption system for constant inlet humidity and flow rate of air stream, the breakthrough patterns were obtained to quantify the adsorption performance of water vapor on synthetic zeolites.

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