

# A simulation model for transient response of a gas separation module using a hollow fiber membrane

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## ARTICLE INFO

### Article history:

Available online 22 March 2011

### Keywords:

Gas separation  
Tritium  
Membrane  
Polyimide  
Simulation  
Transient response

## ABSTRACT

A simulation model has been developed for transient response of a gas separation module using a hollow fiber membrane for the removal of tritium from the atmosphere of the confinement space. The mass transfer process such as sorption and desorption of gases at the surface of the dense layer and the porous support layer, diffusive transfer in the both layers are treated in the model. Sorption isotherm, mass transfer rate and permeance are estimated through step-wise transient response experiments. The present model represents well not only separation factors and recovery ratio at the steady state but also responses to the multi-step wise change in the sweep gas rate.

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## 1. Introduction

For future fusion reactors, where a huge amount of tritium will be handled, it is necessary to establish the technology for the removal of tritium from the atmosphere of the confinement space. A conventional method is to oxidize tritium by a catalytic reactor and to remove tritium by a molecular sieve bed [1]. Some dozens of molecular sieve beds and a complex switching control are required for continuous processing with a large throughput because molecular sieve beds need desorption treatment before the breakthrough time. In addition, desorption process consumes enormous energy. These problems will be fatal defects for a future fusion reactor which needs a quite large confinement space.

One of the alternatives is a gas separation system using a hollow fiber membrane. The advantages of the membrane system are compact scale, low energy consumption, and high reliability for operation without a complex switching control. A number of studies have been presented in order to apply gas separation membranes to tritium removal and confinement systems of fusion reactors [2–5]. Separation factor and recovery ratio of water vapor from the air at steady state were mainly reported. Although it is very important to investigate transient responses of such membrane systems in practical use, the simulation method has not been established yet. The concentration of water vapor at the outlet and the permeated flow rate of the membrane module are very slow

to respond against the change in humidity at the inlet or any other operational conditions of the module. These slow responses cannot be simulated by the conventional model which does not take into account transient phenomena such as the change of liquid-holdup in the membrane material.

The purpose of the present study is to develop a mass transfer model which enables us to simulate transient response of a membrane module.

## 2. Simulation procedure

### 2.1. Simulation model

A schematic illustration of mass transfer through the membrane is shown in Fig. 1. The hollow-filament type membrane consists of two layers: a thin dense layer on the inside and a thick porous support layer on the outside. The competitive sorption of the gas molecules at the surface of dense layer, the diffusion in the dense layer, desorption at the interface between dense and porous layers, the Knudsen's diffusion in the porous layer and the sorption–desorption equilibrium are considered in the present model with time variation.

The molar fluxes of penetrants through dense and porous layers can be expressed as

$$N_d = D_d \frac{dC}{dl} \frac{D_d S}{L_d} (p_h - p_l) = \frac{P_d}{L_d} (p_h - p_l), \quad (1)$$

$$N_p = D_p \frac{dC}{dl} = \frac{D_p}{RT} \frac{dp}{dl}. \quad (2)$$

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## Nomenclature

$a_{sorp}$	slope of the sorption isotherm [mol/m <sup>3</sup> ]
$a_p$	coefficient in Eq. (5) [mol/(m <sup>2</sup> s Pa)]
$C$	mole concentration [mol/m <sup>3</sup> ]
$D$	diffusion coefficient [m <sup>2</sup> /s]
$k_{sorp}$	rate constant of the sorption [s <sup>-1</sup> ]
$l$	position in the permeate direction [m]
$L$	thickness of the membrane [m]
$N$	permeation flux [mol/(m <sup>2</sup> s)]
$p$	partial pressure [Pa]
$P$	total pressure [Pa]
$P$	permeance [mol/(m <sup>2</sup> s Pa)]
$q$	flow rate [mol/s]
$r$	sorption rate of water vapor [mol/s]
$R$	gas constant [J/(K mol)]
$s$	section of the calculation cell [m <sup>2</sup> ]
$S$	solubility coefficient [mol/(m <sup>3</sup> Pa)]
$t$	time [s]
$T$	temperature [K]
$V$	volume of the calculation cell [m <sup>3</sup> ]
$x$	mole fraction of water vapor

## Greek letters

$\varepsilon$	void ratio in the porous layer
$\eta$	recovery ratio
$\theta$	cut ratio

## Subscripts

0	value of air without water vapor
d	dense layer
F	feed stream
h	high pressure side
j	number of the calculation cell along the axis
l	low pressure side
p	porous layer
P	permeate stream
R	retentate stream
S	sweep stream
s	saturated state

A constant pressure gradient is assumed in the dense layer because the layer is very thin enough. The diffusion coefficient  $D_p$  is estimated as Knudsen's diffusion coefficient in Eq. (2).

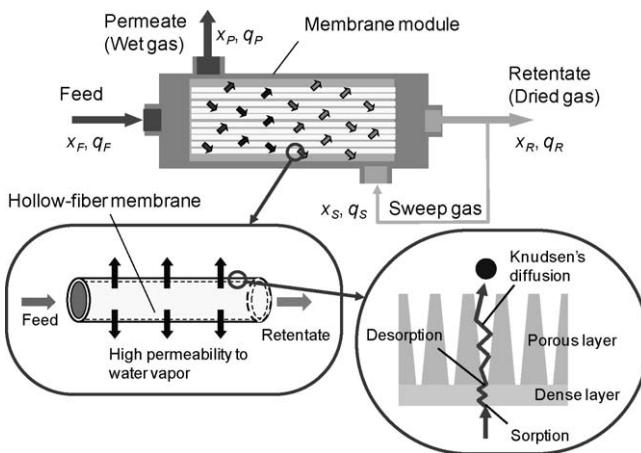


Fig. 1. Water vapor separation with the hollow fiber membrane module.

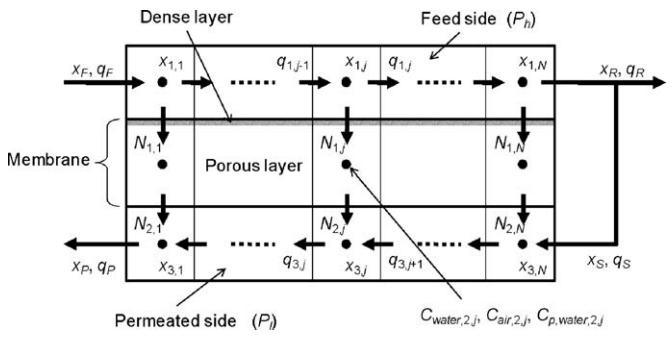


Fig. 2. Layout of parameters for numerical calculation.

### 2.1.1. Sorption of water vapor in the polyimide film

Because of water–polymer interaction polyimide membranes absorb moisture easily at high activities of water vapor. This adsorption capacity of water vapor is not negligible for transient response simulation of water-vapor separation membrane. Typical sorption isotherms of water vapor in polyimide films are summarized in the literature [6]. The sorption capacity of water vapor at the equilibrium increases almost linear with the activity of water vapor [6]. In the present study, water vapor content in the unit volume of the membrane at the equilibrium is assumed by the following equation,

$$\bar{C}_{p,water} = a_{sorp} \left( \frac{p_{water}}{p_s} \right) \quad (3)$$

Sorption rate of water vapor is, then,

$$r = k_{sorp} (\bar{C}_{p,water} - C_{p,water}). \quad (4)$$

### 2.1.2. Competitive sorption between water vapor and air in the dense layer of polyimide film

It is known that a very low partial pressure of a condensable species such as water vapor in the feed stream to a membrane module can significantly reduce the permeability of the other constituent relative to its permeability as a pure component [7]. One of the most widely known approaches is “dual-mode sorption” model, though there is no indisputable explanation applicable to varied conditions [8–11]. In the present study, the permeability coefficient of air is assumed by the following equation at relatively low water vapor activity.

$$P_{d,air} = P_{d,air,0} - a_p \left( \frac{p_{water}}{p_s} \right) \quad (5)$$

### 2.2. Calculation procedure

The assumptions used in the model are (i) the feed gas is a binary mixture of water vapor and air, (ii) the pressure drop along the membrane is negligible and (iii) the system is adiabatic and the temperature of the gas mixture is constant. To simulate the profile of water vapor concentration the module is divided into small sections along the axis as shown in Fig. 2 and the local mass balances are applied.

$$V_1 C_1 \frac{dx_{1,j}}{dt} = q_{1,j-1} x_{1,j-1} - q_{1,j} x_{1,j} - N_{water,1,j} s_1 \quad (6)$$

$$V_1 C_1 \frac{d(1-x_{1,j})}{dt} = q_{1,j-1} (1-x_{1,j-1}) - q_{1,j} (1-x_{1,j}) - N_{air,1,j} s_1 \quad (7)$$

$$V_2 \varepsilon \frac{dC_{water,2,j}}{dt} = N_{water,1,j} s_1 - N_{water,2,j} s_2 - r \quad (8)$$

$$V_2 \varepsilon \frac{dC_{air,2,j}}{dt} = N_{air,1,j} s_1 - N_{air,2,j} s_2 \quad (9)$$

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