Building and Environment 73 (2014) 64–74

Contents lists available at ScienceDirect

Building and Environment

journal homepage: www.elsevier.com/locate/buildenv

Development and systematic validation of an adsorption filter model

Golnaz Shaverdi [a], Fariborz Haghighat [b,*], Wahid Ghaly [a]

[a] Department of Mechanical and Industrial Engineering, Concordia University, Montreal, Canada
[b] Department of Building, Civil and Environmental Engineering, Concordia University, Montreal, Canada

ARTICLE INFO

Article history:
Received 5 September 2013
Received in revised form
9 November 2013
Accepted 28 November 2013

Keywords:
Indoor air quality
Adsorption
Modeling
Gas phase filtration

ABSTRACT

An analytical model is developed to study the performance of gas-phase filters. This model is validated systematically with experimental results obtained from a small scale and a full scale experimental setup, at various inlet concentrations. The prediction made by the model is then compared with predictions made by two existing models and the experimental data: The developed model performs much better than the others. The validated model is applied to study the effect of the diffusivity within the porous pellets, the air volume flow rate, and the particle size on its performance. The variations of initial efficiency and breakthrough time with respect to changes in these parameters are discussed.

1. Introduction

Air cleaning devices can be used to keep the level of pollutants in an acceptable range, thereby reducing the ventilation rates and the associated energy requirements. Adsorption filters are a type of air cleaning devices, and they may also be designed for a wide range of other applications by choosing the appropriate adsorbent, and by considering the physical and chemical characteristics of the adsorbent and the adsorbate [1–3]. However, there are some limitations to their application: their efficiency decreases over time, and they need to be frequently replaced or, in some cases, regenerated. Furthermore, in order to design efficient filters, one should take into account many operating parameters affecting the filter performance. Thus, by developing efficient tools to predict their performance, one may hope to overcome their current limitations and to allow for a wider application of this technology in non-industrial buildings.

Packed bed filters are one of the most common types of adsorption filters. Their operating parameters include the shape, size and distribution of the granules and the packing density of the bed, all of which affect the bed porosity. Other important parameters for these filters are the airflow rate, which affects the convective mass transfer coefficient, and the type of adsorbent used, which determines the diffusivity within the granules and the adsorption parameters.

The trend of the variation of efficiency over time indicates the proper time of filter replacement. Therefore, a first step is to obtain a model that can accurately predict the filter performance. Mass transfer models of adsorption filters have been developed to predict breakthrough time. The inputs of these models are the inlet fluid conditions and the filter characteristics, and the output is the effluent concentration, or the efficiency of the bed.

Indeed, finding a proper and reliable model for packed bed adsorption filters has been an important issue for many years; it has been addressed by many researchers and a number of models have been developed for specific and general cases [4–11]. To address certain limitations arising from these methods, an efficient and reliable model to quantify the performance of packed bed adsorption filters for a wide range of operation is developed here, and is validated against experimental data. In addition, using the developed model, a parametric study of a packed bed adsorption filter is carried out so as to evaluate its performance.

2. Model development

Unlike previously developed packed-bed mass transfer models, this work starts by solving analytically the mass diffusion equation of a single spherical particle. This yields the adsorption amount of one single particle, and this computation is then extended to the whole bed by considering the position of the pellets within the bed.

2.1. Adsorption in a single porous pellet

The contaminant mass transfer in packed bed adsorption filters occurs in several stages. First, the adsorbate molecules convect

* Corresponding author.
E-mail addresses: Fariborz.Haghighat@concordia.ca, haghi@bcee.concordia.ca (F. Haghighat).

0360-1323/$ – see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.buildenv.2013.11.022

from the bulk flow to the laminar layer at the surface of the particle; next, the diffusion and adsorption occur in parallel within the particle. Thus, the mass flux of the contaminant molecules that diffuses within the particle and is adsorbed there is equal to the convective mass flux, N_A:

$$N_A = h_m\left(C_b - C^*\right) \tag{1}$$

where C^* is the laminar layer gas concentration at the surface of the pellet, C_b is the bulk gas concentration in the bed, and h_m is the convective mass transfer coefficient.

In order to compute C^*, the concentration in the pellets, C_{avg}, which takes into account both gas and sorbed phases, is defined by

$$\begin{aligned} C_{avg} &= \frac{\text{Adsorbent mass in gas and sorbed phases within the pellet}}{\text{Volume of the pellet}} \\ &= \frac{V_p(1-\varepsilon_p)Q + V_p\varepsilon_p C_p}{V_p} = \frac{V_p(1-\varepsilon_p)KC_p + V_p\varepsilon_p C_p}{V_p} \\ &= \left[(1-\varepsilon_p)K + \varepsilon_p\right]C_p = K'C_p \end{aligned} \tag{2}$$

Here V_p is the particle volume, ε_p is the particle porosity, Q is the sorbed phase concentration, C_p is the gas phase concentration within the pores of the particle and K is the linear adsorption isotherm, which relates the sorbed phase concentration to the gas phase concentration, assuming they are in equilibrium at a constant temperature. The adsorption isotherm coefficients are obtained in the standard way by plotting the gas and sorbed phase concentrations at the saturation point, at which these phases are considered to be in equilibrium. Safari et al. also used, for C_p, the inlet concentration (equal to outlet concentration) at saturation point. They used the total amount of adsorption during the process, divided by the total mass or volume of adsorbent, as the sorbed phase concentration [12]. Note that the total amount of adsorption comprises the adsorbate present in the gas phase within the pores of the pellets, plus the sorbed phase of the pellets. As shown by equation (2), this amount divided by the volume of the pellet is equal to C_{avg}. Therefore, plotting C_p versus C_{avg} yields K'.

The mass transfer in a single pellet is governed by the following equation from Ref. [13], where we have substituted C_{avg} with $K'C_p$:

$$\frac{\partial(K'C_p)}{\partial t} = D_e\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial(K'C_p)}{\partial r}\right)\right] \tag{3}$$

With the following boundary and initial conditions:

$$\frac{\partial(K'C_p(0,t))}{\partial r} = 0 \tag{4}$$

$$h_m\left(C_b - C^*\right) = D_e\frac{\partial(K'C_p(R_p,t))}{\partial r} \tag{5}$$

$$C_p(r,0) = C_0 \tag{6}$$

Here r is the radial distance from center of the spherical particle, t is the time, D_e is the diffusion coefficient, R_p is the pellet radius and C_0 is the initial concentration at time zero. An analytical solution to the above equation can be found in many heat and mass transfer textbooks (see e.g. Ref. [14]):

$$\begin{aligned} \frac{(C_b - C_p(r,t))}{(C_b - C_0)} &= \sum_{n=1}^{\infty} 4\exp\left(\frac{-\lambda_n^2 D_e t}{R_p^2}\right)\left(\frac{\sin\lambda_n - \lambda_n\cos\lambda_n}{2\lambda_n - \sin(2\lambda_n)}\right) \\ &\times\left(\frac{\sin(\lambda_n(r/R_p))}{\lambda_n(r/R_p)}\right) \end{aligned} \tag{7}$$

where λ_n is obtained from the characteristic equation:

$$1 - \lambda_n\cot\lambda_n = \mathrm{Bi} = \frac{h_m R_p}{D_e K'} \tag{8}$$

C^* can be obtained from the gas phase concentration at the pellet surface, i.e. at $r = R_p$:

$$C_p(R_p,t) = C^*(t) \tag{9}$$

Hence

$$\begin{aligned} \frac{(C_b - C^*(t))}{(C_b - C_0)} &= \sum_{n=1}^{\infty} 4\exp\left(\frac{-\lambda_n^2 D_e t}{R_p^2}\right)\left(\frac{\sin\lambda_n - \lambda_n\cos\lambda_n}{2\lambda_n - \sin(2\lambda_n)}\right) \\ &\times\left(\frac{\sin\lambda_n}{\lambda_n}\right) \end{aligned} \tag{10}$$

Therefore, the amount of adsorbate diffusing and being adsorbed in a time period t within a single pellet is:

$$J(t) = \int_0^t S_a h_m\left(C_b - C^*(t)\right)\mathrm{d}t \tag{11}$$

where S_a represents the available surface area for mass transfer, that is, $4\pi R_p^2$. It should be noted that since the pellets within a packed bed overlap, the available surface area is less than the external surface area of a pellet (see Section 4.1).

Inserting the expression of $C_b - C^*$ from (10) into (11) yields:

$$\begin{aligned} J(t) &= (C_b - C_0)S_a h_m \times \int_0^t \sum_{n=1}^{\infty} 4\exp\left(\frac{-\lambda_n^2 D_e t}{R_p^2}\right) \\ &\times\left(\frac{\sin\lambda_n - \lambda_n\cos\lambda_n}{2\lambda_n - \sin 2\lambda_n}\right)\left(\frac{\sin\lambda_n}{\lambda_n}\right)\mathrm{d}t \end{aligned} \tag{12}$$

2.2. Adsorption in the pellets of a packed bed filter

The amount of adsorption in a single pellet inside a packed bed can be obtained under certain simplifying assumptions. The total adsorption in the bed can then be calculated as the sum of the adsorption amount of all the pellets.

The model developed here is based on a discretization of the adsorption filter in space and time, which is common practice when solving PDEs numerically. The assumptions made here are similar to those made in the development of the existing packed beds filters mass transfer models, however they are applied here using a different approach. Indeed one important characteristic of this model is that it substitutes algebraic mass balance equations with differential equations that are relatively straightforward to solve: This provides a simplification in comparison with previous models. The assumptions made in this model are:

1. The pellets are identical and uniformly distributed in the bed,
2. The bed is divided into N equal sections. The length of each section is dx: