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

\[ F_n = k_{OV,n} \cdot A \cdot \left( p_{L,n} - p_{G,n} \right) \]  

(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).

\[ \frac{1}{k_{OV,n}} = \frac{1}{k_{L,n}} + \frac{1}{k_{M,n}} \]  

(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.

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...
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 mem-
brane are technically the same.

Because of the very high vacuum, the resis-
tance on the vapor side can be ignored. 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 char-
acteristic curves of the flow rates can also be found
in scientific literature. The resistance of the liquid
side boundary layer makes up only an infinitesimal
part of the total resistance of the pervaporation pro-
cess. All this is accountable to favourable flow condi-
tions, which in turn cause advantageous condi-
tions 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 con-
centration polarisation, which increases liquid-side
resistance, is lowered.

The “dissolve-diffuse” model is understood to
mean that the adsorbing/dissolving molecules dis-
perse between the membrane and the liquid-side
boundary layers. This is how equilibrium is created.
With the continuation of pervaporation, the mole-
cules concentrate in the boundary layer and the liq-
uid 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 ca-
pacity as possible, in addition to liquid phase con-
ductance.

Fig. 3 shows the transport properties of the mem-
branes in the study, and from this it is clear that iso-
propyl 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 mem-

branes at 45 and 55 °C yield moderate transport. At
65 °C, CMC-CE-02 approaches the performance of
CMC-CA-01.

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).

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

$$F - \text{permeate flow rate, mol s}^{-1}$$
$$F_n - \text{water flow rate, mol s}^{-1}$$
$$F_m - \text{isopropyl-alcohol flow rate, mol s}^{-1}$$
$$k_{M,m} - \text{isopropyl-alcohol mass transfer coef}-
ficient of the membrane in case of dif-
ference in partial vapour pressure, mol
m^{-2} Pa^{-1} s^{-1}$$
$$P_{L,m} - \text{partial vapour pressure of isopropyl-al-
cohol at the liquid side, Pa}$$

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. The final
equation reflects that the running of the selectivity
corresponds to a hyperbolic function depending on
the feed mass fraction (Fig. 5).

$$s_n = \frac{1}{(1 - w_{F,n} \cdot \Psi) \cdot \Psi - 1} + 1$$ (4)

$$s_n - \text{water selectivity}$$
$$w_{F,n} - \text{water mass fraction, kg kg}^{-1}$$
$$\Psi - \text{constant,}$$
$$\gamma_n - \text{water activity coefficient calculated by the UNIQUAC method}$$
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.

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.

References
