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Membrane Flash Index: Powerful and Perspicuous Help for Efficient Separation System Design

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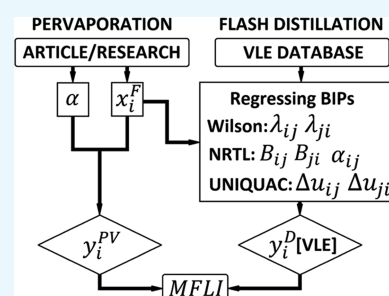Read Online

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ABSTRACT: There are different factors and indices to characterize the performance of a pervaporation membrane, but none of them gives information about their capabilities in the area of liquid separation compared to the most convenient alternative, which is distillation. Membrane flash index (MFLI) can be considered the first and only one that shows if the membrane is more efficient or not than distillation and quantifies this feature too. Therefore, the MFLI helps select the best separation alternative in the case of process design. In this study, the evaluation and capabilities of membrane flash index are comprehensively investigated in the cases of six aqueous mixtures: methyl alcohol–water, ethyl alcohol–water, isobutyl alcohol–water, tetrahydrofuran–water, N-butyl alcohol–water, and isopropanol–water. It must be concluded that the separation capacity of organophilic type membranes is remarkably lower than hydrophilic membranes in all cases of separation. The study of the MFLI is extended with the consideration of other binary interaction parameters like separation factor, permeation flux, selectivity, and pervaporation separation index (PSI) in order to find a descriptive relationship between them. For the same membrane material type, descriptive function can be determined between feed concentration and MFLI and PSI and separation factor, which can be used to calculate each other's value. On the basis of the indices and especially the MFLI, a significant help can be given to the process design engineer to select the right liquid separation alternative and, in the case of pervaporation, find the most appropriate membrane.

1. INTRODUCTION

Flash distillation is a specific method within the whole of rectification and distillation processes, where a liquid mixture is warmed up and pumped into the distillation apparatus of reduced pressure with permanent stream. In steady-state operations, the combinations of two phases are permanent and in equilibrium. The liquid and vapor phases are fed into a decanter (phase separator) where they are treated separately.[1,2]

Pervaporation is a current operation for the treatment of aqueous mixtures with organic content. The pervaporation (PV) technology is mostly applied for dehydration of organic substances,[3–9] separation of organic mixtures,[10–13] and takeout of low-concentration organic substances from their mixtures.[14–20] The separated mixture passes over a phase change in the thin film material (membrane) on account of the used vacuum at the product part that results in the permeate being in the vapor phase.[21–23] The mixture is separated by the sorption and diffusion features of a rather passing substance over a thin film membrane.[1]

Depending on the passing substance, pervaporation is classified into two major categories: hydrophilic pervaporation (HPV) and organophilic pervaporation (OPV).[1,23–27] An enormous number of practical operations and publications represent the relevance of pervaporation as a separation process in the category of membranes.[28,29] The effectiveness

and the slight functional circumstances make pervaporation a profitable process in the field of separation methods.[1,30]

Inorganic zeolite and composite polydimethylsiloxane (PDMS) are the most used materials for organophilic pervaporation for discharge organic compounds from their mixtures.[31] Polyvinyl alcohol (PVA) is the generally used membrane type for hydrophilic pervaporation.[1,32]

PV can be evaluated by various factors. Equation 1 describes the flux[33] as

$$J_i = \frac{P_i}{\Delta t \cdot A} \tag{1}$$

where P_i is the amount of substance i in the permeate side, A is the membrane surface area, and Δt is the duration of the separation process.[34,35] Equation 2 represents the calculation of separation[35] as

Table 1. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in Methanol−Water Separation (AVE, Average; SDV, Standard Deviation; MAX, Maximum)

org or hydr	membrane category	MFLI			PSI			separation factor		
		AVE[1]	SDV[1]	MAX[1]	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes	PDMS	1.2	0.5	2.6	5	5	16	8	5	23
	hydrophobic zeolite	2.3	0.7	3.6	17	28	95	30	28	100
	all type	1.8	0.8	3.6	11	20	95	19	23	100
hydrophilic membranes	polyvinyl alcohol (PVA)	14.5	9.2	24.2	112	275	889	481	602	1534
	other hydrophilic	15.7	6.4	25.0	237	598	1889	246	450	1260
	all type	15.1	7.7	25.0	175	457	1889	363	531	1534

Table 2. Comparison of MFLIs with Separation Factors (α), Pervaporation Separation Indexes (PSIs), and Selectivities (β) in Methanol−Water Pervaporation

org or hydr	membrane category	α [−]	PSI [kg/m^{2}h]	β [−]	MFLI [−]	ref.
orgPV	PDMS/silica nanocomposite	23	8	4.1	2.6	Shirazi et al., 2012[42]
	silicalite-1, SS support	14	13	2.3	1.8	Liu et al., 1996[43]
	B-ZSM-5, α-support s.	12	1	1.9	1.6	Bowen et al., 2003[44]
hydrPV	Polyamide-6	891	15	4097	24.8	El-Gendi and Abdallah, 2013[45]
	composite PVA/P(AA-co-AN/SiO$_2$)	1534	889	963	24.2	Peng et al., 2006[46]
	cross-linked chitosan	9	4	714	15.5	Won et al., 2003[47]

$$\alpha = \frac{y_i/y_j}{x_i/x_j} \tag{2}$$

where x_i, x_j and y_i, y_j are concentrations of substances i and j in the feed side and the permeate side. It must be mentioned that the separation factor (α) is (dimensionless).[35] Equation 3 shows the calculation of the pervaporation separation index (PSI):

$$\text{PSI} = J \cdot (\alpha - 1) \tag{3}$$

Permeance can specify the performance of pervaporation membranes, which is normalized substance flux by the pressure divergence as impulsion:[1,36]

$$\frac{P_i}{\delta} = \frac{J_i}{\gamma_{i1} \cdot x_{i1} \cdot p_{i0} - y_i \cdot p_3} \tag{4}$$

The ratio of permeances gives the selectivity (β):[1]

$$\beta = \frac{P_i/\delta}{P_j/\delta} \tag{5}$$

In the literature, the pervaporation separation index, flux, and separation factor are generally applied for ranking the separation performances of different pervaporations.[23] The listed factors are the functions of the inside attributions of the used material of membranes. However, the selectivity also depends on the functional circumstances, mainly permeate pressure, temperature, and compositions of feed.[23] It can be mentioned that the promising direction of evaluation pervaporation achievement is the determination of selectivity;[36] nevertheless, a few research papers describe this parameter.

It has to be mentioned that the literature do not show a comprehensive clear approach for the comparison of separation effectiveness of pervaporation and its separation alternative, which is distillation.[36] The relative vaporization in the distillation process is involved in the interpretation of selectivity by Baker.[1,29] Nevertheless, this comparison does not result in a direct and simple correlation between distillation and pervaporation for process engineers. Hinchliffe and

Porter[37−39] have reported the cost-based comparison of membrane separation and distillation. Cost permeability has been defined and case studies have been plotted in the function of effective selectivity and this parameter. However, it is informative and really helpful for practice but very specific and difficult to generalize the comparison. Furthermore, the membrane prizes change quickly because this sector is innovative.

Considering pervaporation and flash distillation options, pervaporation can be compared to the characteristics of elementary flash distillation. Toth et al.[1] created a simply method, which is mainly based on the comparison of available theoretical maximum distillate compositions. The main formula of the so-called membrane flash index (MFLI) is as follows:

$$\text{MFLI} = \frac{y_i^{PV}}{y_i^{D}[\text{VLE}]} \tag{6}$$

where y_i^{PV} is the permeate concentration and $y_i^{D}[\text{VLE}]$ is the equilibrium distillation value. The comparison perspective of the MFLI focuses only on the separation abilities of the distillation and pervaporation operations. The prime preference of the membrane flash index is simplicity and accuracy because only two practical (experimental) data (α_i and x_i^F) and the appropriate vapor−liquid equilibrium (VLE) data are enough for evaluation. The membrane flash index presents explicit comparison of distillation and pervaporation in the process and chemical engineering area. The separation achievement of PV is preferable than the application of flash distillation if the MFLI is above 1.[1]

In our previous paper,[1] the calculation of the MFLI was described with one equilibrium model in detail. The purpose of this study is to evaluate the MFLI in the aspects of other descriptive quantities and to extend its calculation.

2. RESULTS AND DISCUSSION

In general, 10−15 assorted samples (membrane) with the highest membrane flash indexes are inspected in every case of the main group of membrane material types. Organophilic and

hydrophilic separations are also investigated. The comparison and evaluation of pervaporation and flash distillation are introduced on the joint liquid−vapor equilibrium figure of binary mixtures.[31,40,41] Calculated MFLIs and liquid−vapor equilibrium figures is found in the Supporting Information (Parts II, III, IV, V, VI, and VII). In decreasing order, the membrane flash indexes are shown in tables.

2.1. Separation of Methyl Alcohol−Water Mixture. Separation factors, MFLIs, and PSIs of pervaporation membranes of methanol−water binary mixtures are summarized in Table 1.

It can be concluded that PVA and other dehydration membranes are dominant in every hierarchy and organophilic pervaporation shows significantly worse separation efficiency than methanol dehydration. Table 2 introduces the highest results of MFLIs in the case of the different membrane types for which selectivity values were available in the research paper. The best three selectivities are introduced. In addition, the corresponding separation factors and PSI values are given to the comparison. The complete data set can be seen in Supporting Information, Part II/3.

It must be mentioned that there is no accordance between separation factor and PSI, e.g., the highest separation factor of the membrane type is not the highest in PSI value. In contrast, the membrane with the highest MFLI value has also the highest selectivity. Figures 1−3 introduce a functional relationship between methanol feed weight fractions and PSIs and MFLIs and separation factors in the case of PDMS membranes.
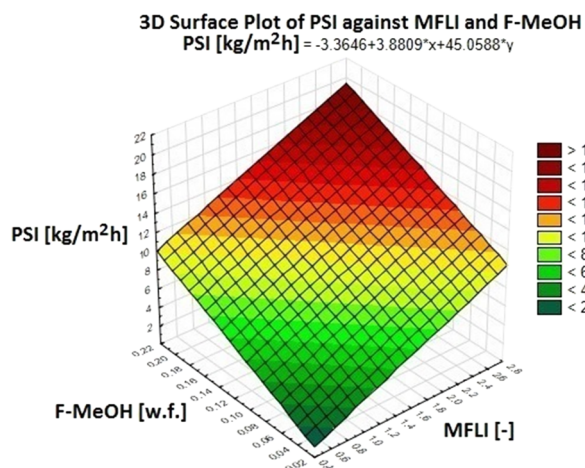

Figure 1. Influence of the PSIs and MFLIs on the methanol feed weight fractions in the case of methyl alcohol−water separation with PDMS membranes.

Figures 4−6 present a functional relationship between methanol feed weight fractions and PSIs and separation factors and MFLIs in the case of PVA type membranes. The Supporting Information contains the figures about zeolite membranes in the part of II/3.

2.2. Separation of Ethyl Alcohol−Water Mixture. Table 3 introduces the MFLI of pervaporation membranes of ethyl alcohol−water mixtures.

It can be mentioned that the parameters of dehydration membranes are dominant as seen with methanol−water separation. The highest values of MFLIs in the case of organophilic and hydrophilic types for which selectivity values
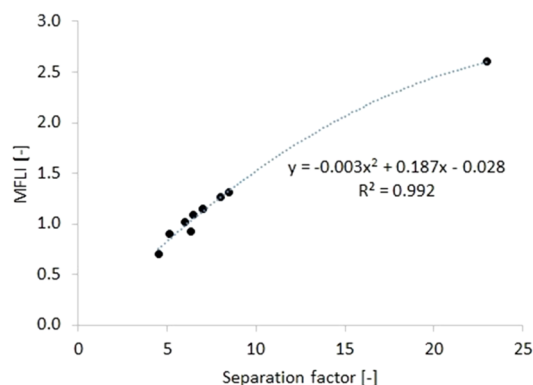

Figure 2. MFLI values in the function of separation factors in the case of methyl alcohol−water separation with PDMS membranes.
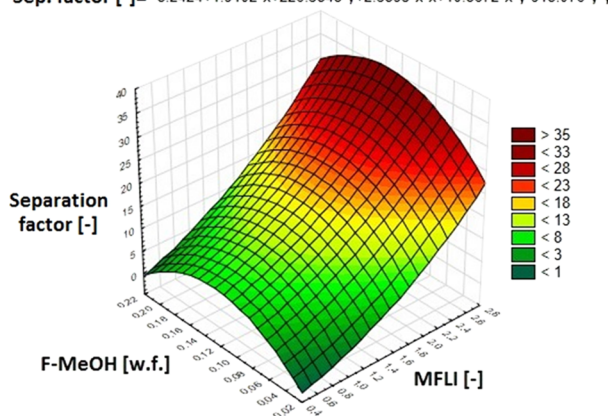

Figure 3. Influence of the separation factors and MFLIs on the methanol feed weight fractions in the case of methanol−water separation with PDMS membranes.
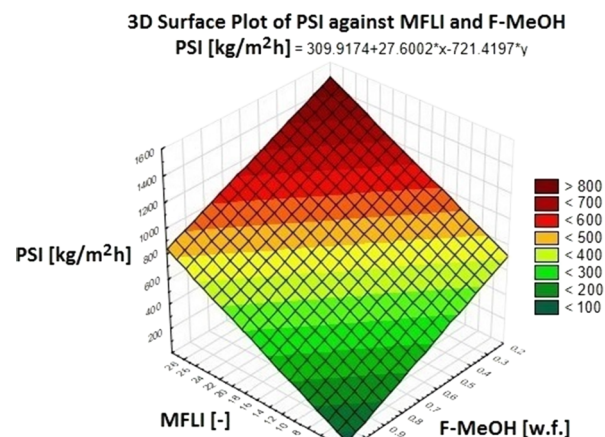

Figure 4. Influence of the PSIs and MFLIs on the methanol feed weight fractions in the case of methyl alcohol−water separation with polyvinyl alcohol membranes.

were available in the research paper can be seen in Table 4. Separations and PSI values were added; the complete data set can be seen in Supporting Information, Part III/3.

It can be said that the highest MLFIs have the highest selectivities too and there is no accordance between MFLIs and PSI values. The Supporting Information contains the
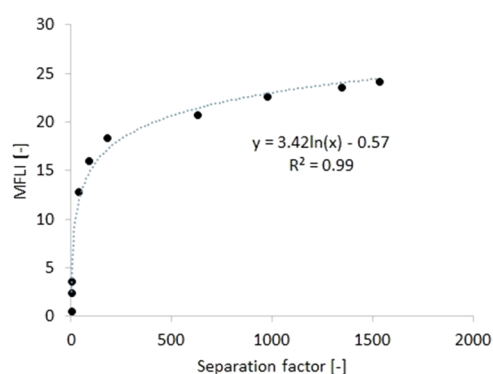
Figure 5. MFLI values in the function of separation factors in the case of methyl alcohol−water with PVA membranes.
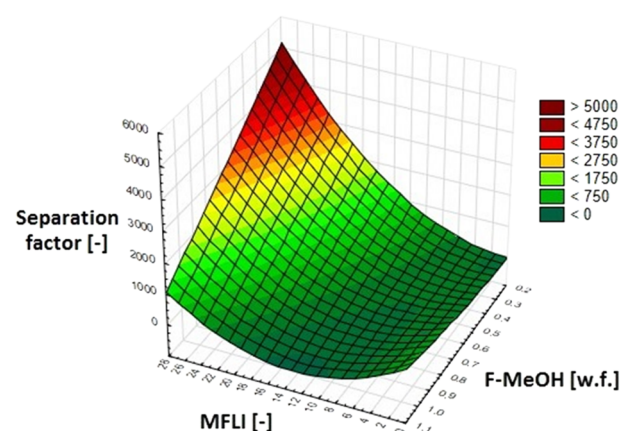

Figure 6. Influence of the separation factors and MFLIs on the methanol feed weight fractions in the case of methyl alcohol−water separation with polyvinyl alcohol membranes.

figures about the functional relationship between ethanol feed weight fractions and PSIs and separation factors and MFLIs in the case of PDMS, PVA, zeolite type membranes, and membranes containing charged group in the part of III/3.

2.3. Separation of Isobutanol−Water Mixture. It must be mentioned that there is remarkably less OPV and HPV membrane type for separation of heterogeneous azeotropic compounds from water. Table 5 introduces the MFLIs of membranes in the organophilic and hydrophilic pervaporations of isobutanol−water mixture.

Table 6 shows the comparison of the main descriptive quantities of IBU−water mixture.

Same tendencies and experience can be determined in separation of IBU−water binary mixture as in the case of ethyl alcohol and methyl alcohol. The Supporting Information contains a functional relationship between isobutanol feed weight fractions and PSIs and MFLIs in the case of PDMS and PVA membranes in the part of IV/3.

2.4. Separation of Tetrahydrofuran−Water Mixture. The comparison of separation factors, MFLIs, and PSIs of tetrahydrofuran−water mixture is summarized in Table 7.

2.5. Separation of N-Butanol−Water Mixture. Table 8 summarizes the comparison of separation factors, MFLIs, and PSI of N-butanol−water mixture.

2.6. Separation of Isopropanol−Water Mixture. Table 9 summarizes the comparison of separation factors, MFLIs, and PSI of isopropanol−water mixture.

3. CONCLUSIONS

In the case of process synthesis, the final decision about the design of a liquid separation system has to consider environmental impacts, cost elements of methods, controllability, etc., in many cases. Membrane flash index (MFLI) gives preliminary information about the selection between pervaporation and distillation methods to help find the appropriate separation method. Moreover, if the membrane flash index value is relative high, the membrane separation should be preferred by far. So, a high value of MFLI shows not only the priority of pervaporation but gives also a heuristic judgment how far it is better. As our examples show that the MFLI can be only a bit higher than 1, showing that pervaporation could be better, but the MFLI can be several orders of magnitude higher than 1 shows a superior performance of pervaporation over the distillation. On the contrary, if the membrane flash index is low, that is, near 1, flash distillation should be selected because that seems to be the better choice.

The separation capacities of six binary, aqueous mixtures are investigated. MFLIs, separation factors, total fluxes, pervaporation separation indices, and selectivity values are evaluated. Three thermodynamic models are introduced for the calculation of MFLIs to generalize the description. It can be determined that the dehydration type membranes have remarkably higher separation capacities in all investigated cases than the organophilic membranes.

To harmonize the MFLI with the other membrane parameters/indices, it is necessary to find the connection between these evaluation parameters to give support for

Table 3. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in Ethanol−Water Separation

org or hydr	membrane category	MFLI			PSI			separation factor		
		AVE[1]	SDV[1]	MAX[1]	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes	PDMS	1.4	0.3	1.9	5	6	20	10	2	14
	other polymeric	2.2	0.2	2.7	11	14	49	23	7	46
	hydrophobic zeolite	3.2	0.7	4.5	36	38	129	57	28	125
	silicalite-silicone rubber mixed matrix	2.0	0.6	3.1	2	3	9	21	16	59
	all type	2.2	0.8	4.5	15	25	129	28	25	125
hydrophilic membranes	polyvinyl alcohol (PVA)	13.0	5.1	20.2	32	52	178	367	267	893
	chitosan-based	15.5	6.1	25.0	171	357	1175	2173	3013	10,491
	membranes containing charged groups	16.5	7.2	33.2	1397	3315	10,299	2966	4455	11,600
	membranes formed from polysalts	11.0	4.5	20.6	746	623	2000	1082	1635	5000
	all type	14.4	6.2	33.2	675	2004	10,299	1810	3157	11,600

Table 4. Comparison of MFLIs with Separation Factors (α), Pervaporation Separation Indexes (PSIs), and Selectivities (β) in Ethanol−Water Pervaporation

org or hydr	membrane category	α [−]	PSI [kg/m²h]	β [−]	MFLI [−]	ref.
orgPV	silicalite-1 with PDMS coating - SS s.	125	17	41	4.5	Matsuda et al., 2002[48]
	silicalite-1 - SS s.	60	45	18	3.9	Sano et al., 1994[49]
	silicalite-1 - SS s.	59	13	18	3.8	Sano et al., 1997[50]
hydrPV	Alg/DNA-Mg²⁺	6500	65	3883	33.2	Uragami et al., 2015[51]
	cationic PVA/GA	709	63	2680	24.6	Praptowidodo, 2005[52]
	anionic PVA/GA	837	72	2587	24.5	Praptowidodo, 2005[52]

Table 5. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in Isobutanol−Water Separation

membrane category	MFLI			PSI			separation factor		
	AVE[1]	SDV[1]	MAX[1]	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes	7.2	2.8	9.8	150	114	295	33	4	40
hydrophilic membranes	8.0	7.7	21.7	2862	4056	12,533	1301	1964	6010

Table 6. Comparison of MFLIs with Separation Factors (α), Pervaporation Separation Indexes (PSIs), and Selectivities (β) in Isobutanol−Water Pervaporation

org or hydr	membrane category	α [−]	PSI [kg/m²h]	β [−]	MFLI [−]	ref.
orgPV	(TX-PDMS)$_n$	38	248	760	9.8	Schnabel et al., 1998[53]
	(T-PDMS)$_n$	37	295	569	9.5	Schnabel et al., 1998[53]
	Sulzer PERVAP 4060	30	29	450	3.2	Toth et al., 2015[23]
hydrPV	Sulzer PERVAP 1510	6010	3005	10,000	21.7	Toth et al., 2015[23]
	Sulzer PERVAP 1510	890	3760	2200	21.2	Valentínyi et al., 2014[54]
	zeolite LTA, porous Al₂O₃	2811	12,533	1400	5.7	Huang et al., 2014[55]

Table 7. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in Tetrahydrofuran−Water Separation

membrane category	MFLI			PSI			separation factor		
	AVE	SDV	MAX	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes	9.7	7.4	20.4	80	119	308	96	36	170
hydrophilic membranes									
zeolite	17.0	1.2	18.4	5634	8305	21,358	6128	8056	20,000
PVA	17.3	2.8	21.3	99	87	217	369	204	591
other	14.2	3.8	21.9	7882	11,953	46,986	23,854	38,186	89,900
all type	15.4	3.5	21.9	6010	10,303	46,986	15,862	31,334	89,900

Table 8. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in N-Butanol−Water Separation

membrane category	MFLI			PSI			separation factor		
	AVE	SDV	MAX	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes									
PDMS	1.5	0.5	2.4	38	38	129	36	14	66
other	1.0	0.4	1.5	136	299	979	31	30	104
all type	1.3	0.5	2.4	77	192	979	34	21	104
hydrophilic membranes	2.9	0.3	3.5	27,026	49,435	125,099	18,402	35,761	90,000

Table 9. Evaluation and Summary of MFLIs, PSIs, and Separation Factors in Isopropanol−Water Separation

membrane category	MFLI			PSI			separation factor		
	AVE	SDV	MAX	AVE	SDV	MAX	AVE	SDV	MAX
organophilic membranes	0.8	0.3	1.4	7	8	22	11	8	32
hydrophilic membranes									
PVA	8.7	0.7	9.1	265	330	1272	2865	5186	17,991
chitosan	8.8	2.4	14.9	491	497	1339	1493	1276	4277
other	9.2	1.9	15.0	6039	13,462	47,398	5178	8163	30,000
all type	8.9	1.7	15.0	2260	8042	47,398	3214	5746	30,000

chemical process design. It is determined that the parameters can be calculated from each other for the different membrane alternatives. It is found that the membrane of the highest MFLI has also the highest selectivity. However, this is not the case

with the other membrane characterizing parameters. Therefore, an algorithm is presented for the calculation of the different membrane characterizing parameters for the efficient support of chemical process design. First, the calculation of the MFLI is suggested to determine the selection between pervaporation and distillation. If the MFLI suggests one to use pervaporation, the determination of selectivity is recommended for the recognition of optimal operating parameters, pressure, temperature, etc. Lastly, the calculation of PSI can summarize the information of purity with separation factor value, yield, and fluxes.

4. COMPUTATIONAL METHODS

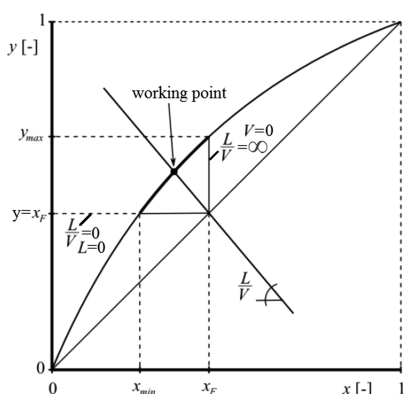Figure 7 introduces the possible operating boundaries of flash distillation.

Figure 7. Possible operating boundaries of flash distillation in liquid−vapor equilibrium.[1] Reprinted with permission from ref 1. Copyright 2018 American Chemical Society.
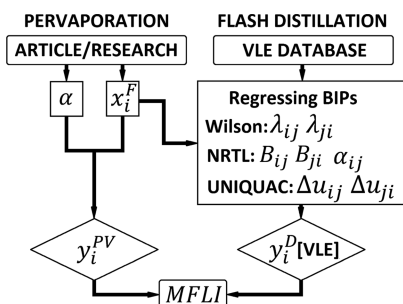

Figure 8. General process of the determination of MFLIs.

The available theoretical maximum vapor data (y_{max}) is the equilibrium composition of the feed, and the corresponding y_i^D

data has to be established as a function of x_i^F, as can be seen in Figure 7.

Refereed vapor−liquid equilibrium data has to be applied to find the appropriate y_i^D. Information can be found in the Vapor−Liquid Equilibrium (VLE) Data Collection from DECHEMA[56] in the database of flowsheet simulators (ChemCAD, Aspen Plus, Aspen Hysys, etc.). In most of the cases, enough exact VLE data is not available. Thus, regression processes of thermodynamic models are offered for the definition of accurate and appropriate y_i^D. Three thermodynamic models are described, which is offered for the calculation of y_i^D in the case of the determination of MFLIs. The paper extends the calculation of MFLI with this presentation.

The activity coefficient model presented by Wilson[57] aims to incorporate two adjustable interaction parameters and clean constituent's molar volumes and to specify the excess Gibbs energy of binary solution, therefore modeling equilibrium. The activity coefficients can be calculated by eq 7:[58]

$$\ln \gamma_k = 1 - \ln\left(\sum_i x_i \Lambda_{ki}\right) - \sum_j \left(\frac{x_j \Lambda_{jk}}{\sum_i x_i \Lambda_{ji}}\right) \tag{7}$$

where the values of Λ_{ij} can be calculated from liquid molar volumes of clean constituents (V_i, V_j) and λ_{ij} and λ_{ij} are interaction parameters of the Wilson model given in cal/g·mol:

$$\Lambda_{ij} = (V_j/V_i) \times \exp[-(\lambda_{ij} - \lambda_{ji})/RT] \tag{8}$$

The main equation of the "non-random two-liquid model" (NRTL)[59] model is displayed as

$$\ln \gamma_i = \frac{\sum_j^n x_j \tau_{ji} G_{ji}}{\sum_k^n x_k G_{ki}} + \sum_j^n \frac{x_j G_{ij}}{\sum_k^n x_k G_{kj}}\left(\tau_{ij} - \frac{\sum_m^n x_m \tau_{mj} G_{mj}}{\sum_k^n x_k G_{kj}}\right) \tag{9}$$

where

$$G_{ij} = \exp(-\alpha_{ij} \times \tau_{ij}) \tag{10}$$

and

$$\tau_{ij} = A_{ij} + \frac{B_{ij}}{T} + C_{ij} \times \ln(T) + D_{ij} \times T \tag{11}$$

B_{ij}, B_{ji}, and α_{ij} are used by the NRTL equation under the regression of binary interaction parameters (BIPs) in the flowsheet simulator, e.g., ChemCAD.[1]

The "universal quasichemical model" (UNIQUAC)[60] combines together an enthalpic (residual contribution) term and an entropic (also called combinatorial contribution) term for the determination of activity coefficients. The combinato-
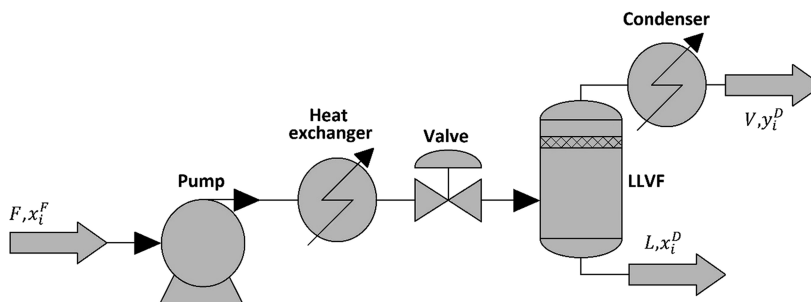

Figure 9. Schematic figure of flash distillation.[31] Reprinted with permission from ref 31. Copyright 2016 Elsevier.
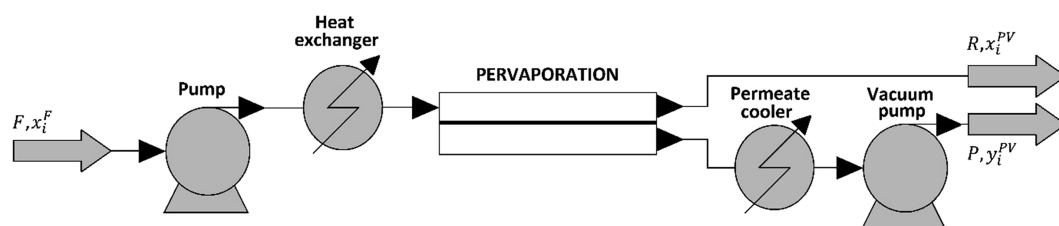
Figure 10. Schematic figure of pervaporation.[31] Reprinted with permission from ref 31. Copyright 2016 Elsevier.

Table 10. Examined Mixtures (100 kPa)[61]

mixtures	NRTL parameter			azeotropic comp.	
	B_{ij} [−]	B_{ji} [−]	α_{ij} [−]	[w.f.]	[°C]
water−methyl alcohol	307.166	−24.4933	0.3001		
water−ethyl alcohol	670.441	−55.1681	0.3031	95.7	78.3
water−isobutyl alcohol	1068.12	95.5182	0.3291	67.7	89.6
water−tetrahydrofuran	953.251	449.411	0.4306	93.3	63.4
water−N-butanol	1468.34	215.427	0.3634	57.5	92.7
water−isopropanol	832.981	20.0554	0.3255	88.0	80.1

rial term is the effect coming from the molecule shape (that could be calculated from group contributions), the residual term from interactions between molecules:[58]

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \tag{12}$$

$$\ln \gamma_i^C = (1 - V_i + \ln(V_i)) - \frac{z}{2} q_1 \left(1 - \frac{V_i}{F_i} + \ln\left(\frac{V_i}{F_i}\right)\right) \tag{13}$$

$$\ln \gamma_i^R = q_i \left(1 - \ln \frac{\sum_j q_j x_j \tau_{ji}}{\sum_j q_j x_j} - \sum_j \frac{q_j x_j \tau_{ij}}{\sum_k q_k x_h \tau_{kj}}\right) \tag{14}$$

where $\tau_{ij} = \exp(-\Delta u_{ij}/RT)$, where Δu_{ij} is the binary interaction parameter. The values are defined as $\Delta u_{ij} = u_{ij} - u_{ii}$, incorporating the interactions between different and similar molecules.[58] It must be mentioned that the applied thermodynamic model has to be remarked in every cases. The selection of the model should be confirmed in the literature.

Using eq 15, y_i^{PV} can be calculated easily:

$$y_i^{PV} = \frac{\alpha \times x_i^F}{(\alpha - 1) \times x_i^F + 1} \tag{15}$$

It has to be also mentioned that the comparison is based on the best available permeate concentration. The main permeable component has to be distributed by each other: organic concentration in the permeate product at organophilic PV with an appropriate equilibrium organic concentration and, in contrast, water concentration in the permeate product at hydrophilic pervaporation with an appropriate equilibrium water concentration. Figure 8 introduces the general determination process of membrane flash index (MFLI).[1]

The Supporting Information contains an example of the determination of MFLIs in Part I. Figures 9 and 10 present the figures of two unit operations, simple flash distillation, and pervaporation. These figures show the parameters to pair each

other: liquid equilibrium with vapor equilibrium value (y_i^D) in flash distillation and y_i^{PV} with the y_i^D.[1]

Six binary aqueous mixtures are selected for the exemplification of correlation between distillation and pervaporation (see Table 10). In the case of vapor−liquid equilibrium data, the "non-random two-liquid model" (NRTL) thermodynamic model[59] is applied.

The comparison of PV and flash distillation is studied only for such separation cases, where the target is not azeotrope fractionation.[1] It can be mentioned that improved separation achievement can be gained by applying rectification, although pervaporation is often the preferred solution in the case of the treatment of the azeotropic mixtures.[31,62]

■ ASSOCIATED CONTENT

ⓈI Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.0c01063.

> Example calculation for membrane flash index (MFLI), separation of methanol and water, separation of ethanol and water, separation of isobutanol and water, separation of tetrahydrofuran and water, separation of N-butanol and water, separation of isopropanol and water, nomenclature, and references (PDF)

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Notes
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■ NOMENCLATURE

A	membrane transfer area $[m^2]$
B_{ij}	NRTL interaction parameter
B_{ji}	NRTL interaction parameter
F	feed
i	component number
j	component number
J_i	flux of component i $[kg/(m^2 h)]$
L	liquid equilibrium
P	permeate
p_{i0}	pure i component vapor pressure $[bar]$
p_3	pressure on the permeate side $[bar]$
P_i/δ	permeance of component i $[kg/(m^2 h bar)]$
R	retentate
s.	support
t	time $[h]$
T	temperature $[°C]$
V	vapor equilibrium
x_i^F	feed alcohol or water weight fraction $[-]$
x_{i1}	concentration of component i in the feed $[m/m\%]$
x_i^D	equilibrium liquid alcohol or water weight fraction $[-]$
y_i^D	equilibrium vapor alcohol or water weight fraction $[-]$
x_i^{PV}	retentate alcohol or water weight fraction $[-]$
y_i^{PV}	permeate alcohol or water weight fraction $[-]$

Abbreviations

AVE	average
BIPs	binary interaction parameter
EtOH	ethanol, ethyl alcohol
HPV	hydrophilic pervaporation
hydr	hydrophilic
IBU	isobutanol, isobutyl alcohol
IPA	isopropanol
MAX	maximum
MeOH	methanol, methyl alcohol
MFLI	membrane flash index
NBU	n-butanol, n-butyl alcohol
NRTL	non-random two-liquid model
OPV	organophilic pervaporation
org	organophilic
PDMS	polydimethylsiloxane
PSI	pervaporation separation index $[kg/(m^2 h)]$
PVA	polyvinyl alcohol
PV	pervaporation
SDV	standard deviation
THF	tetrahydrofuran
Δu_{ij}	UNIQUAC interaction parameter
Δu_{ji}	UNIQUAC interaction parameter
VLE	vapor−liquid equilibrium
w.f.	weight fraction

Greek Letters

α	separation factor
α_{ij}	NRTL interaction parameter
α_{ji}	NRTL interaction parameter
β	selectivity
γ_{i1}	activity coefficient of component i in the feed
δ	membrane thickness $[\mu m]$
λ_{ij}	Wilson interaction parameter
λ_{ji}	Wilson interaction parameter

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