# Modelling of Pervaporative Dehydration of Isopropyl-alcohol on Hydrophilic Membranes

**L. Takács and G. Vatai***
Corvinus University of Budapest, Faculty of Food Science,
Department of Food Engineering, H-1118 Budapest Ménesi út 44

Note
Received: May 18, 2009
Accepted: September 17, 2010

The main goal of this article is mathematical modeling according to Oliveira's mass transfer and linear resistance model,[1] gained with regard CMC-CA-01, CMC-CE-01 and CMC-CE-02 membranes in the isopropyl-alcohol pervaporative dehydration system of ATRA.[2,3] According to Oliveira[1] the flow rate of the certain component "n (water)" can be expressed by the following equation:

$$F_n = k_{OV,n} \cdot A \cdot (p_{L,n} - p_{G,n}) \tag{1}$$

$F_n$ – water flow rate, mol $s^{-1}$

$k_{OV,n}$ – overall water mass transfer coefficient in case of a difference in partial vapour pressure, mol $m^{-2}$ $Pa^{-1}$ $s^{-1}$

$A$ – area of membrane, $m^2$

$p_{L,n}$ – partial vapour pressure of water at the liquid side, Pa

$p_{G,n}$ – partial vapour pressure of water at the vapor side, Pa.

In line with the model, the reciprocal value of the overall mass transfer coefficient is equal to the reciprocal value of the total amount of mass transfer coefficients in the case of the applied membrane and the applied isopropyl alcohol-water mixture's liquid side (eq. 2).

$$\frac{1}{k_{OV,n}} = \frac{1}{k_{M,n}} + \frac{1}{k_{L,n}} \tag{2}$$

$k_{L,n}$ – water mass transfer coefficient in case of a difference in partial vapour pressure on the liquid side, mol $m^{-2}$ $Pa^{-1}$ $s^{-1}$

$k_{M,n}$ – water mass transfer coefficient of membrane in case of a difference in partial vapour pressure, mol $m^{-2}$ $Pa^{-1}$ $s^{-1}$.

According to average values, the mass transfer coefficients on the liquid side have a lower order of magnitude than in the case of membrane and the overall mass transfer data at every temperature (Fig. 1). Fig. 1 shows that, considering the coefficients of transport over the entire pervaporation period, the liquid side mass transfer factor is greater by one order of magnitude than the other two transfer characteristics. Therefore, the conductance of the liquid side boundary layer is negligible.

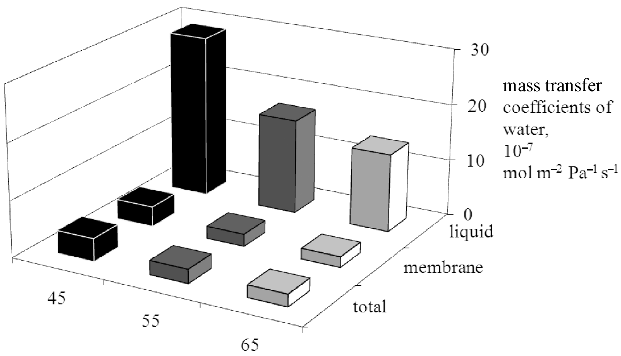



Fig. 1 – *Transport coefficient of the membrane throughout the whole pervaporation process, and the liquid side transport coefficient. Further, the factor of the entire mass transfer at various temperatures with a CMC-CE-02 membrane in isopropanol dehydration.*

Based on the linear resistance model, it can be seen that the mass transfer coefficient of the membrane is equal to the overall mass transfer coefficient. Therefore, in every case the mass transfer is determined by the membrane and its structure.

These coefficients have similar running in case the values depend on the driving force, too (Fig. 2). This means that the resistance on the liquid side in

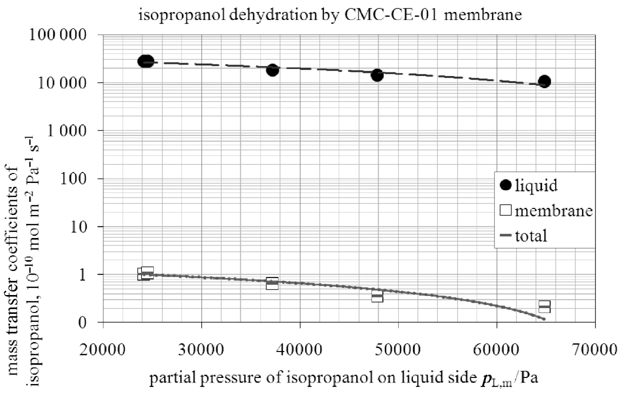



Fig. 2 – *Mass transport coefficients of isopropanol with a CMC-CE-01 membrane, at 45 °C*

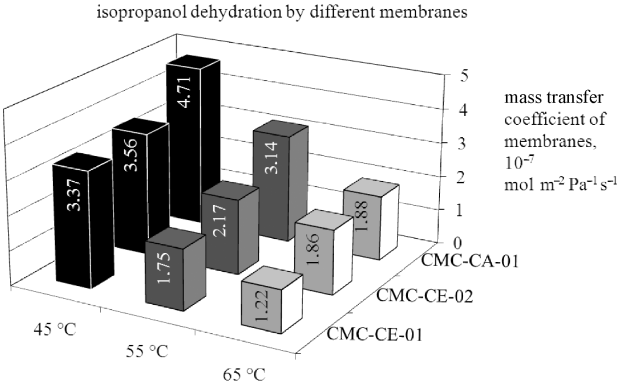
*Corresponding author: gyula.vatai@uni-corvinus.hu
Tel: +36-1-482-6232, Fax: +36-1-482-6323

case of the partial vapor pressure driving force can be neglected. This way, the resistance of the overall membrane process and the resistance of the membrane are technically the same.

Because of the very high vacuum, the resistance on the vapor side can be ignored.[4] According to the model, the running of the partial flow rates corresponds to a zero point fixed linear function and depends on the feed concentration. These characteristic curves of the flow rates can also be found in scientific literature.[5,6] The resistance of the liquid side boundary layer makes up only an infinitesimal part of the total resistance of the pervaporation process. All this is accountable to favourable flow conditions, which in turn cause advantageous conditions for mass transfer. This on the one hand helps transport by way of the well-known physical and hydrodynamic properties, and on the other hand causes difficulties in creating balanced distribution between the boundary layer and the membrane. Thus, dissolving is expedited and the degree of concentration polarisation, which increases liquid-side resistance, is lowered.

The "dissolve-diffuse" model is understood to mean that the adsorbing/dissolving molecules disperse between the membrane and the liquid-side boundary layers. This is how equilibrium is created. With the continuation of pervaporation, the molecules concentrate in the boundary layer and the liquid diffuses towards the solid phase. The driving force of diffusion reduces the dissolving action in the membrane. Therefore, it is important that the membrane structure has as good an adsorption capacity as possible, in addition to liquid phase conductance.

Fig. 3 shows the transport properties of the membranes in the study, and from this it is clear that isopropyl dehydration was best with the CMC-CA-01 membrane. The best indicators were at 45 °C, a temperature which suits the membrane structure very well. CMC-CE-01 and CMC-CE-02 membranes at 45 and 55 °C yield moderate transport. At 65 °C, CMC-CE-02 approaches the performance of CMC-CA-01.




F i g . 3 – *Mass transfer coefficient of membranes and their partial pressure driving force at various temperatures, isopropanol pervaporative dehydration*

The permeate flow rate can be determined by the total amount of the water and isopropyl-alcohol partial flows (eq. 3). This connection shows a very good fit between the measured permeate flow rate and the model values (Fig. 4).

$$F = F_n + F_m = A \cdot (k_{M,n} \cdot p_{L,n} + k_{M,m} \cdot p_{L,m}) \quad (3)$$

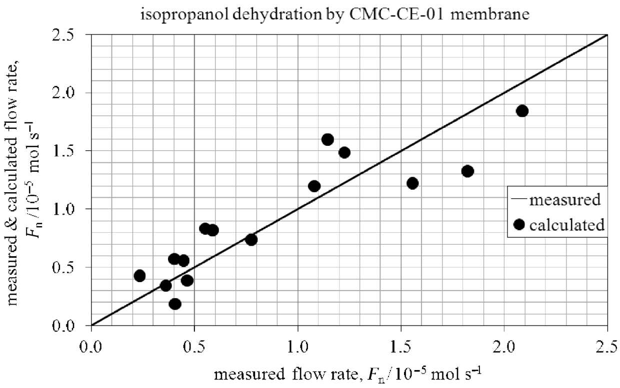
$F$ – permeate flow rate, mol s$^{-1}$

$F_n$ – water flow rate, mol s$^{-1}$

$F_m$ – isopropyl-alcohol flow rate, mol s$^{-1}$

$k_{M,m}$ – isopropyl-alcohol mass transfer coefficient of the membrane in case of difference in partial vapour pressure, mol m$^{-2}$ Pa$^{-1}$ s$^{-1}$

$p_{L,m}$ – partial vapour pressure of isopropyl-alcohol at the liquid side, Pa




F i g . 4 – *Permeate flow rate with CMC-CE-01 membrane isopropanol pervaporative dehydration*

The selectivity of the membrane can be given by the quotient of the related component partial flow rate and the permeate flow rate, thereby the mass transfer model can be written, too.[4] The final equation reflects that the running of the selectivity corresponds to a hyperbolic function depending on the feed mass fraction (Fig. 5).

$$s_n = \frac{1}{(1 - w_{F,n}) \cdot (\Psi - 1) + 1}$$

$$Y = \frac{k_{M,m} \cdot \gamma_m \cdot p_m \cdot \rho_{L,m} \cdot M_n}{k_{M,n} \cdot \gamma_n \cdot p_n \cdot \rho_{L,n} \cdot M_m} \quad (4)$$

$s_n$ – water selectivity

$w_{F,n}$ – water mass fraction, kg kg$^{-1}$

$\Psi$ – constant, –

$\gamma_n$ – water activity coefficient calculated by the UNIQUAC method[7]

$\gamma_m$ – isopropyl-alcohol activity coefficient calculated by the UNIQUAC method[7]

$p_n$ – saturated pressure of water at a given temperature, Pa

$p_m$ – saturated pressure of isopropyl-alcohol at a given temperature, Pa

$\rho_{L,n}$ – liquid density of water at a given temperature, kg m$^{-3}$

$\rho_{L,m}$ – liquid density of isopropyl-alcohol at a given temperature, kg m$^{-3}$

$M_n$ – water molar mass, kg kmol$^{-1}$

$M_m$ – isopropyl-alcohol molar mass, kg kmol$^{-1}$

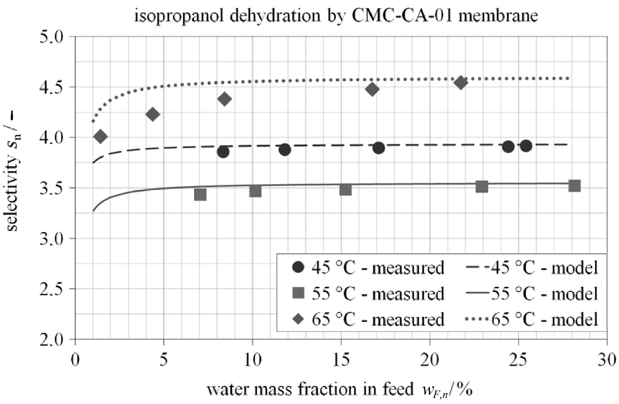



Fig. 5 – *Water selectivity as a factor of total feed solution, at various temperatures using CMC-CA-01 membrane during isopropanol dehydration*

Water selectivity varies with feed solution mass fraction as a hyperbola and reaches a maximum at an infinitely large concentration.

For isopropyl dehydration, whereas the CMC-CE-01 and CMC-CE-02 membranes have the best selectivity at 55 °C, the CMC-CA-01 membrane does well at 65 °C, but every membrane's selectivity is the worst at 45 °C.

Among the three membranes examined, the best one for component transport (and isopropanol pervaporative dehydration) was the CMC-CA-01 membrane. From the point of view of the membranes studied, and their mass transfer characteristics, the liquid side resistance is not significant during pervaporation. Pervaporative resistant is influenced by the material of the membrane and how it is constructed. The use of definitive membrane characteristic of the linear resistance model guarantees a base for industrial application and technological design.[8]

Use of the linear resistance model's definitive membrane characteristic guarantees a base for industrial application and technological design. Evaluation of pervaporative indicators are the way of the future for industry and for calibrating process parameters. In addition, the process lends itself to economic examination and provides data for simulation with hybrid technology, using computers.[9–13]

## References

1. *Oliveira, T., Scarpello, T., Livingston, A.,* Journal of Membrane Science **195** (2002) 75.
2. *Atra, R., Vatai, Gy., Békássy-Molnár, E.,* Chemical Engineering and Processing **38** (1999) 149.
3. *Atra, R.,* Application of membrane separation processes in dairy and beverage industry – in Hungarian (Membránszeparációs műveletek tej- és szeszipari alkalmazásai), PhD. Dissertation, Szent Istvan University, Budapest, Hungary, 2000.
4. *Huang, R. Y. M.,* Pervaporation membrane separation processes. Amsterdam-Oxford-New York-Tokyo, Elsevier, 1999.
5. *Ji, W., Sikdar, S. K., Hwang, S.-T.,* J. Membr. Sci. **128** (1997) 195.
6. *Jonquieres, A., Clement, R., Lochon, P., N'eel, J., Dresch, M., Chretien, B.,* J. Membr. Sci. **206** (2002) 87.
7. *Reid, R. C., Prausnitz, J. M., Poling, B. E.,* The Properties of Gases and Liquids, Fourth Edition McGraw-Hill Book Company, 1985, p. 247.
8. *Urtiaga, A. M., Gorri, E. D., Ortiz, I.,* Separation and Purification Technology **49** (2006) 245.
9. *Sommer, S., Melin, T.,* Ind. Eng. Chem. Res. **43** (2004) 5248.
10. *Kreis, P., Gorak, A.,* Chemical Engineering Research and Design **84** (A7) (2006) 595.
11. *Koczka, K., Mizsey, P., Fonyo, Z. S.,* CEJC **5** (4) (2007) 1124.
12. *Lovász, A., Mizsey, P., Fonyo, Z. S.,* Chem. Eng. J. **133** (2007) 219.
13. V*erhoef, A., Degreve, J., Huybrechts, B., Van Veen, H., Pex, P., Van der Bruggen, B.,* Computers and Chemical Engineering **32** (2008) 1135.