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MODELING OF GAS FLOW WITH VOCS ADSORPTION ON A FIXED BED PRECONCENTRATOR

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ABSTRACT

In several cases the concentrations of gaseous volatile organic compounds (VOCs) are too small to be detected by BTEX micro-analyzers and therefore a preconcentration unit should be coupled to the analytical instrument in order to increase the injected concentration of the pollutants and improve then detection sensitivity. The present work is focused on the modeling of the preconcentrator by simulating first only the main flow and secondly the adsorption process coupled to the main flow with. The introduced model is validated by comparison with published results.

The main flow is described by the continuity and Navier–Stokes equations supplemented by a source term to model flow through the porous medium [1]:

$$\nabla \cdot u_i = 0 \quad (1)$$

$$\rho u_j \frac{\partial}{\partial x_j} (u_i) = - \frac{\partial p}{\partial x_i} + \mu \frac{\partial \tau_{ij}}{\partial x_j} + S_i \quad (2)$$

$$S_i = \frac{\mu}{\alpha} u_i + c_2 (0.5 \rho u_i |u_i|) \quad (3)$$

Here, p is the pressure, ρ is the density, u_i is the flow velocity, α is the viscose resistance which is function of porosity and particle diameter and c_2 is inertial resistance coefficient . No-slip boundary conditions are applied at the preconcentrator walls. Also, the gas flow rate at the inlet is given, while the pressure at the outlet is fixed. Once equations (1-3) are solved, the inlet pressure as well as the velocity field of the main flow are obtained.

Next, in order to simulate the adsorption process, the time evolution of the concentrations of the k -th VOC in the gas phase $c_{k,x}$ and in the solid phase $q_{k,x}$ along the flow direction x are obtained by solving the following time dependent equations [2]:

$$\varepsilon_b \frac{\partial c_{k,x}}{\partial t} + u_i \frac{\partial c_{k,x}}{\partial x} - \varepsilon_b D_{lk} \frac{\partial^2 c_{k,x}}{\partial x^2} + \rho_b \frac{\partial q_{k,x}}{\partial t} = 0 \quad (4)$$



$$\rho_b \frac{\partial q_{k,x}}{\partial t} = k_{ai} \varepsilon_b \left(1 - \frac{q_{k,x}}{Q_k}\right) c_{k,x} - k_{d,k} \rho_b q_{k,x} \quad (5)$$

Here, ε_b is the bed porosity, D_{li} is the axial dispersion coefficient, ρ_b is the bed density and Q_k is the maximum monolayer adsorption capacity, while k_{ak} and $k_{d,k}$ are the adsorption and desorption rate constants respectively. It is noted that u_i is the flow velocity obtained from Eqs. (1-3). The associated boundary and initial conditions are:

$$\begin{aligned} t=0 \quad 0 < x \leq H_b \quad c_{k,x=0}, q_{k,x} = 0 & ; & t=0 \quad x=0 \quad c_{k,x}=c_{k0}, q_{k,x} = 0 \\ t > 0 \quad x=0 \quad c_{k,0} = const & ; & t > 0 \quad x=H_b \quad \partial c_{k,x}(H_b,t) / \partial x = 0 \end{aligned}$$

The above model is introduced to simulate nitrogen flow through the micro preconcentrator built at In'Air Solution. Equations (1-3) are solved for three flow rates with the outlet pressure fixed at 4 bar using various permeability coefficients and the results are shown in Fig. 1a. In all cases as the flow rate is increased the inlet pressure is increased to overcome the increased pressure drop. In addition, as the permeability coefficient is increased the pressure drop is always decreased. In order to validate the implemented model of the main flow comparison with corresponding experimental results is under way. Then, Eqs. (1-5) are solved for flow through a porous tube with diameter 1.8 cm and length 29 cm. to compute the main flow field as well as the concentrations $c_{k,x}$ and $q_{k,x}$. Results of the latter one are shown in Fig. 1b, where the adsorption capacity of fixed-bed silica gel for acetone versus time are plotted. These curves, also known as the breakthrough curves, are compared with corresponding results in the literature [2] and as it is seen a very good agreement is observed.

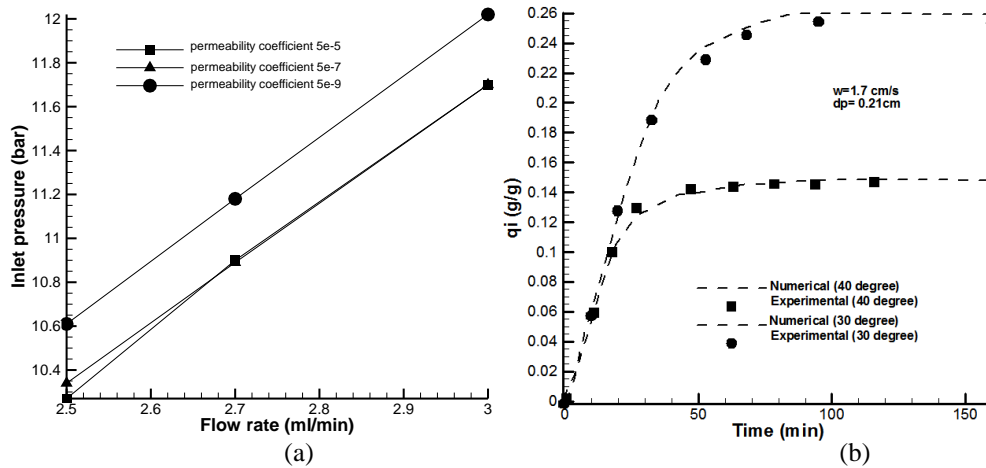


Figure 1: (a) Pressure drop in the In'Air Solution preconcentrator for different adsorbents and flow rates. (b) Experimental and numerical simulation data of acetone adsorption onto fixed-bed silica gel

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References and Citations

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