Prediction of Ionic Liquids Performance for Hydrogen Sulfide Absorption from Natural Gas using COSMO-RS

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Abstract. The capability of ionic liquids (ILs) in various applications makes them attracted by many researchers. They have potential to be developed as “green” solvents for gas separation, especially hydrogen sulfide (H₂S) gas. In this work, it is attempted to predict the solubility of H₂S in ILs by COSMO-RS method. Since H₂S is a toxic pollutant, it is difficult to handle in the laboratory, therefore an appropriate model will be necessary in prior work. The COSMO-RS method is implemented to predict the Henry’s law constants and activity coefficient of H₂S in 140 ILs with various combinations of cations and anions. It is found by the screening that more H₂S can be absorbed in ILs with chloride ([Cl]-) and acetate ([Ac]-) anion. The solubility of H₂S in ILs with different alkyl chain at the cations not much affected and with different type of cations are slightly influence H₂S capture capacities. Even though the cations do not affect much in solubility of H₂S, the effectiveness of cation still need to be considered in different way. The prediction results only show their physical absorption ability, but the absorption of H₂S need to be consider chemically to get high capacity of absorption of H₂S.

1 Introduction
H₂S is an acid gas contaminant produced along with methane (CH₄), and carbon dioxide (CO₂) in natural gas fields, crude petroleum, biogas and syngas [1]. The problem with the presence of H₂S gas in natural gas, it is corrosive and can erode the metals in tanks, piping, valves and pumps, moreover its highly toxic which can cause environmental catastrophe [2]. In addition to hazardous effects of H₂S to human health like olfactory paralysis if the H₂S exposure concentration is more than 140 ppm and can cause to death if the H₂S concentration is more than 700 ppm [3]. Therefore, removal of H₂S from the raw natural gas is important for safe transportation, storage and fuel-source utilization.

H₂S and CO₂ from natural gas stream are usually removed using several technologies like absorption [4], adsorption [5], and conversion [6] process. Among all the technologies, absorption process is widely applied in large capacity gas treatments. Aqueous alkanolamine solutions is widely used industry solvent to remove H₂S from industrial natural gas. However, in the commercial use of alkanolamine solutions, there are some drawbacks, including loss of the alkanolamine, transfer of water to the gas stream during the desorption process and the form of corrosive by-production in the degradation of alkanolamines, which make the process economically expensive [7]. Furthermore, the absorption selectivity remains
unsatisfactory and hence, the need for substituent solvent with efficient absorption capacity is always on demand.

ILs are the alternative materials which are investigated as new potential solvents for natural gas industry treating processes. ILs are greener solvents that can potentially replace the use of amines for H₂S absorption. The uniqueness of ILs is the possibility of tuning the properties of ILs depending on the application by altering the anion-cation combination. Physicochemical properties like viscosity, density, melting point, acidity, basicity, water miscible and polarity of ILs can be controlled by selection of the cation and anion [8]. In recent years, a lot of studies were focused on CO₂ capture and there are various ILs were reported [9]. However, only a few studies have been reported for H₂S capture using ILs. In the last 10 years, the studies have been carried out to evaluate the ability of conventional room temperature ILs (RTILs) or functionalized ILs in H₂S absorption process [10]–[15]. It is reported that H₂S separation is possible using ILs by experimentally. However, the solubility of H₂S remain low at atmospheric pressure or at low pressure. In this study, new ILs is proposed to achieve high absorption capacity of H₂S at low pressure. ILs can be functionalized to be task specific ILs, ensuring highly efficient and selective separation.

In order to select suitable ILs for H₂S absorption, the screening of ILs is very important to predict the interaction between ILs with H₂S. While in recent years experimental data on ILs have been studied, predictive models have always been useful in the design of chemical engineering processes. and only small number of literatures has been reported. There are several methods that have established correlations for the prediction of ILs properties such as Equation of States (EOS) [16], [17], Molecular Simulation [18], Group Contribution Models (GCM) [19] or Correlation Model [20], [21]. However, the limitation of models which is unable to predict accurately the solubility of the systems and limitation to explore wide range combination of different cation and anion to classify suitable solvent or ionic liquid for H₂S absorption. COSMO-RS is an advanced software tool developed by Klamt et al. [22] that provides another approach to predicting thermodynamics properties of fluids for different systems, including ILs. In this work, COSMO-RS is used to screen the solubility of H₂S in variety of cations and anions combinations. By using the COSMO-RS models, the thermodynamic properties such as the Henry’s law constant and activity coefficient will be predicted, accordingly ILs will be selected for further functionalization to produce task specific ILs for the selective absorption of H₂S.

2. Computational Methods

2.1 COSMO-RS Method

COSMOthermX is a Graphical User Interface to the COSMOtherm command line program [23]. It allows for the Interactive use of the COSMOtherm program such as compounds selection, input files preparation, program runs and show of the calculation results. The flow chart of COSMO-RS software operation for screening ILs is shown in Figure 1.
Figure 1. COSMO-RS operation for screening ILs.

The COSMO-RS calculation start with the selection of compounds from database or the file manager in COSMOTHERM and the new compounds can be search in all database or online by name, SMILES, CAS-Number, 2D structure and 3D structure. A 3D structure can also be generated using TURBOMOLE [1]. Then, followed by the selection of setting for the calculation of properties. Different input might be required for each property and usually the solvent composition and the temperature must be given. The mixture properties for ILs and H2S are set at temperature 25°C and atmospheric pressure [23].

The two ILs components (cation and anion) are given as individual compounds in the COSMOTHERM input file. Therefore, it should be noted in the interpretation of the COSMOTHERM results for the calculated thermodynamic properties. As per suggested by Diedenhofen et al., ILs are considered as equimolar mixtures of cations and anions ($n_{\text{ion}} = n_{\text{cation}} = n_{\text{anion}}$) in COSMOTHERM calculation [24]. With that boundary condition, the calculation is based on a ternary mixture: cation, anion, solute i (H2S). Hence for ternary system the composition of solute in the ternary system is given by equation (1):

$$x_{i}^{\text{ternary}} = \frac{n_i}{n_i + 2n_{\text{ion}}}$$  \hspace{1cm} (1)

On the other hand, experimental determination of the thermodynamic properties of the ILs assumes a binary system consisting of the IL and the solute as stated in equation (2):

$$x_{i}^{\text{binary}} = \frac{n_i}{n_i + n_{\text{IL}}}$$  \hspace{1cm} (2)
These two definitions are just different perspectives on the same system. Therefore, any calculated value corresponds to both the mole fraction definitions. Where,

\[ x^\text{binary}_i = \frac{x^\text{ternary}_i}{x^\text{ternary}_i + x^\text{ion}_i} \]  

(3)

2.2 Property Calculation

The mixture properties for ILs and H$_2$S are set at temperature 25°C and atmospheric pressure. All the COSMO-RS calculations were implemented with the COSMOtherm program, which offers an efficient performance of the COSMO-RS method.

2.2.1 Henry’s Law Constant. Henry’s Law constants can be determined directly from COSMOtherm program and is defined as:

\[ K_H = \frac{p}{x_{(i)}} \]  

(4)

where \( K_H \), \( p \), and \( x_{(i)} \) are the Henry’s Law constant, the studied pressure and the solubility of the gaseous solute in the solvent (ILs) expressed in mole fraction, respectively.

2.2.2 Selectivity and Capacity of ILs at Infinite Dilution. Activity coefficients \( (\gamma^\infty) \) of H$_2$S and CO$_2$ in ILs at infinite dilution were calculated using COSMOtherm program. The selectivity (S) and the capacity of ILs at infinite dilution were derived in equation (5).

\[ S^\infty_1 = \left( \frac{\gamma^\infty_2}{\gamma^\infty_1} \right)^{IL \ phase} \]  

(5)

Where ‘1’ and ‘2’ refer to H$_2$S and CO$_2$, respectively. The capacity \( (C^\infty_1) \) of ILs to accommodate H$_2$S was calculated by the equation (6).

\[ C^\infty_1 = \left( \frac{1}{\gamma^\infty_1} \right)^{IL \ phase} \]  

(6)

The performance index (PI) showed the overall performances of the ILs, considering both capacity and selectivity.

\[ PI = C^\infty_1 \times S^\infty_1 = \left( \frac{1}{\gamma^\infty_1} \right)^{IL \ phase} \times \left( \frac{\gamma^\infty_2}{\gamma^\infty_1} \right)^{IL \ phase} \]  

(7)

Therefore,

\[ PI = \left( \frac{\gamma^\infty_2}{(\gamma^\infty_1)^2} \right)^{IL \ phase} \]  

(8)
2.3 Hunting the ILs for H₂S Absorption by Solubility Prediction

2.3.1 Screening of common cations and anions.

By combining various cations and anions, the ILs can be designed. There are two stage of selection type of cations and anions. For the first stage, 20 cations and 5 anions are chosen to combine 100 ILs. The cations include imidazolium, pyridinium, pyrrolidinium and piperidinium with 4 alkyls substituted. The anions include tetrafluoroborate, hexafluorophosphate, bis (trifluoromethyl-sulfonyl) imide, chloride and acetate. Note that all the cations and anions are the common ILs used by researchers. All the structure of ILs are listed in Error! Reference source not found.. They are identified for H₂S-ILs screening in COSMO-RS simulations. The listed ILs will be screened for their suitability for H₂S absorption.

| Name of Cation and Anion | Abbreviation | Structure |
|--------------------------|--------------|-----------|
| 1-‘R’-3-methylimidazolium; R=C₂H₅, C₄H₉, C₆H₁₃, C₈H₁₇ | [‘R’ mim]⁺ | ![Structure](structure1.png) |
| 1-‘R’pyridinium; R=C₂H₅, C₄H₉, C₆H₁₃, C₈H₁₇ | [‘R’ py]⁺ | ![Structure](structure2.png) |
| 1-‘R’-1-methylpyrrolidinium; R=C₂H₅, C₄H₉, C₆H₁₃, C₈H₁₇ | [‘R’ mpyrr]⁺ | ![Structure](structure3.png) |
| 1-‘R’-1-methylpiperidinium; R=CH₃, C₄H₉, C₆H₁₁, C₈H₁₃ | [‘R’ mpip]⁺ | ![Structure](structure4.png) |
| 1,1-dimethyl-ethyl-ammonium | [DiEAmm]⁺ | ![Structure](structure5.png) |
| Triethylpentylammonium | [TriPAm]⁺ | ![Structure](structure6.png) |
| Tetramethylammonium | [TemAm]⁺ | ![Structure](structure7.png) |
| Tetra-ethylammonium | [TeEAmm]⁺ | ![Structure](structure8.png) |
| Hexafluorophosphate | [PF₆]⁻ | ![Structure](structure9.png) |
| Bis(trifluoromethylsulfonyl)imide | [Tf₂N]⁻ | ![Structure](structure10.png) |
| Tetrafluoroborate | [BF₄]⁻ | ![Structure](structure11.png) |
| Chloride | [Cl]⁻ | Cl⁻ |
2.3.2 Screening of specific (amine-based) ILs.

New ILs are designed based on the results in this work by tuning the selected cation. Then the designed ILs are screened using COSMO-RS method prior to detailed experimental measurements of specific 
task of the ionic liquids. The selection of cations and anions are based on the previous screening work 
using common ionic liquids. Ammonium was selected as a type of cation, while for anions were acetate 
and chloride. In order to get highly effective ILs for H\textsubscript{2}S absorption, tertiary amine-based was selected 
for cation and for anions were halide to predict the Henry’s law constant, capacity, selectivity and 
performance index. The structure of all cations and anions to be screening shown in Table 2.

Table 2. Chemical structure of specific cations and anions.

| Name of Cation and Anion | Abbreviation | Structure |
|--------------------------|--------------|-----------|
| N,N,N',N' – tetramethylene – 1,2 – diamine | [TMEDA]+ | ![Structure](image1) |
| N,N,N’,N’ – tetramethyl – 1,3 – propanediamine | [TMPDA]+ | ![Structure](image2) |
| N,N-dimethylethanolamine | [DMEA]+ | ![Structure](image3) |
| N,N,N’,N’ – tetramethyl – 1,6-hexanediarnine | [TMHDA]+ | ![Structure](image4) |
| N,N – dimethylbutylamine | [DMBA]+ | ![Structure](image5) |
| Bis(2,2-morpholinoethyl)ether | [BDMPEE]+ | ![Structure](image6) |
| Bis(2-dimethylaminoethyl) ether | [BDMAEE]+ | ![Structure](image7) |
| Chloride | [CL]- | ![Structure](image8) |
| Bromide | [BR]- | ![Structure](image9) |
| Acetate | [AC]- | ![Structure](image10) |
| Propionate | [PRO]- | ![Structure](image11) |
| Butyrate | [BU]- | ![Structure](image12) |
3. Results and Discussion

3.1 Screening of Common Cations and Anions

3.1.1 Henry’s law constant.

The Henry’s Law constants of H$_2$S in 100 ILs are predicted by COSMO-RS method at 25°C and at atmospheric pressure, given in Table 3. A graphical comparison of different effect of anion, cation and alkyl group are given in Figure 2, Figure 3 and Figure 4.

Table 3. The Henry’s law constant (bar) of H$_2$S in 100 ILs predicted by COSMO-RS at 25°C and at atmospheric pressure.

| Cation | Anion | \[PF_6\] | \[Tf_2N\] | \[BF_4\] | \[Cl\] | \[Ac\] |
|--------|-------|----------|----------|----------|------|----------|
| [Emim] | 2.1435 | 1.8643 | 1.8391 | 0.9552 | 1.0896 |
| [Bmim] | 1.8568 | 1.7523 | 1.6035 | 0.9758 | 1.0265 |
| [Hmim] | 1.9195 | 1.8535 | 1.6930 | 1.1488 | 1.1743 |
| [Omin] | 1.9011 | 1.8749 | 1.6742 | 1.1900 | 1.2005 |
| [Epy]  | 2.1334 | 1.8304 | 1.8695 | 0.9952 | 1.1327 |
| [Bpy]  | 1.9393 | 1.8027 | 1.7194 | 1.1119 | 1.1646 |
| [Hpy]  | 1.8721 | 1.8079 | 1.6651 | 1.1803 | 1.1958 |
| [Opy]  | 1.8494 | 1.8277 | 1.6392 | 1.2209 | 1.2199 |
| [Empyr] | 2.1801 | 1.8641 | 1.6555 | 0.6518 | 0.6950 |
| [Bmpyr] | 2.0482 | 1.8510 | 1.6274 | 0.7732 | 0.7477 |
| [Hmpyr] | 2.0076 | 1.8672 | 1.6219 | 0.8453 | 0.7805 |
| [Ompyr] | 1.9933 | 1.8915 | 1.6186 | 0.8909 | 0.8051 |
| [Mmpip] | 2.0129 | 1.8272 | 1.5664 | 0.7144 | 0.7028 |
| [Bmpip] | 1.9888 | 1.8348 | 1.5703 | 0.7615 | 0.7271 |
| [Penmpip] | 1.9791 | 1.8466 | 1.5740 | 0.7917 | 0.7391 |
| [Hmpip] | 1.9693 | 1.8581 | 1.5757 | 0.8223 | 0.7580 |
| [DIEAm] | 2.6643 | 2.5032 | 3.3646 | 3.5318 | 3.8382 |
| [TriPAm] | 1.7301 | 1.6961 | 1.3062 | 0.5936 | 0.5331 |
| [TeAmm] | 2.8260 | 2.0038 | 2.2761 | 0.6843 | 0.9384 |
| [TeEAmm] | 1.8027 | 1.6896 | 1.3186 | 0.5288 | 0.5177 |

From the equation (4), the higher Henry’s Law constant indicates the lower solubility. Based on Figure 2, it can be found that the ILs with anions [Cl] and [Ac] can capture more H$_2$S. With same cation, for example [TriPAm] the Henry’s law constants are 1.73, 1.70, 1.31, 0.59 and 0.533 bar for anions \[PF_6\], \[Tf_2N\], \[BF_4\], [Cl] and [Ac] respectively. The solubility of H$_2$S in [TriPAm][Cl] is about three times higher than in [TriPAm][PF$_6$]. It shows that the small and highly coordinating anion can give
strong hydrogen bond interactions. Therefore, the effect of anion needs to be considered in designing new task specific ionic liquids.

Figure 2. Effect of anions on the solubility of H$_2$S in [TriPAmm]-based ILs at 25°C and at atmospheric pressure.

In addition, the ILs with different type of cation include imidazolium, pyridinium, pyrrolidinium, piperidinium and ammonium were slightly influence the solubility of H$_2$S in those ILs. As shown in Figure 3, the lowest value of Henry’s law constant was from group ammonium though [DiEAm] was the highest among all the screening ILs.

Figure 3. Effect of cation types on the solubility of H$_2$S in [Cl]-based ILs at 25°C and at atmospheric pressure.

The interaction between anion and cation should be weak with the longer alkyl chain, which allowed more space for the accommodation of H$_2$S. The predicted results from Figure 4. shows that henry’s law constant slightly increases with the increase of alkyl chain length for [Cl]-based ILs and the value almost the same around 1.0 to 1.2 bar. The predicted solubility of H$_2$S might affected moderately by the increasing of alkyl chain at cation. However, the alkyl chain important in the selection of ILs based on
their physical properties like viscosity and toxicity of cations. The viscosity and toxicity of ILs increased as the carbon chain increases from ethyl to octyl [25]. Therefore, it is better to choose potential ILs with low alkyl chain.

Figure 4. Effect of alkyl group on the solubility of H$_2$S in [Cl]-based ILs at 25°C and at atmospheric pressure.

From the predicted data of Henry’s Law constant by COSMO-RS software, the chosen of anion is important in designing new TSILs and even though the cations slightly affected the solubility of H$_2$S, the effectiveness of cation in H$_2$S absorption still need to be considered in different way. The prediction results only show their physical absorption ability, but the absorption of H$_2$S need to be considered chemically to get high capacity of absorption of H$_2$S.

3.2 Screening of Amine-based ILs

3.2.1 Henry’s law constant.

The Henry’s Law constants of H$_2$S in new designed ILs are predicted by COSMO-RS method at 25°C and at atmospheric pressure, given in Table 4. The effect of anion needs to be considered in designing new task specific ionic liquids. Based on the Table 4, it can be found that [TMPDA][Cl], [TMPDA][Br] and [TMPDA][MoAc] were the lowest value of Henry’s law constant which means highest solubility of H$_2$S in the ILs. It can be found that the ILs with anions [Cl] and [Br] have high H$_2$S. For example, the Henry’s law constants of [TMPDA]-based ILs were decreased from 1.179, 1.168, 1.158, 0.998, 0.885 and 0.880 bar for anions order [Pro] > [Bu] > [Ac] > [MoAc] > [Br] > [Cl]. The solubility of H$_2$S in [TMPDA][Cl] is higher than others. Furthermore, the prediction of Henry’s law constant of lowest value among cations was [TMPDA]. Then, the most effective ILs were from [Cl]-based and [TMPDA]-based ILs.

Table 4. The henry’s law constant (bar) Of H$_2$S in amine-based ILs predicted by COSMO-RS at 25°C and at atmospheric pressure.
3.2.2 Performance of ILs in H$_2$S Absorption.

Table 5 shows the prediction of COSMO-RS on ILs’ performance in the absorption of H$_2$S. Based on the PI results, [TMPDA][CL], [DMEA][CL], [TMPDA][MOAC], [DMBA][CL], BDMAEE][MOAC], [TMEDA][CL], [BDMAEE][CL] and [TMHDA][MOAC] were predicted to be the best ILs. PI was influenced by anions where the order [CL] > [MOAC] > [AC] > [PRO] > [BU] > [BR] decreased. The PI of [TMPDA]$^+$ was highest than other cations. This showed that [TMPDA]-based ILs could provide better results compared to other ILs in actual H$_2$S absorption experiment.

From the predicted data the selectivity of ILs at infinite dilution by COSMO-RS software, the chosen of anion is important in designing new TSILs. The selectivity was affected by anions. The order of the anions for selectivity data same observation as performance index data. The two highest results were [CL]$^-$ and [MOAC]$^-$. Meanwhile, [AC]$^-$ shows highest result among ester functional group. Anions with long alkyl chain were found to have low selectivity. The selectivity results of [MOAC]$^-$ was higher than [AC]$^-$ which means the additional oxygen in the chain can give high results. However, in halide group, chloride shows the highest value while bromide was the lowest among the anions.

The order of the capacity affected by anions slightly different from selectivity and PI values. However, [CL]$^-$ and [MOAC]$^-$ anions were still predicted to be the highest capacity. However, capacity values for [BR]$^-$ different based on cations. For cations, capacity value not much different when we compare the all the cations with same anion based. It can be observed that the cations did not give significant effect in H$_2$S absorption.

4. Conclusion

In this work, a series of ILs with different combinations of cations and anions are screened for H$_2$S absorption process. The prediction of Henry’s law constant, capacity, selectivity and performance index of ILs at infinite dilution are successfully identified by COSMO-RS model. Anions generally play more important role than cations, and common anions such [Cl], [Ac], [PF$_6$], [BF$_4$] and [TF$_2$N] were proposed in prediction of Henry’s law constant. Low Henry’s law constant indicates high solubility. [Cl] and [Ac] showed lowest Henry’s law constant and the results of both anions are around 0.5 bar. The solubility of [Cl] was about three times higher than [PF$_6$]. While type of cations was slightly influence H$_2$S solubility and the highest H$_2$S solubility predicted from the COSMO-RS was ammonium-based ILs.

The second part of screening method was prediction of capacity, selectivity and performance index of functionalized ILs at infinite dilution. The prediction result shows the best performance of ILs in H$_2$S absorption was [TMPDA][Cl] which is 53.55. The performance of ILs was not much affected by altering different cations. However, anions can affect the performance of ILs in H$_2$S absorption and the best performance of anion was [Cl]-based ILs. The longer alkyl chain in anions, the lower performance can be observed. Therefore, the best ILs for the H$_2$S absorption experiment was [Cl]-based ILs.

Table 5. COSMO-RS results on ILs’ performance in absorption of H$_2$S.

| COSMO-RS Prediction | Cation | Anion | [CL] | [BR] | [AC] | [PRO] | [BU] | [MOAC] |
|---------------------|--------|-------|------|------|------|-------|------|-------|
| [TMHDA]             | [BDMAEE] | [BDMPEE] | [TMEDA] | [TMPDA] | [DMEA] | [DMBA] | [TPMDA] | [TSIL] |
| 1.3160              | 1.2725 | 1.2181 | 1.2593 | 0.8808 | 1.8418 | 1.5246 | 1.6548 | 1.4089 |

| Anion | [Cl] | [Br] | [Ac] | [Pro] | [Bu] | [MoAc] |
|-------|------|------|------|-------|------|--------|
| [Cl]  | 1.3160 | 1.5618 | 1.3056 | 1.3531 | 1.3632 | 1.1788 |
| [Br]  | 1.2725 | 1.5353 | 1.2861 | 1.3386 | 1.3517 | 1.1718 |
| [Ac]  | 1.2181 | 1.4339 | 1.2265 | 1.2726 | 1.2842 | 1.1301 |
| [Pro] | 1.2593 | 1.3223 | 1.5007 | 1.5496 | 1.5467 | 1.3079 |
| [Bu]  | 0.8808 | 0.8852 | 1.1580 | 1.1792 | 1.1677 | 0.9976 |
| [MoAc]| 1.8418 | 2.3468 | 2.2720 | 2.3846 | 2.3755 | 2.0040 |
| [DMBA]| 1.5246 | 1.8597 | 1.5889 | 1.6548 | 1.6627 | 1.4089 |
| Capacity (C) | [TMHDA] | 9.5037 | 6.8273 | 9.4817 | 8.8634 | 8.6576 | 10.6179 |
|-------------|---------|--------|--------|--------|--------|--------|--------|
| Selectivity (S) | | 4.0446 | 2.6077 | 3.8161 | 3.5369 | 3.3634 | 3.9651 |
| Performance Index (PI) | | 38.4384 | 17.8033 | 36.1833 | 31.3487 | 29.1192 | 42.1004 |
| Capacity (C) | [BDMAEE] | 10.7909 | 7.5039 | 9.7941 | 8.9238 | 8.5867 | 10.6749 |
| Selectivity (S) | | 4.0047 | 2.7419 | 3.9843 | 3.7303 | 3.5477 | 3.9651 |
| Performance Index (PI) | | 43.2149 | 20.5751 | 39.0225 | 33.2884 | 30.4630 | 43.8487 |
| Capacity (C) | [BDMPEE] | 10.0061 | 7.4927 | 9.3605 | 8.6416 | 8.3615 | 10.1047 |
| Selectivity (S) | | 3.6944 | 2.6935 | 3.7396 | 3.5405 | 3.3902 | 3.8050 |
| Performance Index (PI) | | 36.9661 | 20.1816 | 35.0044 | 30.5957 | 28.3472 | 43.8487 |
| Capacity (C) | [TMEDA] | 10.3543 | 8.5451 | 7.7695 | 7.0564 | 6.8746 | 8.9742 |
| Selectivity (S) | | 4.2094 | 2.9003 | 3.8596 | 3.6066 | 3.4337 | 4.1244 |
| Performance Index (PI) | | 43.5849 | 24.7831 | 29.9871 | 25.4497 | 23.6052 | 37.0126 |
| Capacity (C) | [TMPDA] | 11.7012 | 11.7981 | 8.9234 | 8.4013 | 8.3550 | 10.4457 |
| Selectivity (S) | | 4.4911 | 2.9941 | 4.0591 | 3.8276 | 3.6817 | 4.3150 |
| Performance Index (PI) | | 52.5514 | 35.3242 | 32.2024 | 32.1569 | 30.7608 | 45.0730 |
| Capacity (C) | [DMEA] | 18.9596 | 11.6698 | 6.4287 | 4.7088 | 4.1888 | 6.2425 |
| Selectivity (S) | | 2.6141 | 2.3161 | 3.2445 | 3.1222 | 3.1222 | 3.5435 |
| Performance Index (PI) | | 49.5617 | 27.0288 | 20.8577 | 15.3382 | 13.0781 | 22.1205 |
| Capacity (C) | [DMBA] | 10.2871 | 6.7198 | 8.1410 | 7.2405 | 6.9499 | 9.1858 |
| Selectivity (S) | | 4.3738 | 2.9730 | 4.1143 | 3.8115 | 3.5976 | 4.3482 |
| Performance Index (PI) | | 44.9932 | 19.9778 | 33.4945 | 27.5969 | 25.0028 | 39.9419 |

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