CFD analysis of flow in tubular zeolite membrane modules

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Introduction

Flow analysis in membrane modules is essential for establishing the scale-up rules of membrane module, leading to optimization of module structure and operation conditions. Although there have been many studies on the development of membranes, flow inside a membrane module at high temperature and pressure has rarely been studied. In this study, the flow in a single element zeolite membrane module was numerically simulated using a thermal flow analysis software, RFLOW, as for vapor permeation through a zeolite membrane. A flow analytical model taking into account the effects of both molecular and turbulent diffusion of flow was developed.

Methods

The numerical analysis using the k-epsilon model was conducted with Navier-Stokes equations for incompressible fluid, equations of continuity, and convection-diffusion equations. **Figure 1** shows a schematic illustration of single element membrane module. The mesh size in the single element membrane module is given in **Figure 1**. For modeling of membrane permeation, the permeation flux, *S*, is given by:

$$S = -K(A/V)c \tag{1}$$

where *K* is the membrane permeability coefficient, *A*, the membrane surface area of cell element, *V*, the volume of cell element, and *c*, the volume fraction of a permeable component. **Eq. 1** is used only for the cells adjoining membrane surface.

Assuming that *K* was an experimental constant which depends on only membrane properties, the value of *K* was determined so as to agree the calculated results with the experimental ones under specific conditions where permeation flux was independent of the flow rate of feed. The validity of our model was also investigated by comparing with the experimental results of vapor permeation separation through a zeolite membrane. In this experiment, a mixture of ethanol and water was fed and water was permeated selectively.

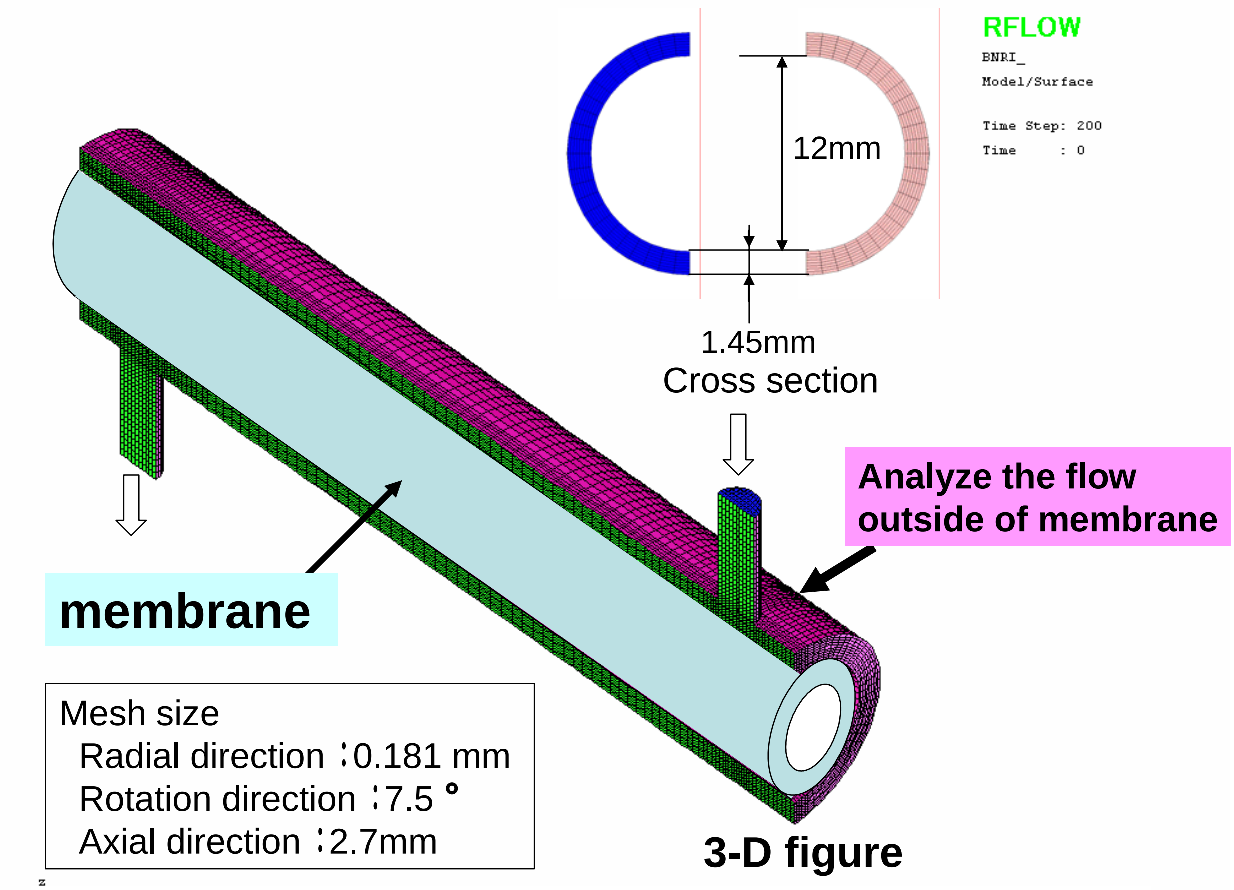

Figure 1 Schematic illustration of single element membrane module.

Results and Discussion

In order to elucidate the contribution of turbulent and molecular diffusion to the flow in the module and the fluxes of ethanol and water, the numerical analyses were carried out by taking into accounts the effects of both turbulent and molecular diffusion and only the effect of turbulent diffusion. **Table 1** gives insights on the effects of turbulent and molecular diffusion on the water concentration of the outlet by changing the feed rate. The value of *K* used for calculation was determined using the experimental value in Case-1.

The magnitude of the effects of turbulent and molecular diffusion would depend on the flux, i.e. the Re number of the flow. When the Re number of the flow exceeded 5000, the fluxes were large enough for the effect of turbulent diffusion on the flow to given the flow pattern in the module: turbulent diffusion was more significant than molecular diffusion at these high Re numbers. In these cases, i.e. the turbulent diffusion-controlled region, the values of the water concentrations at the outlet were hardly affected by molecular diffusion.

On the other hand, molecular diffusion became significant with decreasing Re number, explaining the experimental results well. The discrepancy between calculated and experimental data became smaller when both turbulent and molecular diffusion were taken into account. These results obtained in this study illustrated that this analysis model can be applied for the flow in the wide range of Re number.

Table 1 Experimental and calculated results.

<table>
<tr><th>Case</th><th>Feed rate [kg/hr]</th><th>Re number [-]</th><th>Volume fraction of water in feed [-]</th><th>Experimental results of the water concentration of the outlet [-]</th><th>Calculated results of the water concentration of the outlet [-] (by taking into accounts only the effect of turbulent diffusion)</th><th>Calculated results of the water concentration of the outlet [-] (by taking into accounts the effects of both turbulent and molecular diffusion)</th></tr>
<tr><td>Case-1</td><td>15</td><td>16700</td><td rowspan="4">0.221</td><td>0.176</td><td>0.177</td><td>0.177</td></tr>
<tr><td>Case-2</td><td>10</td><td>11100</td><td>0.162</td><td>0.159</td><td>0.158</td></tr>
<tr><td>Case-3</td><td>5</td><td>5560</td><td>0.137</td><td>0.118</td><td>0.113</td></tr>
<tr><td>Case-4</td><td>1</td><td>1110</td><td>0.053</td><td>0.025</td><td>0.058</td></tr>
</table>

Conclusions

A flow analytical model which can be applied for the flow in the wide range of Re number was developed by taking into account the effects of both molecular and turbulent diffusion of flow.

Acknowledgement

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Symbols

S: permeation flux [$m^3/(m^3 \cdot s)$]
K: membrane permeability coefficient [m/s]
A: membrane surface area of cell element [m^2]
V: volume of cell element [m^3]
c: volume fraction of permeation component [-]