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Vacuum assisted removal of volatile to semi volatile organic contaminants from water using hollow fiber membrane contactors II: A hybrid numerical-analytical modeling approach

Christopher Ian McDermott [a,*], Shamsul Abedin Tarafder [b], Olaf Kolditz [a], Christoph Schüth [c]

[a] *University of Tübingen, Center for Applied Geoscience, Chair of GeoSystems Research, Sigwartstr. 10, D-72076 Tübingen, Germany*
[b] *University of Tübingen, Center for Applied Geoscience, Applied Geology Group, Sigwartstr. 10, D-72076 Tübingen, Germany*
[c] *Technical University of Darmstadt, Institute of Applied Geosciences, Hydrogeology Group, Schnittspahnstr. 9, D-64287 Darmstadt, Germany*

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Abstract

Applying a new hybrid numerical and analytical approach in the finite element simulator RockFlow/GeoSys for hydraulic flow and mass transport, the efficiency of the removal of organic contaminants from water using a microporous polypropylene hollow fiber membrane module (HFM) was accurately modeled for a large range of operating conditions. The modeling results were validated against 177 experimental measurements under a wide range of operating conditions for 12 organic compounds with different diffusion coefficients and a wide variety of Henry's law constants, from Naphthalene at circa 0.017 to 1,1-dichloroethene with circa 1.19. The hybrid numerical analytical approach enables prediction of the removal efficiencies within a few minutes, whereas a pure numerical approach would require several hours to days due to numerical stability controls. The input parameters for the model are defined by the geometry of the HFM and the operating conditions, no empirical formulations are applied. This model allows the investigation of the main factors controlling the removal characteristics, e.g., the dependency on Henry's law coefficient, gas side diffusional resistance, and aqueous diffusion limitation, and also enables the efficient design of further organic removal systems based on the HFM technology.

Keywords: Hollow fiber membrane; Vacuum stripping; Water treatment; Mass transfer resistance; Organic contaminants

1. Introduction

Membrane air stripping (MAS) is a very efficient technology for the removal of volatile organic compounds from liquid streams. The basic principal comprises the separation of the contaminated liquid, e.g. water, from the sweep gas by a porous membrane enabling an independent control of gas and liquid flow rates. Especially hollow fiber membrane (HFM) modules provide a large surface area for mass transfer while having a very small footprint. Additionally a vacuum can be used to enhance stripping efficiencies or to decrease the volume of strip gas that has to be treated.

The driving force for the mass transfer in HFM modules from the water phase to the gas phase is the concentration gradient between the two phases. Theoretically, the mass transfer is limited then by three resistances: (1) diffusion from the bulk aqueous solution through a liquid boundary layer to the membrane surface, (2) diffusion through the air filled pores of the membrane, and (3) diffusion through the gas boundary layer outside the membrane pore into the stripping gas.

As the mass transfer resistance is the reciprocal of the mass transfer coefficient K (m/s), the overall mass transfer resistance ($1/K$) is typically expressed in a series model as follows [1]:

$$\frac{1}{K} = \frac{1}{k_\mathrm{L}} + \frac{1}{k_\mathrm{m} H} + \frac{1}{k_\mathrm{a} H} \tag{1}$$

where k_L is the local liquid phase mass transfer coefficient (m/s), k_m the membrane mass transfer coefficient (m/s) and k_a is the local gas phase mass transfer coefficient (m/s). In the gas phase the Henry's law coefficient H of the stripped compound has to be taken into account. To calculate the removal efficiency of a

* Corresponding author. Tel.: +49 7071 2975041; fax: +49 7071 5059.
E-mail address: chris.mcdermott@uni-tuebingen.de (C.I. McDermott).

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HFM module, a series of empirically based formulations have been to determine k_L, k_m, and k_a [2].

Typically, high strip gas flow to water flow conditions are chosen to operate HFM modules and under these conditions, mass transfer is in general limited by the liquid phase. However, for a set of recently performed laboratory experiments, the empirically based formulations failed to predict removal efficiencies for a large variety of organic compounds under low strip gas flow to water flow conditions with mass transfer limitations on the gas side [3]. Therefore, a process based hybrid model applying both numerical finite element techniques and analytical source term solutions to define the flow and transport problem [4–7] was developed to describe mass transfer in HFM modules. Modeling involved a geometrical simplification of the flow system, the application of the finite element model RockFlow/GeoSys [8] to solve the hydraulic and mass transport equations mathematically and the inclusion of analytical source terms to describe diffusive flux across the membrane. Input parameters for the model are the geometry of the HFM module [3], the diffusion coefficients of the stripped compounds in air and water dependent on temperature and pressure, the tabulated Henry's law coefficients [3], and the operation conditions.

By applying the proposed model, the different effects of the various parameters involved during HFM stripping (e.g., HFM module geometry, aqueous and gaseous flow rates, compounds Henry's law coefficients) can be investigated and the results can be used to predict removal efficiencies and to develop more efficient stripping schemes. The model is verified using the data set for the removal of organic contaminants from water by HFM filtration presented in an accompanying paper [3].

2. Conceptual model

In HFM modules, the water enters the module at one side and flows either over the shell side (outside) or the lumen side (inside) of the hollow fibers to the outlet on the other side. The strip gas is applied on the respective opposite side of the membrane in counterflow. The mass transfer of an organic contaminant from the water phase into the gas stripping phase takes place across the membrane walls forming the hollow fibers. The membrane is porous, does not allow water to move across it, but does allow the diffusion of organic compounds in the gaseous phase. To model these processes, the overall mass transfer is broken down into the different steps, i.e., advective flow as a result of the pressure gradient and mass transport due to flow and diffusive gradients. Fig. 1 illustrates the path of a typical organic molecule through a HFM module, and the processes taken into account during modeling. After entering the HFM system (a), the molecule is transported some distance inside the solute tube as a result of advective and diffusive transport. At some point the molecule reaches the edge of the solute tube, and the interface between the water in the solute tube with the gas in the membrane. The organic molecule then leaves the water phase, and enters the pore space of the membrane (b). The relationship between the concentration of the organic molecules in the water and in the gas is governed at the boundary by Henry's law. Once in the pore space of the membrane, concentration driven diffusion occurs across the membrane following Fick's first law of diffusion (c). After leaving the membrane the molecule is again transported by advective and diffusive transport out of the system in the gas phase in counterflow (d).

Fig. 2 illustrates the geometry of the HFM module. The strip gas flow tubes (GFT) are assumed to be almost perfectly hexagonally packed. The spaces between the GFT form the solute flow tubes (SFT), carrying the dissolved organic contaminant in counterflow. In HFM modules, flow in the SFT is conventionally along the length of the GFT (Fig. 2, left). For the model development, a Liqui-Cel© 2.5 in. × 8 in. extra flow hollow fiber module was taken as a reference for a HFM module geometry. The main characteristics of the module are summarized in an accompanying paper [3]. In Liqui-Cel© extra flow modules with a central baffle, flow also has a radial component transverse to the GFT

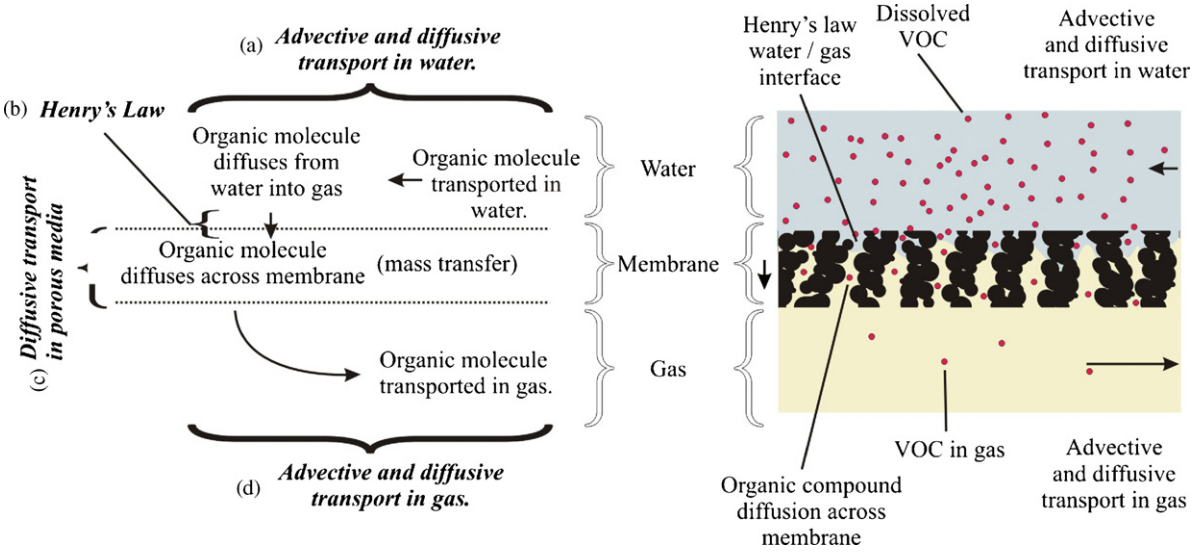

Fig. 1. Conceptual model of the transport of the organic molecule (VOC) in the HFM module.