

Modeling and Dynamic Simulation for a Tritiated Water Vapor Adsorber

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1. Introduction

The recovery of tritiated water vapor from the waste gas stream is important with respect to reduction of tritium emission to environment. Use of adsorption systems has been more prevalent for an application in the airborne tritium decontamination during recent years [1,2,3,4]. Both the design and operation of the detritiation adsorber are related to the characteristic breakthrough curves in which readily measured effluent concentration is plotted as a function of elapsed time. To maintain the gaseous tritium emission below the approved emission limits, they have routinely dried air to a dew-point of -60°C or below. The regulatory guidance relevant to airborne tritium is based on the derived air concentration (DAC) that when breathed for 2,000 hours work-year equals effective dose of 5rem.

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.

In designing a fixed bed dryer and preparing an advanced dryer control, it is necessary to quantify the bed utilization and dynamic behavior against an inlet humidity and a flow rate. In this study, a mathematical model and dynamic simulation are studied for the prediction of operating performance of the atmospheric detritiation dryer.

2. Mathematical Model

The dynamics of a fixed bed is described by a set of diffusion equations, coupled with source terms due to adsorption and diffusion inside the adsorbent particles. Prediction of the breakthrough curves is based on correct mathematical model formulation of a fixed bed adsorber.

An adsorber is considered as an isothermal fixed bed column with a constant void fraction(ϵ_b) arising from the gaps. The fixed bed is composed of cylindrical pellets of adsorbent with a uniform diameter(d_p). The adsorbent is a porous solid with a constant porosity(ϵ_p) as shown in Figure 1. The governing equation for the bulk-fluid phase of the adsorption column can be written as follows:

$$\frac{\partial C}{\partial t} = E_m \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial z} - \frac{2k_f}{R} \frac{1 - \epsilon_b}{\epsilon_b} \left(C - \frac{q|_{r=R}}{q_m b - b q|_{r=R}} \right) \quad (1)$$

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

$$E_m \frac{\partial C}{\partial z} \Big|_{z=0} = v(C - C_f), \quad \frac{\partial C}{\partial z} \Big|_{z=L} = 0, \quad C|_{t=0} = 0$$

In case of a single microporous adsorbent particle such as a zeolite crystal, accumulation in the solid phase and a radial diffusion in the cylindrical particle are described by the following equation.

$$\frac{\partial q}{\partial t} = D_{ef} \left(\frac{\partial^2 q}{\partial r^2} + \frac{1}{r} \frac{\partial q}{\partial r} \right) \quad (2)$$

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

$$q = \frac{a}{1 - \epsilon_b} \frac{bC}{1 + bC} = q_m \frac{bC}{1 + bC} \quad (3)$$

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.

$$\frac{\partial q}{\partial r} \Big|_{r=0} = 0, \quad D_{ef} \frac{\partial q}{\partial r} \Big|_{r=R} = k_f \left(C - \frac{q|_{r=R}}{q_m b - b q|_{r=R}} \right), \quad q|_{t=0} = 0$$

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

We obtain a system of ordinary differential equations for both the bulk-fluid and particle phase by applying the method of lines (space discretization of the governing PDEs) [6].

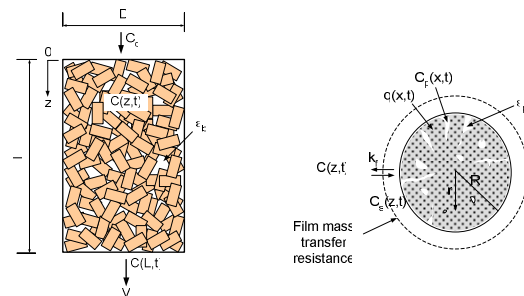


Figure 1. Model of the fixed bed column.

3. Results and Discussion

3.1 Numerical Simulation

The model equations are solved using explicit method of finite difference technique with the appropriate initial and boundary conditions. 50 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 [6].

3.2 Breakthrough Behavior

Understanding the dynamics of the fixed bed adsorption columns for modeling is a demanding task due to the strong nonlinearities in the equilibrium isotherms, mass transfer resistances between fluid phase and solid phase, and fluid dynamic dispersion.

The case to consider here is a microporous adsorbent particle such as a zeolite crystal, exposed to a step change in adsorbate concentration at the external surface of the cylindrical particle at time zero. The outlet concentration at different time is calculated and breakthrough patterns are generated as shown in Figure 2.

The physical parameters in the model are the solid diffusion coefficient, axial dispersion coefficient, and external mass transfer coefficient. These model parameters could be adjusted to give the best-fit curve.

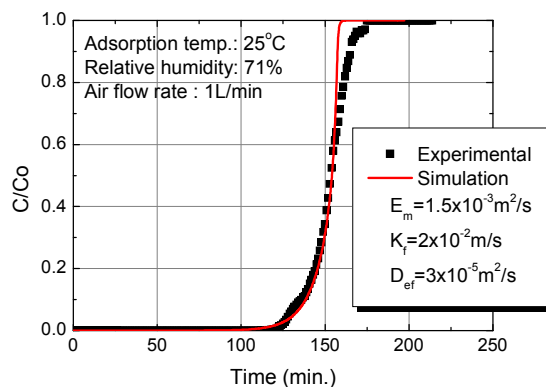


Figure 2. Breakthrough curve at different time.

4. Conclusion

To predict the operating performance in air leaving a detritiation dryer, a 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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