Prediction of the service life time of cartridges for personal protection: Discussion on the pertinence of 3 models

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The main objective of the study is to determine the optimal model to predict the service life of gas masks in order to avoid contaminating a worker in a polluted atmosphere. Three models dedicated to dynamic adsorption of single Volatile Organic Compounds (VOC) in dry conditions have been compared to fit experimental measurements realized on a column filled with PICA activated carbon in order to predict the breakthrough time of a respirator cartridge. A comparison between the widely used Wheeler Jonas (WJ) model and the Linear Driving Force (LDF) approach is made. Through the LDF approach, we develop two different models: an analytical solution called the Linear Driving Force Constant Pattern model and a numerical model solved with Comsol Multiphysics® software. The experimental isotherm of the VOC is first modeled using Langmuir's equation. The breakthrough curves are calculated using the Wheeler Jonas equation and the analytical solution obtained [1] with the LDF approach. The performance of both models is discussed in terms of comparison with experimental results.

The Wheeler Jonas equation is the model used by several national safety institutes. It gives a prediction of the service life of a respirator cartridge for a single component toxic VOC. The model provides a symmetrical breakthrough curve. Furthermore the predictive calculation of the kinetic parameter k_v can be accurate using published correlations [2]. However this model lacks physical sense which reduces its reliability for multicomponent modeling, since symmetrical breakthrough curves are rare.

Contrary to WJ model, the linear driving force approach is dependent on physical equations based on the adsorption phenomena. Because of the curvature of the isotherm, asymmetrical breakthrough curves adapted to experimental measurements can be represented with the analytical solution in which we make the assumption of a constant pattern behavior of the curve C(x) inside the adsorption column. To better understand this behavior, the VOC adsorption in a 1D isothermal adsorption column packed with porous adsorbent is modeled. The mathematical model obtained is a set of coupled nonlinear partial and ordinary differential equations, based on a mass balance in the system:

$$\varepsilon \frac{\partial C}{\partial t} + \rho \frac{\partial q}{\partial t} + u \frac{\partial C}{\partial x} = 0$$

Where C, q, u, x, ρ and ε are the concentration of VOC in the gas phase, the adsorption capacity, the gas velocity, the length of activated carbon bed, the density of activated carbon and the bed void fraction respectively. Expressions for the equilibrium isotherm equation and the rate of mass transfer equation are also included in the model. We solve the equations using the numerical Comsol Multiphysics® software.

Numerical approaches provide better results owing to better agreement with the curvature of the breakthrough curve. An analytical solution is available for specific conditions. Because of the small size of the bed in the case of a respiratory cartridge, the hypothesis of constant pattern behavior is significant and must be verified. We suggest in this case a numerical study to determine the behavior of the curve.

References:

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