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A Comparison of Models to Describe the Maximal Retention of Organic Molecules in Nanofiltration

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ABSTRACT

Nanofiltration is used in a growing number of applications for the treatment of drinking water, wastewater, and process water. Trial-and-error is generally used to test the applicability of nanofiltration and to select the membranes. In particular for organic molecules, a model that describes retention as a function of molecular parameters and membrane characteristics has not yet been established. In this paper four models for maximal retention, represented by the reflection coefficient, were compared: the steric hindrance pore model, the model of Zeman and Wales, the log-normal model, and an adapted version of the log-normal model. The calculated results were compared to reflection coefficients determined experimentally for a broad range of relatively small organic molecules. Each of the models yielded acceptable results, although the steric hindrance pore model and the model of Zeman and Wales are based on a somewhat idealized view of membrane structure. The log-normal model calculates reflection coefficients from a distribution of pore sizes. The adapted log-normal model also includes hydrodynamic lag, caused by sterical hindrance in the membrane pores. It was found that this effect is very small. The log-normal model appeared to be most useful to predict reflection coefficients in practical applications.

Key Words. Nanofiltration; Reflection coefficient; Modeling

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INTRODUCTION

Nanofiltration is a pressure-driven membrane process, intermediate between reverse osmosis and ultrafiltration. The number of applications for nanofiltration is still growing due to the availability of new membranes and improved insight into membrane structure and the interactions between the membrane and molecules in solution. One of the main advantages of nanofiltration is the combined removal of (charged) inorganic and organic compounds (1, 2). A well-known example of this is the combined removal of hardness and pesticides from groundwater (3, 4). Furthermore, the energy requirements are much lower than with reverse osmosis because the transmembrane pressures applied in nanofiltration are significantly lower than those in reverse osmosis.

For a given separation, trial-and-error is generally used to learn whether nanofiltration can be applied and for the selection of the nanofiltration membranes. A model that describes the retention of a given compound restricts the number of experiments needed for an industrial application.

In this paper, different models for the retention of (uncharged) organic molecules are discussed: the steric hindrance pore model, the model of Zeman and Wales, and the log-normal model. The applicability of these models to describe the maximal retention of organic molecules is studied. Moreover, a new model in which elements from the model of Zeman and Wales are combined with elements from the log-normal model is presented.

The calculated retention corresponds to the retention at an infinite pressure, which is the maximal retention that can be obtained. The retention is slightly lower at realistic pressures due to the contribution of diffusion to the transport process, but the pressure dependence of retention is not included in the models.

THEORETICAL BACKGROUND

An interpretation of the transport mechanisms through a nanofiltration membrane is necessary for the description of the retention of unchanged molecules. Transport of uncharged molecules is a combination of diffusion and convection. This is expressed in the transport equations of Spiegler and Kedem (5) for water flux and for the flux of a dissolved component:

$$J_v = L_p(\Delta P - \sigma\Delta\pi) \tag{1}$$

$$J_s = -P\Delta x\frac{dc}{dx} \pm (1 - \sigma)J_v c \tag{2}$$

Diffusion is represented by the first term in Eq. (2); the second term represents the contribution of convection to the transport of uncharged molecules.

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The retention of a given molecule can be calculated from Eqs. (1) and (2) as

$$R = \frac{\sigma(1 - F)}{1 - \sigma F} \tag{3}$$

with

$$F = \exp\left(-\frac{1 - \sigma}{P} J_v\right) \tag{4}$$

The permeability P is a measure of the transport of a molecule by diffusion. The reflection coefficient σ of a given component is the maximal possible retention for that component. From Eqs. (3) and (4), it can be seen that this corresponds with retention at an infinite water flux. A model for σ would provide the necessary information about retention at relatively high water fluxes and, correspondingly, at high pressures. The resulting curve for the reflection coefficient as a function of the molecular diameter (retention curve) can be used to estimate the maximal retention that can be obtained with a given membrane.

In the *steric hindrance pore model* (SHP model) (6–8) the reflection coefficient is calculated from the pore size of the membrane and the diameter of the molecule. It is assumed that all pores have the same size. Therefore, the uniform pore size should not be interpreted as a real value for the diameter of the pores. The calculated pore size corresponds with the pore size of an imaginary membrane with uniform pores, for which the retention of uncharged molecules is equal to retention with the real membrane. In reality, not every pore has the same cylindrical diameter; the model is an approximation of the membrane's structure.

The membrane is thus represented as a bundle of cylindrical pores through which molecules in solution can permeate. During the transport these molecules encounter a certain amount of sterical hindrance and interactions with the pore wall. A molecule which is smaller than the diameter of the membrane is partially retained through these effects. A molecule with the same size as the pore diameter is completely retained.

The reflection coefficient can thus be calculated as

$$\sigma = 1 - H_F S_F \tag{5}$$

with

$$H_F = 1 + (16/9)\eta^2 \tag{6}$$

$$S_F = (1 - \eta)^2[2 - (1 - \eta)^2] \tag{7}$$

$$\eta = d_s/d_p \tag{8}$$

H_F is a "wall-correction parameter" that represents the effect of the pore wall, S_F is a parameter that represents sterical hindrance during transport through

the pores. The diameter of a molecule and the diameter of a pore are symbolized by d_s and d_p, respectively.

The *model of Zeman and Wales* (9) also uses the Ferry formula (10); it describes the retention of a sphere through a capillary (reflection coefficient) as

$$\sigma = 1 - 2(1 - \eta)^2 + (1 - \eta)^4 \tag{9}$$

which can be written as

$$\sigma = 1 - (\eta(\eta - 2))^2 \tag{10}$$

The pores are assumed to have a uniform cylindrical diameter. Furthermore, a parabolic velocity dependence in the pore is assumed.

Zeman and Wales introduced a factor $v_{\text{molecule}}/v_{\text{water}} = K_2/K_1$ (K_2 and K_1 are constants) in this equation to represent steric hindrance during convectional transport. This sterical hindrance gives rise to a hydrodynamic lag in the membrane pores. Based on experimental data, they assumed that the K_2/K_1 factor can be expressed as $\exp(-\alpha\eta^2)$, where α is a dimensionless constant. Equation (10) then becomes

$$\sigma = 1 - [(\eta(\eta - 2))^2] \exp(-\alpha\eta^2) \tag{11}$$

In the *log-normal model* the pore size is assumed to not be constant, in contrast to the SHP model and the model of Zeman and Wales. A log-normal distribution is assumed for the pore size. No steric hindrance in the pores or hydrodynamic lag is taken into account, but it is assumed that a molecule permeates through every pore that is larger than the diameter of the molecule. Moreover, the contribution of diffusion to transport through the membrane is considered to be negligible. Therefore, the (maximal) retention can be expressed by

$$\sigma(r^*) = \int_0^{r^*} \frac{1}{S_p\sqrt{2\Pi}} \frac{1}{r} \exp\left(-\frac{[\ln(r) - \ln(\bar{r})]^2}{2S_p^2}\right) dr \tag{12}$$

This equation involves two variables, S_p and $\bar{r}$, where S_p is the standard deviation of the distribution. This standard deviation is a measure for the distribution of the pore sizes. As the retention curve corresponds to an integrated log-normal distribution, a small "S_p" represents a large slope of the retention curve; a large "S_p" represents a small slope, $\bar{r}$ is a mean pore size; namely, the size of molecule that is 50% retained.

Finally, the log-normal model was optimized by taking hydrodynamic lag in the pores into account. For this purpose the velocity ratio $v_{\text{molecule}}/v_{\text{water}}$, given as $v_{\text{molecule}}/v_{\text{water}} = \exp(-\alpha\eta^2)$ by the model of Zeman and Wales, was introduced into the log-normal model.

For this new model it is assumed that a molecule is completely retained by a pore smaller than the molecular diameter. If the pore is larger than the

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molecular diameter, the molecule is partly retained to the extent that its velocity in the pores is lower than the water velocity. The reflection coefficient can thus be written as the sum of the fraction of the pores that are smaller than the molecular diameter and a term representing the fraction of molecules that are retained by pores that are larger than the molecular diameter.

The equation for the reflection coefficient then becomes

$$\sigma(r^*) = \int_0^{r^*} \frac{1}{S_p\sqrt{2\Pi}} \frac{1}{r} \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) dr + \int_{r^*}^{\infty} \left(1 - \exp\left(-\alpha\left(\frac{r^*}{r}\right)^2\right)\right) \frac{1}{S_p\sqrt{2\Pi}} \frac{1}{r} \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) dr \quad (13)$$

$$= 1 - \int_{r^*}^{\infty} \exp\left(-\alpha\left(\frac{r^*}{r}\right)^2\right) \frac{1}{S_p\sqrt{2\Pi}} \frac{1}{r} \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) dr \quad (14)$$

The two-parameter log-normal model is thus extended to a three-parameter model for the reflection coefficient (α $\bar{r}$, and S_p).

EXPERIMENTAL

Three nanofiltration membrane types were selected for the modeling: NF70 (Dow/FilmTec), UTC-20 (Toray), and NTR 7450 (Nitto-Denko). The characteristics of these membranes are summarized in Table 1.

Before modeling, the different factors that have an influence on the retention of an organic molecule had to be determined (11). Molecular size is the most important parameter that determines the retention of an uncharged organic molecule by nanofiltration. Nanofiltration membranes work as sieves, retaining molecules that are larger than the membrane pores. The dipole moment plays a secondary role (11) due to interactions between the dipole and the charged membrane. The molecule is directed toward the membrane charge in such a way, that the side of the dipole with the opposite charge is closer to

TABLE 1
Membranes Used

Membrane type	Manufacturer	Membrane material	Charge (neutral pH)	MWCO (estimate)
NF70	DOW/Film Tec	Crosslinked aromatic polyamide	Negative	250
NTR 7450	Nitto-Denko	Sulfonated polyethersulfone	Negative	600–800
UTC-20	Toray	Polyamide	Positive	180

the membrane. Therefore, the molecule can more easily enter into the membrane structure. As a consequence, the retention is lower.

The molecules that were used for the modeling were not charged and their dipole moment did not exceed a chosen limit of 3-D. Molecular size therefore remained as the only parameter determining retention (11, 12). For the calculation of the molecular diameter, an energetic optimization procedure was used: in an iterative procedure using the computer program HyperChem (13), the molecular energy was minimized by adjusting the configuration of the molecules. In this way a complete view of the molecular structure and shape was obtained. The smallest cylinder around the molecule (with the diameter of the ground surface smaller than the height of the cylinder) was then determined. The axis of the cylinder was supposed to form an angle α with the surface of the membrane. The projection of the cylinder on the membrane surface can then be calculated as

$$\text{Height in projection} = a \cos \alpha + b \sin \alpha$$

where a = height of the cylinder and b = diameter of the cylinder.

The probability of an arbitrary angle α is proportional to the surface of a spherical shell (Fig. 1), which leads to a probability distribution $p(\alpha) = \cos \alpha$. The mean height in projection, the molecular diameter d_s, can then be calculated as

$$\begin{aligned} d_s &= \text{mean height in projection} \\ &= \frac{1}{\pi/2} \int_0^{\pi/2} (a \cos \alpha + b \sin \alpha) p(\alpha) d/\alpha \\ &= a/2 + b/\pi \end{aligned}$$

Table 2 represents the molecules that were used for the modeling together with the calculated diameter and the permanent dipole moment. For every molecule the reflection coefficient was calculated from experimental data for the retention as a function of the water flux through the membrane. These data

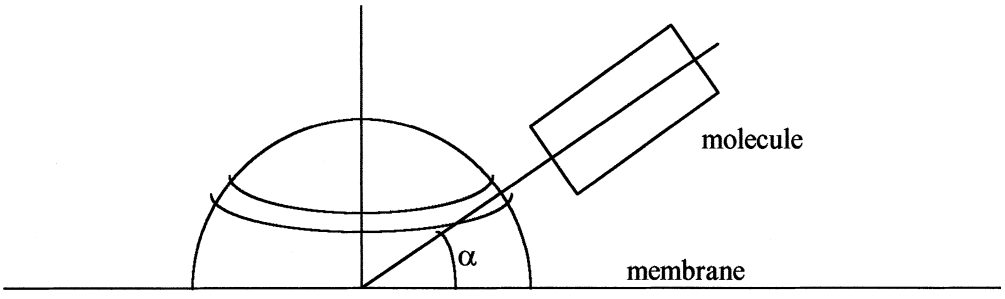

FIG. 1 Probability distribution for the angle α between the molecule and the membrane.

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TABLE 2
Permanent Dipole Moment and Retention of the Uncharged Molecules Used

Molecule	Diameter (nm)	μ° (Debye)	Reflection coefficient (%) NF70	NTR 7450	UTC-20
Methanol	0.27	1.6	26.1	2.3	4.7
Ethanol	0.34	1.7	31.8	3.4	22.2
Isopropanol	0.39	1.8	82.1	23.6	39.0
Methyl ethyl ketone (MEK)	0.42	2.8	88.0	8.6	
Ethyl acetate	0.48	1.7	72.0		32.4
Cyclohexanone	0.45	2.8	89.4		67.8
Aniline	0.49	1.5	62.5	3.0	4.4
Phenol	0.49	1.7	53.7	7.2	4.4
Toluene	0.50	0.4	75.0		
Methyl metacrylate	0.52	2.0	91.1	24.7	
Isobutyl methyl ketone (BMK)	0.52	2.7	72.5	18.2	35.8
Benzyl alcohol	0.54	1.7	77.5	29.5	13.3
Xylose	0.55	1.0	86.3	37.6	92.0
Galactose	0.66		84.1	31.3	94.1
Maltose	0.82		96.5	50.1	94.2
Raffinose	0.94		99.6	67.0	96.5

were obtained with a lab-scale nanofiltration unit (Amafilter, Test Rig PSSITZ) with an effective membrane area of 0.0044 m^2 and with pressures ranging from 2 to 20 bar (11). The temperature was set at 25°C. The feed velocity was set at 6 m/s in all the experiments.

RESULTS

Equations (3) and (4) were used to determine σ and *P* with a least-squares method. The results are represented for the membranes NF70, NTR 7450, and UTC-20 in Table 2.

The modeling of the reflection coefficient as a function of the molecular diameter was done for the different models by fitting the relevant equations to the experimental data using a least-squares method. This led to an optimal value for the parameters of the model.

Steric Hindrance Pore Model

The pore diameter of the membrane for every molecule was calculated from Eqs. (5) to (8) using the molecular diameters from Table 2 and the experimental reflection coefficient. Only molecules with a reflection coefficient above 5% were used for the calculation of the pore diameter; the rela-

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TABLE 3
Membrane Pore Sizes According to the SHP Model

	NF70	NTR 7450	UTC-20
Pore size (nm)	0.68	1.28	0.86
Standard deviation (nm)	0.06	0.10	0.09
Number of measurements	16	9	8

tive error is too high for lower values of σ. The results are summarized in Table 3.

With the calculated pore diameter and Eqs. (5) to (8), the reflection coefficient can be calculated as a function of the molecular diameter. The resulting retention curves are presented in Fig. 2 for NF70, in Fig. 3 for NTR 7450, and in Fig. 4 for UTC-20. In the same figures a comparison is made between the SHP model and the other models.

Zeman and Wales

The factor α from eq. (11) was derived from the experimental data for NF70, NTR 7450, and UTC-20 with a least-squares method. The results are summarized in Table 4; the retention curves (reflection coefficient as a function of the molecular diameter) are presented in Figs. 2–4.

Log-Normal Model

The two parameters used in the log-normal model were calculated from the experimental data (Table 5). A comparison among the three membranes re-

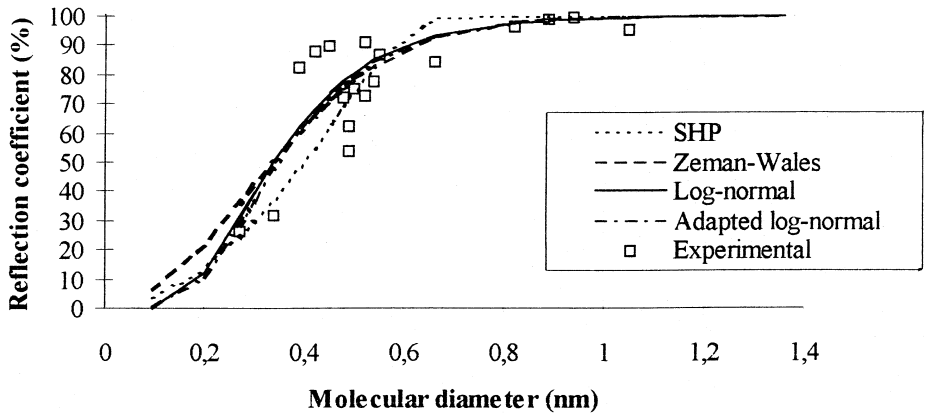

FIG. 2 Modeling of the reflection coefficient for NF70 and comparison with experimental data.

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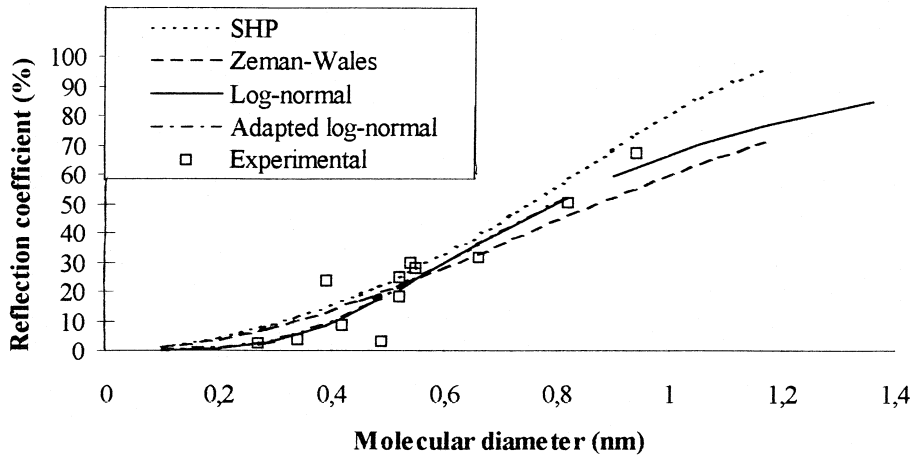

FIG. 3 Modeling of the reflection coefficient for NTR 7450 and comparison with experimental data.

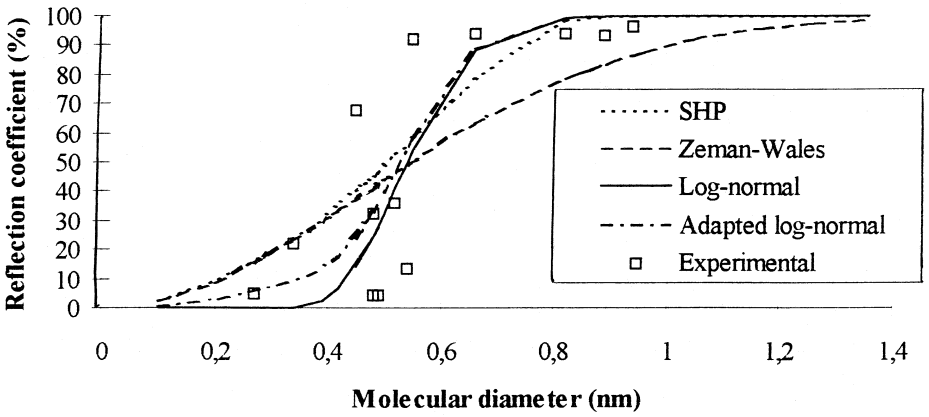

FIG. 4 Modeling of the reflection coefficient for UTC-20 and comparison with experimental data.

TABLE 4
Calculated α-Values from the Model of Zeman and Wales

	NF70	NTR 7450	UTC-20
α (—)	66.0	150.4	383.9

TABLE 5
Membrane Parameters for the Log-Normal Distribution

	NF70	NTR 7450	UTC-20
r (nm)	0.34	0.80	0.54
α (nm)	0.54	0.52	0.17

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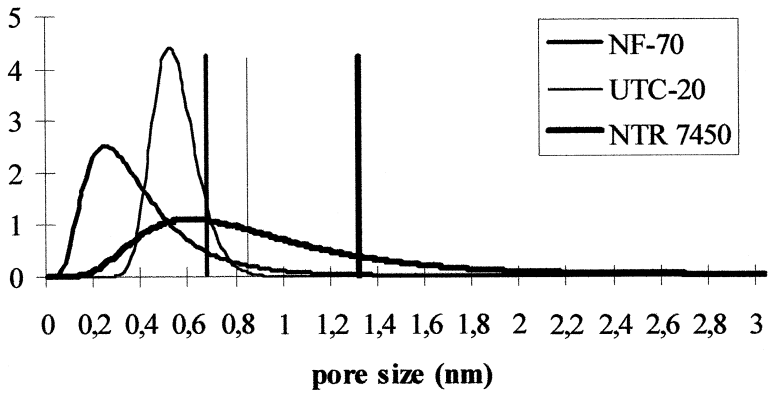

FIG. 5 Pore size distribution calculated with the log-normal and pore size calculated with the SHP model (vertical line).

veals that the mean pore diameter is the largest for NTR 7450 and the smallest for NF70, in agreement with the SHP model. However, with the log-normal model the steepest retention curve is obtained for UTC-20, in contrast with the model of Zeman and Wales where NF70 has the steepest retention curve. The information obtained with the log-normal model indicates that very small molecules will be better retained with NF70 than with UTC-20; above a certain molecular diameter the retention with UTC-20 will be higher than with NF70. The retention curves are presented in Figs. 2–4.

With the parameters $\bar{r}$ and α and the assumption that no hydrodynamic lag is involved in the transport of uncharged molecules, the pore size distribution can be obtained. This is represented in Fig. 5 for the three membranes. It should be remarked that this is a distribution of the effective pore area and not a distribution of the number of pores. Larger pores will have a greater influence on the permeation than smaller pores.

The differences between NF70 and UTC-20, as discussed, are obvious. NF70 has a smaller mean pore size, but a broader distribution of pores. NTR 7450 has a much broader range of pore sizes. The membrane pore size that was calculated with the SHP model is marked with a vertical line in Fig. 5.

Adapted Log-Normal Model

The retention curve obtained with the log-normal model was adjusted by taking the hydrodynamic lag into account through the parameter α. For each of the membranes an optimal value for α was chosen for the values of $\bar{r}$ and σ that were obtained with the log-normal model (Table 5). The calculated α-values are: 0.000 for NF70. 0.236 for UTC-20 and 0.043 for NTR 7450. A large value for α corresponds with an important hydrodynamic lag. The results suggest that hydrodynamic lag is not important for the studied nanofiltration

membranes. No improvement can be obtained for NF70 by taking hydrodynamic lag into account. The resulting retention curves are given in Figs. 2–4.

DISCUSSION

Due to the deviations of the experimental data, none of the models is obviously the best. These deviations are caused by two factors: a deviation of the calculated reflection coefficient (vertical in the retention curve) and a deviation of the molecular diameter (horizontal in the retention curve). Therefore, the retention curve is an estimate of the reflection coefficient and not an exact calculation. The standard deviation of the estimate of the reflection coefficient is represented in Table 6 for the different models. From this table it can be concluded that each model can be valuable. The relatively simple log-normal model has proved to give excellent results. The SHP model and the model of Zeman and Wales, which are based on idealized representations of the membrane, are not very meaningful physically in our opinion. In the log-normal model, no assumptions of this kind are made; the membrane has a distribution of pore sizes instead of a single pore size, and the pores do not have to be cylindrical. On the other hand, it can be seen from Figs. 2, 3, and 4 that there is only a small difference between the log-normal and the adapted log-normal model. The standard deviations given in Table 6 for the adapted log-normal model are not much lower than those of the log-normal model. The retention curves differ only slightly. This means that there is only a small influence of hydrodynamic lag. The log-normal model, where the hydrodynamic lag is neglected, can thus be considered to be the most practical model to predict reflection coefficients because it avoids the difficult integral calculations involved in the adapted log-normal model.

In addition to the comparison between experimental and modeled reflection coefficients, the mathematical conditions for the models can be evaluated. This corresponds to physical insight into the filtration process. These conditions are:

- The retention increases with the molecular diameter
- A molecule with an infinite diameter is completely retained

TABLE 6
Standard Deviation of the Reflection Coefficient as Estimated with the Different Models

	SHP	Zeman–Wales	Log-normal	Adapted log-normal
NF70	20.1	14.1	14.0	14.0
NTR 7450	10.0	9.0	9.0	8.9
UTC-20	29.7	25.5	27.3	26.7

Mathematically, this can be translated as $(dR/dr) > 0$ for every $r > 0$, and $\lim_{\eta\to\infty} R(r) = 1$ [or $(dR/d\eta) > 0$ for $\eta > 0$, and $\lim_{\eta\to\infty} R(\eta) = 1$].

For the *SHP model*, Eq. (8) can be rewritten by means of Eqs. (9) and (10) as

$$R = (1/9)(16\eta^6 - 64\eta^5 + 73\eta^4 - 36\eta^3 + 20\eta^2) \tag{15}$$

so that the derived function is obtained as

$$dR/dr = (1/9r_p)96\eta^5 - 320\eta^4 + 292\eta^3 - 108\eta^2 + 40\eta) \tag{16}$$

The SHP model satisfies neither the first neither the second condition because in the interval | 0.∞ | the derivative becomes negative for certain points, and the limit in ∞ is ∞.

For the *model of Zeman and Wales* it follows from Eq. (14):

$$dR/dr = (1/r_p)\ \exp(-\alpha\eta^2)(-2\alpha\eta^5 + 8\alpha\eta^4 + (4 - 8\alpha)\eta^3 - 12\eta^2 + (8 + 2\alpha)\eta) \tag{17}$$

The first condition is not satisfied because the derived function is not strictly positive in the interval | 0.∞ |. The second condition is satisfied.

The *log-normal model* satisfies both conditions, because

$$\frac{dR}{dr} = \frac{1}{S_p\sqrt{2\pi}}\frac{1}{r}\ \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) > 0$$

$$\lim_{r^*\to\infty} R(r^*) = \lim_{r^*\to\infty} \int_0^{r^*} \frac{1}{S_p\sqrt{2\Pi}}\frac{1}{r}\ \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) dr = 1$$

For the *adopted log-normal model*, the derivative was evaluated numerically. It was found that the boundary condition for the derivative was satisfied if $\alpha > 0$. For the second condition:

$$\lim_{r^*\to\infty} R(r^*) = \lim_{r^*\to\infty} \left(1 - \int_{r^*}^{\infty} \exp\left(-\alpha\left(\frac{r^*}{r}\right)^2\right)\frac{1}{S_p\sqrt{2\Pi}}\frac{1}{r} \exp\left(-\frac{(\ln(r) - \ln(\bar{r}))^2}{2S_p^2}\right) dr\right) = 1$$

The SHP model and the model of Zeman and Wales can be adapted by putting forward the limit that the equations are only valid for $\eta < 1$, and that $R = 1$ for $n > 1$. In this way, both conditions are satisfied.

CONCLUSIONS

The SHP model and the model of Zeman and Wales yield acceptable results but they are based on an idealized view of the membrane structure. The log-

normal model provides a good estimate of the reflection coefficient, starting from the distribution of the membrane pores. Nevertheless, hydrodynamic lag is not included in the log-normal model. The adapted log-normal model accounts for hydrodynamic lag in the pores by defining a supplementary membrane parameter. Therefore, the adapted log-normal model must theoretically be considered as the best model for the reflection coefficient.

Nevertheless, because the hydrodynamic lag was found to have a negligible influence on the reflection coefficient, the log-normal model is still applicable in practice. This model consists of only two parameters: a mean pore size and a standard deviation from the mean pore size. These parameters are easily understandable and can be obtained from retention measurements.

The models for the reflection coefficient are only valid in the high pressure limit. For lower pressures the pressure dependency of the retention should be accounted for. Equations (3) and (4) could be used for this purpose if a model to calculate the permeability parameter P for every molecule is established first. The models could thus be extended to the lower pressures used in nanofiltration.

SYMBOLS

c	concentration (mol/m^3)
d_p	pore diameter (m)
d_s	molecular diameter (m)
H_F	Wall correction parameter (—)
J_s	solute flux (mol/m·h)
J_v	water flux (L/m·h)
L_p	water permeability (L/m·hbar)
P	permeability (m^2/h)
R	retention (%)
r	solute or pore size (m)
$\bar{r}$	mean pore size (m)
r_p	pore radius (m)
S_F	sterical hindrance parameter (—)
S_P	standard deviation of pore size (m)

Greek

α	parameter in Zeman and Wales equations (—)
ΔP	transmembrane pressure (bar)
$\Delta\pi$	osmotic pressure difference (bar)
Δx	membrane thickness (m)
η	ratio of molecular diameter to pore diameter (—)
σ	reflection coefficient (%)

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