

Entrainer Selection



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1 Introduction

Although conventional distillation is the most important industrial separation process, there are situations where solvent-enhanced separation, e.g., azeotropic distillation, extractive distillation, liquid-liquid extraction and absorption are a more appropriate choice. Therefore, a software package was developed in order to find a suitable solvent (entrainer) for the above-mentioned separation processes. The entrainer selection is based on azeotropic data, activity coefficients at infinite dilution, liquid-liquid equilibrium (LLE) and gas solubility (GLE) data. These data are taken from factual data banks as well as from thermodynamic models.

The main menu contains three different dialogs for the distillation processes (e.g., azeotropic distillation, extractive distillation and additional selectivity), the liquid-liquid extraction and the absorption. The last two are also able to find solvent mixtures.

2 Distillation Processes

The Distillation Processes dialog contains the controls for three solvent based distillation processes.

The screenshot shows the 'Distillation Process' dialog box with the following details:

- Distillation Process:** Extraction (LLE) | Absorption
- Component 1:** 31 Benzene, Vapor Pressure [kPa]: 36.08 (by Antoine Low - No Validation)
- Component 2:** 50 Cyclohexane, Vapor Pressure [kPa]: 36.17 (by Antoine Low - No Validation)
- Basic Settings:**
 - Separation Process: Extractive Distillation
 - Vapor Pressure Equation: Antoine Low - No Validation
 - System Temperature [K]: 323.15 (selected)
 - System Pressure [kPa]: 101.325
- Separation Process Settings:**
 - Minimum Separation Factor at Infinite Dilution (α_{12} or inverse): 1.5
 - Minimum Vapor Pressure Difference [kPa] Entrainer - Binary Mixture: -10 (> 0 kPa -> Reverse Extr. Dist., type 0. to ignore limit)
 - Ignore components without boiling point data:
 - Activity Coefficient Data Source: DDB Access
 - Azeotropic Information Data Source: DDB Access
 - Discard activity coefficients and azeotropic points marked as doubtful or worse:
- Solvent Settings:**
 - Maximum Melting Point [K] of the Entrainer: 323.15
 - Include Components Without Given Melting Point:
 - Maximum Viscosity [mPas] of the Entrainer: 5
 - Include Components Without Given Viscosity Information:
 - Exclude Ionic Liquids:
 - Preselected Components: 229 components
 - Use All Components (Ignore List):
 - Buttons: Select, Load List, Default List
 - Entrainer Selection: License Server: Success

After specifying the binary separation problem (Component 1 and 2), the vapor pressures or boiling points of the components are shown, depending on the chosen system temperature or pressure and vapor pressure equation in the “Basic Settings”. The component selection is performed by the (DDB-) standard program DDB Components. Beside the temperature and pressure and the vapor pressure equation, the “Basic Settings” allows the user to choose the specific distillations process. This will change the “Separation Process Settings” to show the necessary options and needed data sources:

<i>Process</i>	<i>Input</i>
Extractive Distillation	minimum separation factor at infinite dilution, boiling point (isobaric case) or vapor pressure difference (isothermal case) between entrainer and binary system
Azeotropic Distillation	selection of the new introduced azeotrope (binary or ternary), model for the calculation of the virial coefficients
Selectivity	minimum selectivity at infinite dilution

The data source options allow the user to choose the necessary data sources for given separation processes. If experimental data are selected, a linear regression is used to estimate the values for the separation factor or selectivity and the azeotropic temperature for the given system pressure. The calculation with different thermodynamic models (group contribution methods) is possible: UNIFAC, mod. UNIFAC (Dortmund), mod. UNIFAC (Lyngby), NIST-modified UNIFAC (Dortmund), PSRK, and VTPR.

The “Solvent Settings” offers the possibility to specify the chosen solvent base. This is useful, if the azeotropic data are calculated with a thermodynamic model. Instead of calculating the homogeneous and heterogeneous points for many thousands of components, it is possible to use a limited list of predefined solvent candidates. Use the “Select” button to create a list of solvents with *DDB Components*. Use the “Load List” button to load a list of components from file. Normally a list of common solvents is preselected. This list can be reset by the “Default List” button. If the “Use All Components (Ignore List)” Options is used, the solvent list is ignored and all components of the DDB are tested as potential solvents.

The maximum melting point and the maximum viscosity options allow to exclude components with non-matching conditions. Components, which do not have this information, can either be included or not. The knowledge of the melting point is necessary to avoid a crystallization of the entrainer. Low viscosities help to enhance the mass transfer and minimize the energy costs (pumping costs).

It is possible to exclude ionic liquids completely. Ionic liquids often dominate the result lists because of their specific properties but may not be usable for the process under investigation.

If the program is finished the data finally used are stored and automatically entered in the next run.

2.1 Proposal of Alternative Separation Processes

In some cases, the components can be separated without introducing a third component. The program package first checks the VLE behavior. After the evaluation a proposal with the alternative separation process is given before the entrainer selection starts:

- zeotropic behavior \Rightarrow ordinary distillation
- formation of a heterogeneous azeotrope \Rightarrow heterogeneous azeotropic distillation
- zeotropy at high/low pressures \Rightarrow vacuum (pressure) distillation
- strong pressure dependence of azeotropic composition \Rightarrow pressure swing distillation

2.2 Extractive Distillation

With the help of saturation vapor pressures P_i^s and activity coefficients at infinite dilution γ_i^∞ the separation factor at infinite dilution α_{ij}^∞ for the binary system can be calculated:

$$\alpha_{12}^\infty = \frac{\gamma_1^\infty P_1^s}{\gamma_2^\infty P_2^s}$$

The entrainer should alter the activity coefficients of the components to a different extend, in order to reach separation factors far from 1. Since the entrainer should not introduce new azeotropes, the boiling point or vapor pressure difference between entrainer and binary mixture must be sufficient. For a convenient recovery of the entrainer its boiling point must usually be sufficiently higher (e.g., $\Delta T = 40$ K) than for any component of the mixture to be separated. Recent investigations have demonstrated the use of low-boiling solvents in so-called “reverse extractive distillation” processes, but the amount of solvent has to be increased enormously to ensure a sufficient liquid concentration of the entrainer. Moreover, the enthalpy of evaporation affects the energy balance of the process negatively. Thus, this kind of process will probably only be competitive when no suitable high-boiling solvent is available.

It is also possible to switch off the boiling point/vapor pressure condition when the user puts in the value 0. This allows in one-step to find entrainers both for extractive distillation and reverse extractive distillation.

If the criteria melting point, viscosity and boiling point or vapor pressure difference are fulfilled, all solvents are chosen which show a sufficient separation factor. Additionally, it will be checked, if the new solvents show zeotropic behavior with the components to be separated.

2.3 Azeotropic Distillation

For the azeotropic distillation, there are two different processes available. On the one hand, entrainers are chosen which introduce at least one further extreme-boiling binary azeotrope. On the other hand, entrainers are selected which introduce a low-boiling ternary heterogeneous azeotrope.

Tab.1 Criteria for solvents when components 1 and 2 form a pressure maximum azeotrope or no azeotrope

Case A	Case B
<ul style="list-style-type: none"> • Introduction of at least one further binary azeotrope with pressure maximum 	<ul style="list-style-type: none"> • Introduction of a low boiling ternary azeotrope
<ul style="list-style-type: none"> • Homogeneous or heterogeneous 	<ul style="list-style-type: none"> • Heterogeneous
<ul style="list-style-type: none"> • For a given pressure: $T_{az,1-3}$ or $T_{az,2-3} < T_{az,1-2} - 2.0$ K • For a given temperature: $P_{az,1-3}$ or $P_{az,2-3} > P_{az,1-2} + 20$ mmHg 	<ul style="list-style-type: none"> • For a given pressure: $T_{az,1-2-3} < T_{az,1-2} - 2.0$ K • For a given temperature: $P_{az,1-2-3} > P_{az,1-2} + 20$ mmHg

Tab.2 Criteria for solvents when components 1 and 2 form a pressure minimum azeotrope

Case A	Case B
<ul style="list-style-type: none"> • Introduction of at least one further binary azeotrope with pressure minimum 	There are no ternary heterogeneous azeotropes with a pressure minimum! => The program stops.
<ul style="list-style-type: none"> • Homogeneous 	
<ul style="list-style-type: none"> • For a given pressure: $T_{az,1-3}$ or $T_{az,2-3} > T_{az,1-2} + 2.0$ K • For a given temperature: $P_{az,1-3}$ or $P_{az,2-3} < P_{az,1-2} - 20$ mmHg 	

In all cases, the method for calculating the fugacity coefficients must be specified (ideal, Tsonopoulos or DIPPR), in order to consider the vapor phase reality.

2.4 Selectivity

Beside the extractive and azeotropic distillation it is also possible to evaluate a solvent only on its selectivity. The selectivity is the quotient of the activity coefficients of the two components in the solvent and should be far from 1 for a good solvent. This can be useful if a wider range of solvents with no or little information beside the activity information should be evaluated.

2.5 Results

Exclude from list

Components without Boiling Point Information Components without Viscosity Information

Components without Melting Point Information Components without Density Information

Components without Azeotropic Information for 1-2/1-3 Components with $|T(\alpha)-T(\text{System})| > 5K$

Components without LLE Information Component without Surface Tension Information

Visible columns

Vapor Pressures Surface Tension Separation Factor

Melting Point Names Selectivity

Density Azeotropic Information Capacity

Viscosity LLE Information

Components to be Separated:

DDB No.	Name	Formula	Ps [kPa]	CAS No.
(1) 31	Benzene	C6H6	36.18	71-43-2
(2) 50	Cyclohexane	C6H12	36.25	110-82-7

Given System Temperature = 323.15 [K]

Azeotropic data for system (1)-(2):
homPmax at P = 40.01 kPa

List of Entrainers (Extractive Distillation)

Source of Activity Coefficients: DDB for Activity Coefficients at Infinite Dilution
Source of Azeotropic Information: DDB for Azeotropic Data

Table Sorted by Separation Factors

DDB No.	Entrainer	Ps [kPa]	Tm [K]	Viscosity [mPas]	alpha(1) (T i)
701	Formamide	n.a.	275.65	1.929	0.103 (3
546	Monoethanolamine	n.a.	283.50	7.730	0.105 (3
151	Dimethyl sulfoxide	0.43	291.69	1.344	0.118 (3
1223	N-Formylmorpholine	0.10	295.86	4.176	0.131 (3
956	Butanenitrile	9.09	161.00	0.420	0.138 (3
8	1,2-Ethanediol	0.09	261.65	7.357	0.143 (3
728	Propylene carbonate	n.a.	218.15	n.a.	0.154 (3
284	N-Methyl-2-pyrrolidone	0.25	249.70	1.170	0.156 (3
563	Ethylene glycol diacetate	0.24	242.15	n.a.	0.162 (3
1285	Tetraethylene glycol	n.a.	266.95	n.a.	0.167 (3
227	N,N-Dimethylacetamide	0.98	251.42	0.679	0.182 (3

2.5.1 Limited Views

The display of components can be filtered by several criteria. The *Exclude from list* criterion allows suppressing components for which some of the required information is not available.

The *Visible columns* criteria allow some specified columns to suppress. The normal result table is often too wide even for a landscape mode print. Suppressing unused columns allows the print to fit again.

2.5.2 Sorting

This entrainer list can be arranged by different criteria:

<i>criteria</i>	<i>function</i>
Selectivities	sort by selectivities
Separation factors	sort by separation factors
Boiling points / Vapor pressures	sort by boiling points / vapor pressures
Melting points	sort by melting points
Surface tensions	sort by surface tensions
Viscosities	sort by viscosities
Densities	sort by densities
Component class	sort by component classes (based on mod. UNIFAC (Do) main groups): alkanes, aromatics, alcohols, water, ketones, esters, ethers, amides, halogenated compounds, unsaturated compounds, aldehydes, carbonic acids, other components
DDB code no.	sort by DDB code no.
Azeotropic information	sort by azeotropic information
LLE information	sort by LLE information

2.5.3 Links

The result table contains two types of links (green underlined text): A mouse-click on the DDB component numbers besides the component names opens a context menu allowing to display several further information for the solvent.

The links next to the selectivity columns are links to explanations like

Remark <*>: Extrapolated activity coefficients for at least one component

3 Extraction (LLE)

3.1 Introduction

The “Extraction (LLE)” program adds many new features to the solvent selection for liquid-liquid extraction, like, for example, the search for solvent mixtures or the use of experimental ternary and quaternary liquid-liquid-equilibria. Additionally, the density difference between the two liquid phases is calculated and the program estimates how difficult it would be to separate all components by distillation after the extraction step.

This software package does not only rely on the activity coefficient at infinite dilution for the solvent selection, but it also uses the actual distribution coefficients of the different components between the two liquid phases. The distribution coefficients show a more accurate description of the reality and can be directly used to estimate the value of the solvents for the given separation problems.

3.2 Program Description

The dialog allows users to define the separation problem. Furthermore, the procedure and the weight of different properties for the selection of solvents can be influenced.

On the top of the dialog (“System” area) the components which should be separated can be defined either by DDB Components or by a direct input of their DDB numbers. Two components are allowed if the experimental database is used. If the calculation is based on a predictive model up to 4 components are possible.

The “Check Parameter” button allows the user to control if all needed parameters for the chosen model for the calculation with the given components are available. The “Diluted?” check boxes can be used to mark components which are only available in small concentrations in the feed. These components are not considered to be the primary component of the raffinate phase. This option also allows marking components which should be considered for extraction. If we look for solvents which should extract component A out of a feed consisting of A and B, A can be marked as diluted.

The “Basic Settings” area allows the user to define the extraction temperature and pressure (pressure only for equations of state) and a minimum limit for the separation factor of the liquid-liquid-extraction. The fitting prediction model or experimental database (LLEDDB or ACTDDB) for the solvent selection are chosen with the drop box “database”. For ACTDDB the preferred experimental source can also be defined with the magnifying glass button.

When prediction models are used as database the considered solvents can be defined (“Preselected Components”). The program starts always with a default list of common solvents. This list can be modified with the “Select” or “Load List” button, or the list can be ignored and all components of the DDB are used for the solvent selection (“Use All Components (Ignore List)”). This could lead to a time-consuming calculation.

The “Default list” button resets the list.

Additional settings are given in the “Options area” to specify the process of solvent selection. If the option “Search for Solvent Mixtures” is activated the program tries to find suitable solvent mixtures out of the combination of the suitable pure solvents. Additional mixtures can be defined in the table “User Defined Mixtures” with the help of the DDB numbers of the two solvents and the concentration of the binary mixture. They are considered if the option “Calculate User-Defined Mixtures” is marked.

The program normally uses mole fractions to calculate the distribution coefficients and the solvent loss. It is often more realistic to use weight fractions, so this possibility is given with the option “Use Weight Fractions for Distribution Coefficients”.

The quality of a solvent for the given separation is directly estimated with the help of four criteria. Each of these criteria can be weighted with the given factors in the “Weight Factors” area. If one of the criteria should not be considered it can be set to zero.

The following criteria are used:

- Capacity

The capacity shows how easy a solvent can extract the wanted component and how much solvent is needed. For its calculation the distribution coefficients of the extracted components or, in the case of using the activity coefficient database (ACT), the inverse activity coefficient of the extracted component in the solvent are used.

$$K_i = \frac{X_{i,E}}{X_{i,R}} \quad Sp_i = \frac{1}{Y_{i,S}^\infty}$$

- Selectivity

A high value for the solvent selectivity shows a good separation performance for the given components with a liquid-liquid extraction. The separation factors α are used for its calculation. If the ACT database is used, the quotient of the activity coefficients of the components, which are to be separated, in the solvent "Sa" is a measure for the selectivity.

$$\alpha_{ij}^{ext} = \frac{K_i}{K_j} \quad Sa_{ij} = \frac{Y_{i,S}^\infty}{Y_{j,S}^\infty}$$

- Solvent Loss

A high solvent loss to the raffinate phase leads to an inefficiency in the extraction column because this solvent has to be recycled costly. It can be estimated with the concentration of the solvent in the raffinate phase or the activity coefficient of the solvent at infinite dilution in the raffinate component.

$$solvent\ loss = \frac{1}{Y_{S,R}^\infty}$$

- Distillation

After the extraction the solvent is normally separated from the other components by distillation. The program uses the worst separation factor, which is estimated during the binary VLE calculations between the solvent and each component as the measure for the distillation efforts. It is considered as the bottleneck of this operation.

The equation for the selection criterion combines all these criteria:

$$\left[\sum_{i=1}^{ne} \sum_{j=1}^{nr} \frac{K_{E(i)}}{K_{R(j)}} / (nc - 1) \right]^{ws} \cdot \left[\sum_{i=1}^{ne} \frac{K_{E(i)}}{ne} \right]^{wc} \cdot (1 - X_{S,R})^{wsl} \cdot \log(\alpha_{IS}^{dis})^{wsd}$$

with

nc = number of components

ne = number of components in the extract phase

nr = number of components in the raffinate phase

ws = weight selectivity

wc = weight capacity

wsl = weight solvent loss

wsd = weight distillation

$E(i)$ = component i in the extract phase

$R(j)$ = component j in the raffinate phase

$X_{S,R}$ = solvent in the raffinate phase

α_{IS}^{dis} = Worst separation factor of a connected distillation

K = distribution factor $X_{i,e}/X_{i,r}$

Higher values show always a better property of the examined solvent for this criterion. All criteria are summarized with the help of the selection criterion.

The equation is shown when the “button is used. The best solvent will have the highest values for this selection criterion.

The “Entrainer Selection” button starts the calculation.

The calculation can be interrupted by the “Stop”-button.

3.3 The Calculation

During the calculation the program always estimates which of the given components will be the main component in the raffinate phase for the used solvent. It is the component which shows the least effort to migrate from the feed into the solvent and is not diluted. After that the binary LLE between this component and the solvent and the distribution of the other component/s at infinite dilution between these two liquid phases is calculated. This procedure is reasonable because most of the extraction steps will take place under this condition. Furthermore, the results for all solvents are comparable. Other mixture properties (like azeotropic behavior) are calculated for binary systems between the solvent and each of the given components. The solvent properties are also estimated for the pure solvent and the solvent mixture.

3.4 Results

mod. UNIFAC (Dortmund) T=300 K		Solvent		Distribution Extract--- --->Raffinat e		Distribution Coefficients by Mole Fractions		Separation factors		LLE Component B/Solvent			
#	Selection Criterion	Solvent #1	Solvent #2	Conc. Solvent #1 [mole%]	A	B	K 31	K 50	K(A)/K(B)	Comp. B in extract phase [mole%]	Comp. B in raffinate phase [mole%]	Density extract phase [kg/m ³]	Density raffinate phase [kg/m ³]
35	10.522	[123] N-Formylmorpholine			31	50	0.99668	0.08124	12.27	7.895	97.186	1113.42	781.87
34	5.6882	[168] 2-Pyrrolidone			31	50	0.67002	0.09736	6.88	9.287	95.392	1063.97	783.18
24	4.8138	[443] Triethylene glycol			31	50	0.52355	0.07006	7.47	6.998	99.885	1098.01	772.65

Azeotropic information				Alpha Distillation				Solvent Properties						Solvents		
AZDType 31	AZD y 31 [mole%]	AZDType 50	AZD y 50 [mole%]	alpha for x(31)->1	alpha for x(31)->0	alpha for x(50)->1	alpha for x(50)->0	Ps [kPa] Solvent	Tm [K] Solvent	Sft. [mM/m] Solvent	Vis. [mPas] Solvent	Flash Point [K] Solvent	Lower Explosion Limit [Vol%] Solvent	Upper Explosion Limit [Vol%] Solvent	Name Solvent 1	Name Solvent 2
none		none		39.99	80.50	168.55	8.27	0.0218	295.86		7.420				N-Formylmorpholine	
none		none		57.42	9928.31	99.75	855.49	1.18E-006	266.95		40.665				Tetraethylene glycol	
none		none		72.89	121.41	152.55	39.68	0.00161	299.10		12.129				2-Pyrrolidone	

The “Result table” shows the results of the different databases for the solvent selection. There are some options to adapt the result sheet to the user’s needs. Solvents which have a high viscosity or a low flash point can be excluded from the list. Also, solvents with no information for these two properties can be suppressed. This can also be done for solvents with a homogeneous azeotrope between the solvent and one of the components. If the ACT database is used it can also happen that there is no information about the liquid-liquid equilibria. These solvents can also be excluded. The result list can be sorted by the values of a chosen column when a left click is done on the header of the column.

The different information areas for the solvents are classified by color in the results sheet. Single red cells show a bad property of a solvent.

- the first column contains the selection criterion. The sorting of the table is related to the values in this column.
- the short solvent names and its DDB numbers are given (“Solvent” column). In a case of a binary solvent mixture the concentration of the first named solvent in the mixture is also given.

- the column “Distribution” shows which components are more likely to be extracted (left side) by the given solvent or which components will stay mainly in the raffinate phase. The component in the last column is the main raffinate component for this solvent (see calculation description).
- in the next main column, the distribution coefficients of the different components are displayed.
- the separation factors are calculated in relation to the distribution coefficient of the main component of the raffinate phase.
- the column “LLE Component / Solvent” contains the information of the binary liquid-liquid equilibria between the solvent and the main component of the raffinate phase and the densities of the two liquid phases.
- the following columns (“Azeotropic information”) show the azeotropic behavior at a pressure of 1 bar between the solvent and each component. If an azeotrope was detected its concentration is also given.
- the next columns (“Alpha distillation”) give the separation factor for a distillation at 1 bar between the solvent and the components in their diluted regions.
- the table is closed with the solvent properties and the complete solvent names.

When the experimental database is used, no separation factors α for the distillation are estimated. The activity coefficient database uses also other values for the selectivity and capacity.

Example: The program estimated that N-Formylmorpholine is the best solvent for the separation of Benzene and Cyclohexane (see picture). The third main column shows that it extracts Benzene (DDB number is #DDB=31) out of Cyclohexane (#DDB=50). It shows with $K=0.99660$ a better distribution coefficient for the extracted benzene than the two other shown solvents and it has with 12.27 a higher separation factor. N-Formylmorpholine and Cyclohexane have a wide miscibility gap, too. The raffinate phase nearly completely exists of Cyclohexane (97.186 mole %) which results in a low solvent loss. The density difference ($1119.42 \text{ kg/m}^3 \leftrightarrow 781.87 \text{ kg/m}^3$) is very large, so that the phase separation between the two liquid phases should be fast. The corresponding distillation is also easy because there is no azeotropic behavior between the solvent and the components and the separation factors of the distillation are far away from one. The pure solvent properties show that the solvent is liquid and has a low viscosity.

4 Absorption

4.1 Introduction

Besides the extractive and azeotropic distillation process and liquid-liquid extraction absorption is a further important separation process widely used. The goal of the absorption process is to separate components from a gas stream by using an appropriate absorbent. Contrary to the extractive and azeotropic distillation process which use energy and a solvent the absorption and liquid-liquid extraction processes use only a solvent as separating agent. The program can search for solvent mixtures and can use molality-based Henry coefficients. Additionally, it uses a sophisticated selection criterion for the performance evaluation of the solvents, which consists of the selectivity, the capacity and the solvent loss.

4.2 Program Description

The starting dialog allows to define the separation problem and to weight the criteria for the evaluation of the solvent performance.

On the top of the dialog ("System" area) the components which should be separated can be defined either by DDB Components („Add Component"-button) or by a direct input of their DDB numbers. Two components are allowed if the experimental database is used. If the calculation is based on a predictive model up to 4 components are possible. The „Check Parameter"-button allows the user to control if all needed parameters for the calculation with the given components for the chosen model are available. The "DDB/All Gases" button shows all GLE and HPV datasets of the Dortmund Databank, which contain the given solvents.

The "Basic Settings" area allows the user to define the absorption temperature and a minimum separation factor for the absorption process. The prediction model or experimental database (GLE + HPV) for the solvent selection are chosen with the drop box "database".

The considered solvents can be defined in the "Preselected Components" area. The program starts always with a default list of common solvents. This list can be modified with the "Select" or "Load List" button, or the list can be ignored and all components of the DDB can be used for the solvent selection ("Use All Components (Ignore List)"). This could lead to a time-consuming calculation. The "Default list"-button resets the list. If the experimental database is chosen and the "Use all Components (Ignore List)" option is not used, artificial data can be created by models with the "Create Artificial Data" button. This will open an additional menu, which show all given datasets. The "Add" button opens a calculation menu for the components pair in the same line. The value are returned by the "Predict (Result => Query Result)" button.

Additional settings are given in the "Options" area to specify the process of solvent selection. If the option "Search for Solvent Mixtures" is activated the program tries to find suitable solvent mixtures out of the combination of the suitable pure solvents. Additional mixtures can be defined in the table "User Defined Mixtures" with the help of the DDB numbers of the two solvents and the concentration of the binary mixture. They are considered if the option "Calculate User-Defined Mixtures" is marked. Normally the program uses mole fraction-based Henry coefficients. Often it is better to use molality-based Henry coefficients to compare solvents with a different molecular weight. This feature can be chosen with the button "Use molality-based Henry Coefficients".

The quality of a solvent is directly estimated with the help of the given three criteria which can be weighted with the given factors ("Weight Factors" area):

Capacity

The capacity shows how easy the gas can be solved in the solvent. For the calculation the inverse Henry coefficient is used.

$$C_i = \frac{1}{H_{i,S}}$$

Selectivity

A high value for the solvent selectivity shows a good separation performance for the given gases with the absorption process. The selectivity is the quotient of the Henry coefficients of the given gases in the same solvent.

$$\alpha_{ij}^{\infty} = \frac{H_{j,S}}{H_{i,S}}$$

Solvent loss

A high solvent loss increases the amount of solvent which is needed overtime. It is linked to the vapor pressure of the used solvent.

All criteria are combined in the following equation for the selection criterion:

$$\left[\sum_{i=1}^{na} \sum_{j=1}^{ng} \frac{H_{j,S}}{H_{i,S}} / (nc - 1) \right]^{ws} \cdot \left[\sum_{i=1}^{na} \frac{1}{H_{i,S}} / na \right]^{wc} \cdot \left[\frac{1}{1 + \log(1 + P_S^s)} \right]^{wsl}$$

nc = number of components

na = number of absorbed components

ng = number of components in the vapor phase

ws = weight selectivity

wc = weight capacity

wsl = weight solvent loss

$H_{i,S}$ = Henry coefficient of component i in the solvent phase

P_S^s = vapor pressure of the solvent

Higher values of the different terms show always better properties of the examined solvent for the given separation problem. The selection criterion summarizes all criteria to be able to estimate a global performance value to compare the different solvents. The best solvent will have the highest value for the selection criterion.

The calculation is started with the “Calculate/Search”-button. If “exp. Database (dataset file)” is chosen, the needed dataset file can be opened.

4.3 Calculation

During the calculation the programs estimates how good the different gases can be solved in the given solvents. It sorts the different gases in order of their values of the Henry coefficient for the given solvent and estimates the selectivity between the gases. With the help of these values a list of absorbed and not absorbed gases for each solvent is estimated. This procedure makes the result between the different solvents comparable.

4.4 Results

“The Result table” shows the results of the different databases for the solvent selection. There are some options to adapt the result sheet to the user’s needs. Solvents which have a high viscosity or a low flash point can be excluded from the list. In addition, solvents with no information for these two properties can be suppressed.

PSRK T=300 K		Solvent			Distribution Gas<--- --->Absorbed			Henry Coefficients by Mole Fractions			Separation factors	
#	Selection Criterion	Solvent #1	Solvent #2	Conc. Solvent #1 [mole%]	A	B	C	H 1051 [bar]	H 1065 [bar]	H 1050 [bar]	H(A)/H(B)	H(A)/H(C)
6	4.7612	[15] Formic acid			1051	1050	1065	59682.82400	47.90760	142.06439	420.11	1245.79
16	3.514	[75] 1,4-Dioxane			1051	1050	1065	455.29934	6.31588	56.13468	8.11	72.09
7	3.1913	[18] Methoxybenzene			1051	1050	1065	541.62569	8.96970	71.75166	7.55	60.38
45	2.5743	[284] N-Methyl-2-pyrrol...			1051	1050	1065	1129.83830	6.27546	68.40287	16.52	180.04

Solvent Properties							Solvents	
Ps [kPa] Solvent	Tm [K] Solvent	Sft. [mN/m] Solvent	Vis. [mPas] Solvent	Flash Point [K] Solvent	Lower Explosion Limit [Vol%] Solvent	Upper Explosion Limit [Vol%] Solvent	Name Solvent 1	Name Solvent 2
6.208	281.45	36.813	1.552	315.15	10.0	45.5	Formic acid	
5.329	284.85	32.646	1.154	284.15	1.9	22.5	1,4-Dioxane	
0.5404	235.65	33.301	0.965	314.15	1.2		Methoxybenzene	
0.05284	249.70		1.628	359.15			N-Methyl-2-pyrrolidone	

The different information areas for the solvents are classified by color in the results sheet. Single red cells show a bad property of a solvent.

- The first column contains the selection criterion. The sorting of the table is related to the values in this column.
- The short solvent names and its DDB numbers are given (“Solvent” column). In a case of a binary solvent mixture the concentration of the first named solvent in the mixture is also given.
- The column “Distribution” shows which gases are more likely to be absorbed (right side) by the given solvent or which components will stay mainly in the gas phase. The component in the last column is the best absorbed component for this solvent.
- In the next main column, the Henry coefficients of the different gases are displayed.
- The separation factors are calculated in relation to the Henry coefficient of the least absorbed gas.
- The table is closed with the solvent properties and the complete solvent names.

5 Literature

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