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Model simulation and experiments of flow and mass transport through a nano-material gas filter

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ABSTRACT

A computational model for evaluating the performance of nano-material packed-bed filters was developed. The porous effects of the momentum and mass transport within the filter bed were simulated. For the momentum transport, an extended Ergun-type model was employed and the energy loss (pressure drop) along the packed-bed was simulated and compared with measurement. For the mass transport, a bulk adsorption model was developed to study the adsorption process (breakthrough behavior). Various types of porous materials and gas flows were tested in the filter system where the mathematical models used in the porous substrate were implemented and validated by comparing with experimental data and analytical solutions under similar conditions. Good agreements were obtained between experiments and model predictions.

1. Introduction

Packed-bed filters have been used for decades to remove hazardous gases and vapors from contaminated air flows. Because of their relatively simple but robust structure, these filters have been utilized in different manufacturing industries. The fluid/solid interaction/adsorption is involved in this process. There have been numerous experimental investigations on the adsorption process occurring between the gas flow (e.g. water vapor or ammonia) and the granules (e.g. activated carbon, zeolite compounds) in the packed-bed column, e.g. [1–6]. The breakthrough behavior, which is the typical mechanism in the adsorption process, has been well stated in those publications. Also, there exists a theoretical solution (Wheeler–Jonas equation) that determines the breakthrough time ([7,8]), which can be used to compare with the experimental data.

Mathematical modeling is an efficient way to conduct parametric studies due to its low cost and efficiency. However, a complete study using the transport equation models for momentum and mass transport in gas filtration is very rare compared with typical studies of the packed-bed reactors. To investigate the mass and heat transfer in the reactor, Nijemeisland and Dixon ([9,10]) reviewed the use of computational fluid dynamics (CFD) as a design tool for fixed bed reactors. Their study presented the relationship between the local flow field and the local wall heat flux in a packed bed of spheres, and CFD was used to obtain the detailed velocity and temperature fields. For the filtration problem in the current study, Arturo et al. [11] used an Eulerian 2-D transient model to describe the space-time evolution of clogging patterns developed in deep-bed filtration of the liquids. A local formulation of the macroscopic logarithmic filtration law was proposed, as well as a geometrical model for the effective specific surface area of momentum exchange. The comparison between the simulations and exper-

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iments showed that CFD is useful for the quantitative description of packed-bed clogging. Tung et al. [12] studied the mechanism of the deep bed filtration for submicron and nano-particles suspension by means of a force analysis on the suspended particles flow passing through ordered-packed granular filter beds. The flow fields through the filter beds were calculated. There has not been a complete study of both the momentum and mass transport through a packed-bed filter, especially those filled with nano-materials.

Recently, nano-structured materials (usually made by clustering powders or pellets, e.g. zinc oxide (ZnO), magnesium oxide (MgO)) with high surface areas were proved to be more efficient than the traditional adsorbing filter media [13]. These materials have the potential to enhance the present day science and technological applications. Hence, the adsorption process (breakthrough behavior) of these materials becomes an important subject. Existing knowledge of physical adsorption is not sufficient to predict the performance of nano-materials due to their properties. One of the primary applications of this study is to utilize nano-structured materials in filtration media to benefit indoor air environment (IAE). However, one of the difficulties of testing nano-materials is the unknown transport properties of the new materials, which require either unique experimental measurements or new theoretical models.

At the present time, a platform that combines a series of experimental equipment and numerical models has been developed. Several test facilities (packed-beds) and related numerical models have been designed to evaluate the performance of novel nano-adsorbent materials for removing gas contamination. Although the governing equations for flow and species transport are still in their standard format, this work is to add the data and knowledge base that is rare for the study of gas filtration through nano-structured absorbent materials in the current literature. The current packed-bed model is capable of monitoring real time effects of concentration in the adsorption column. Various types of porous material (e.g. zirconium, activated carbon, zinc oxide, etc.) were used as filter media to test the effectiveness of the system in data replication. Pressure drop measurements have been carried out to validate the function of the packed-bed system. Breakthrough analysis has been done to understand the adsorption kinetics in the filter bed. The results from simulations were in agreement with the experimental data. Thus, the relationships between experiment and numerical simulations can be demonstrated.

This paper has three following parts: Section 2 presents the details of the numerical model based on the experiment setup; Section 3 shows the results comparison and analysis with discussions including the pressure drop estimation and the breakthrough behavior investigation, with the conclusions given in Section 4.

2. Numerical model descriptions and simulation setups

In this section, first, the theoretical model is presented for simulating the filtered flow with species transport in the packed-bed filter. The geometries of the physical models are based on the experimental setup of the modeled problems. The transport equations for both flow and species are then discretized and solved numerically using commercial software FLUENT 6.3 [14]. And the details of the computational fluid dynamics simulations (including the computational domain, numerical schemes, boundary conditions, etc.) will be discussed later in this section.

2.1. Numerical model descriptions

In the current model, we assume the flow is incompressible and Newtonian. The packed-bed is filled with porous material pellets with equal size. The possible reaction between the fluid and the porous material is neglected in the species transport simulation since it is a relatively slow process. The heat generated from the adsorption procedure is not taken into account, either. In the theoretical model for this study, new source terms are added to the momentum and mass transport equations in the porous medium to account for the flow resistance and adsorbing effects of the porous medium (see Fig. 1). The computational domain is divided into two zones: the fluid zone and the porous zone. The theoretical models with the modeled porous materials are first validated by comparing the experimental results, and then applied to predicting the performance

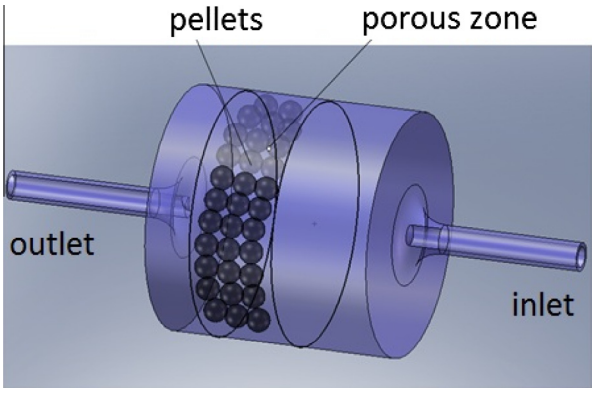

Fig. 1. The concept of the packed-bed simulation with porous substrates.