CHEMICAL ENGINEERING TRANSACTIONS

VOL. 74, 2019

A publication of
AIDIC
The Italian Association
of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Sauro Pierucci, Jiří Jaromír Klemeš, Laura Piazza

ISBN 978-88-95608-71-6; **ISSN** 2283-9216

DOI: 10.3303/CET1974200

A Simple Group Contribution Model to Predict Thermal Conductivity of Pure Ionic Liquids

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Ionic liquids (ILs) have been attracted considerable attention in separation and purification processes as green solvents. Researchers use ILs in many areas, such as micro-extraction and catalysis in biodiesel production. However, there are still few studies about it. A comprehension of ILs thermophysical properties, for example, heat capacity and thermal conductivity may improve new technological processes and minimize energy costs. Since these fluids can be composed of different ions, it is harder to obtain these properties for several ILs. Therefore, this paper evaluated a group contribution (GC) model from the literature due to be accurate and straightforward for thermal conductivity (k) prediction of pure ionic liquids in a wide range of temperatures at atmospheric pressure. Once ILs containing $C(CN)_3^-$, $B(CN)_4^-$, DCA^-, CH_3COO^-, $HOPO_2^-$, SER^-, LIS^-, CYS^-, PRO^-, TAU^-, THR^-, VAL^- and FAP^- groups are commercially used, and the authors did not use an experimental database of ILs containing these anions, the model is unable to predict k for them. In this manner, from ILThermo, a larger experimental database including these anions was used to propose GC parameters for them and reestimate the others. This was done by minimizing the sum of the square of the residues comparing calculated and experimental value to obtain each group contribution parameter, using the generalized reduced gradient algorithm in Excel® and VBA programming. The revised model obtained results with mean deviation of 1.16 % for k prediction, including 13 more GC parameters. Both models were compared to predict k for other data set, not used in the parameters estimation. The proposed model was better in all evaluated cases and increased the amount of ILs to predict k.

1. Introduction

Ionic liquids (ILs) are promising as green solvents and have been evaluated as substitutes for volatile organic compounds, as they have thermal and chemical stability, high selectivity, low toxicity, and can be reused (Amiril et al., 2017). ILs are organic salts with melting point below 100 °C. They are composed of a large organic cation and an organic or inorganic anion whose properties are determined by the chemical interactions. There is a variety of applications for ILs such as micro-extraction and catalysis biodiesel production (Berthod et al., 2018) and aromatic separation (NAVARRO et al., 2018). Since several ILs can be obtained through a combination of ions, prediction of thermophysical properties, such as heat capacity and thermal conductivity, can assist the development of new processes and minimize energy cost. For the selection of an IL in separation processes, the thermal conductivity (k) is one of the main properties required for analyzing energy consumption. Computational modeling stands out as a quick way of predicting k from an experimental database by applying predictive methods. There are different predictive models for ILs, such as the group contribution (GC) method that performs the regression of experimental data and the QSPR (Quantitative Structure Property Relationship) based on quantum mechanics (Coutinho et al., 2012).

Due to be simple and accurate, a GC model from the literature was evaluated to predict thermal conductivity (k) of pure ionic liquids in a wide range of temperatures at atmospheric pressure. The GC model proposed by Gardas and Coutinho (2009) predicted k of ionic liquids with simplicity and good precision, obtaining relative average deviation (RD) of 1.06 %, using 16 ILs based on 107 data points in a interval of 293-390 K. This model is based on linear correlation with experimental data and group contribution (GC) approach to predict k:

Paper Received: 17 March 2018; Revised: 20 August 2018; Accepted: 20 January 2019

Please cite this article as: Soares L.H., Guirardello R., Rolemberg M., 2019, A Simple Group Contribution Model to Predict Thermal Conductivity of Pure Ionic Liquids, Chemical Engineering Transactions, 74, 1195-1200 DOI:10.3303/CET1974200

$$k = A_k - B_k T \quad (1)$$

where [k] = $W^{-1}m^{-1}K^{-1}$, T = absolute temperature, and A_k and B_k are fitting parameters determined by GC method, according to Eqs (2-3):

$$A_k = \sum_{i=1}^{k} n_i a_{i,k} \quad (2)$$

$$B_k = \sum_{i=1}^{k} n_i b_{i,k} \quad (3)$$

where estimated values of $a_{i,k}$ and $b_{i,k}$ are shown in Table 1, n_i is the amount of each group i, and k is the total number of groups present in the molecule.

Table 1: Group contributions parameters $a_{i,k}$ and $b_{i,k}$ in Eqs (2-3) for temperature range 293-390 K.

Species	$a_{i,k}$	$b_{i,k}$ (K^{-1})
	Cations	
1,3-dimethylimidazolium (+)	0.1356	1.564×10^{-5}
1-dimethylpyrrolidinium (+)	0.1325	1.668×10^{-5}
Tetramethyl phosphonium (+)	0.1503	3.230×10^{-5}
	Anions	
PF_6^-	0.0173	9.088×10^{-6}
BF_4^-	0.0874	8.828×10^{-5}
TF_2N^-	0.0039	2.325×10^{-5}
$CF_3SO_3^-$	0.0305	5.284×10^{-5}
$EtSO_4^-$	0.0700	6.552×10^{-5}
Cl^-	0.0166	1.000×10^{-5}
	Groups	
CH_2	0.0010	2.586×10^{-6}
CH_3	0.0042	7.768×10^{-6}

Source: Gardas and Coutinho (2009).

Since Gardas and Coutinho (2009) did not use an experimental database of ILs containing $C(CN)_3^-$, $B(CN)_4^-$, DCA^-, CH_3COO^-, $HOPO_2^-$, SER^-, LIS^-, CYS^-, PRO^-, TAU^-, THR^-, VAL^- and FAP^- groups, the model is limited and cannot be applied to systems with these anions. However, many commercially used ILs are composed of these groups not analyzed by the authors. Then, the purpose of this study is to improve the model to predict them.

2. Methodology

Based on the GC model proposed by Gardas and Coutinho (2009), a new database of experimental data obtained from ILThermo was elaborated, considering 33 ILs and the inclusion of 13 anion groups. This new base has 237 experimental data at atmospheric pressure in a wide range of temperature, 273-390 K, and thermal conductivity 0.105-0.214 $W^{-1}.m^{-1}.K^{-1}$. The methodology was developed with the implementation of spreadsheets in Excel® to validate the results reported by the authors for the analyzed 16 ILs. Following the methodology validation, the model was extended for the 33 ILs with the inclusion of the 13 anions using a new, larger, and comprehensive experimental database for the ILs of this work. From this base, group contribution parameters for $C(CN_3)^-$, $B(CN)_4^-$, DCA^-, CH_3COO^-, $HOPO_2^-$, SER^-, LIS^-, CYS^-, PRO^-, TAU^-, THR^-, VAL^- and FAP^- were proposed, and the GC parameters for others groups were re-estimated. This was done by minimizing the sum of the square of the residues comparing calculated and experimental value of k, using generalized reduced gradient algorithm:

$$S = \sum_{i=1}^{N} \left[\left((A_k - B_k T) - k_{exp} \right)^2 \right]_i \quad (4)$$

where N is the total data points used, A_k and B_k are fit parameters using the new database calculated by Eqs (2-3), k_{exp} is the thermal conductivity experimental data from the new database.

For parameters initial estimate, it was used the group parameters reported by Gardas and Coutinho (2009), and the others were randomly chosen. The minimization of Eq (4) was done with VBA (Visual Basic) programming and the tool Solver from Excel®, obtaining new GC parameters. The relative average deviation (RD) between calculated (k_{cal}) and experimental data was determined to verify the model precision:

$$\text{RD }(\%) = \frac{100\ \text{x}\ \sum_{i=1}^{N} \left|(k_{cal} - k_{exp})/k_{exp}\right|_i}{N} \tag{5}$$

Also, the proposed model in this paper and reported by Gardas and Coutinho (2009) were compared to predict k for five new experimental data set of pure ILs from ILThermo, not used to generate the models.

3. Results

Based on the new database elaborated and in Eq (4), new group contribution parameters $a_{i,k}$ and $b_{i,k}$ in Eqs (2-3), as underlined in Table 2, were proposed for temperature range 273-390 K.

Table 2: Group contributions parameters proposed $a_{i,k}$ and $b_{i,k}$ in Eqs (2-3) for temperature range 273-390 K.

Species	$a_{i,k}$	$b_{i,k}$ (K^{-1})
Cations		
1,3-dimethylimidazolium (+)	1.459×10^{-1}	6.283×10^{-6}
1-dimethylpyrrolidinium (+)	1.363×10^{-1}	1.027×10^{-8}
Tetramethyl phosphonium (+)	1.799×10^{-1}	1.078×10^{-8}
Anions		
PF_6^-	1.405×10^{-2}	3.027×10^{-5}
BF_4^-	7.385×10^{-2}	7.958×10^{-5}
TF_2N^-	1.995×10^{-6}	3.527×10^{-5}
$CF_3SO_3^-$	2.437×10^{-2}	6.471×10^{-5}
$EtSO_4^-$	6.045×10^{-2}	7.360×10^{-5}
Cl^-	1.001×10^{-2}	1.550×10^{-5}
DCA^-	1.115×10^{-1}	2.928×10^{-4}
$C(CN)_3^-$	5.294×10^{-2}	6.451×10^{-5}
$B(CN)_4^-$	6.723×10^{-2}	1.161×10^{-4}
CH_3COO^-	1.324×10^{-1}	2.222×10^{-4}
$OHPO_2^-$	6.705×10^{-2}	5.309×10^{-5}
SER^-	1.213×10^{-2}	6.925×10^{-5}
LYS^-	1.175×10^{-2}	5.921×10^{-5}
CYS^-	3.524×10^{-3}	7.046×10^{-5}
PRO^-	6.222×10^{-4}	4.554×10^{-5}
TAU^-	2.023×10^{-2}	9.870×10^{-5}
THR^-	1.451×10^{-3}	5.080×10^{-5}
VAL^-	9.217×10^{-3}	6.654×10^{-5}
FAP^-	2.248×10^{-7}	8.584×10^{-5}
Groups		
CH_2	7.533×10^{-8}	2.993×10^{-6}
CH_3	7.210×10^{-7}	4.292×10^{-6}

For [$MeOHPO_2$] anion group of an IL was utilized $OHPO_2^-$ and CH_3 groups as GC parameters. The results of thermal conductivity prediction for pure ionic liquids, including new anions groups, are shown in Table 3.

From the new experimental database, the RD was 1.16 % for the proposed model. From these, 39.4 % of the estimated values were within RD 0.00-0.75 %, 33.3 % within 0.75-1.5 %, 18.2 % within 1.5-2.25 %, only 9.10% of thermal conductivity predicted had deviation larger than 2.25 %, with a maximum of 4.37% for [C_{10}mIm][TF_2N]. Analyzes of thermal conductivity behavior with temperature, alkyl chain length and type of anion and cation was realized. Figure 1a shows the thermal conductivity increase with different anions for tetrabutyl phosphonium (TBPh) cation at a fixed temperature of 313.15 K. Then, k for ILs based on TBPh cation increase with this anion trend: [CYS] < [PRO] < [THR] < [VAL] < [SER] = [TAU] < [LYS]. Regarding to ILs based on imidazolium cation, k increases with the following anion trend: [TF_2N] < [CF_3SO_3] ≤ [PF_6] < [DCA] < [$C(CN)_3$] < [$B(CN)_4$] < [$EtSO_4$] < [BF_4] < [$MeOHPO_2$] < [CH_3COO]. According to Figure 1b, thermal conductivity slightly decrease with the increase of temperature. Also, is noted the anion trend for k: [CH_3COO] > [$MeOHPO_2$] > [$EtSO_4$] > [TF_2N]. Considering the thermal conductivity data for ILs with a fixed anion, it was verified that there is a trend in this property prediction with cation variation: [phosphonium] > [imidazolium] > [pyrrolidinium]. In contrast, the alkyl chain length of IL does not follow a notable trend as the others variation, and there is no significant effect in k. Regarding the model proposed validation, the model including new group contributions was compared with the model reported by Gardas and Coutinho (2009) to predict k for a new data set of pure ILs.

Table 3: Thermal conductivity prediction for pure ionic liquids, including new anions groups.

Ionic liquid	Temperature range (K)	Data points	RD (%)	Reference
$[C_4mIm][PF_6]$	294.9-335.1	3	0.64	Tomida et al. (2007b)
	293-353	7	0.85	Nieto de Castro et al. (2010)
$[C_6mIm][PF_6]$	294.1-335.2	3	0.66	Tomida et al. (2007b)
$[C_8mIm][PF_6]$	295.1-335.2	3	1.97	Tomida et al. (2007b)
$[C_2mIm][BF_4]$	300-390	10	2.12	Valkenburg et al. (2005)
$[C_4mIm][BF_4]$	300-390	10	2.25	Valkenburg et al. (2005)
$[C_2mIm][TF_2N]$	293-353	7	1.82	Ge et al. (2007)
$[C_4mIm][TF_2N]$	293-353	7	2.95	Ge et al. (2007)
$[C_6mIm][TF_2N]$	293-353	7	1.30	Ge et al. (2007)
$[C_8mIm][TF_2N]$	293-353	7	0.80	Ge et al. (2007)
$[C_{10}mIm][TF_2N]$	293-353	7	4.37	Ge et al. (2007)
$[C_3mmIm][TF2N]$	300-390	10	0.20	Valkenburg et al. (2005)
$[C_2mIm][EtSO_4]$	293-353	7	1.31	Ge et al. (2007)
$[C_4mIm][CF_3SO_3]$	293-353	7	0.14	Ge et al. (2007)
$[THTDPh][TF_2N]$	293-353	7	0.15	Ge et al. (2007)
[THTDPh][Cl]	293-353	7	0.58	Ge et al. (2007)
$[C_4mPyr][TF_2N]$	293-323	4	0.16	Ge et al. (2007)
$[C_4mIm][DCA]$	293.6-344.2	6	1.48	França et al. (2014)
$[C_4mIm][C(CN)_3]$	283.15-353.15	8	2.48	Koller et al. (2014)
$[C_8mIm][C(CN)_3]$	283.15-353.15	8	1.43	Koller et al. (2014)
$[C_{10}mIm][C(CN)_3]$	283.15-353.15	8	1.25	Koller et al. (2014)
$[C_6mIm][B(CN)_4]$	283.15-353.15	8	1.22	Koller et al. (2014)
$[C_{10}mIm][B(CN)_4]$	283.15-353.15	8	1.21	Koller et al. (2014)
$[C_2mIm][CH_3COO]$	273.15-353.15	9	0.75	Fröba et al. (2010)
$[C_2mIm][MeOHPO_2]$	273.15-353.15	9	0.60	Fröba et al. (2010)
$[C_4mPyr][DCA]$	293.5-343.4	6	0.95	Fröba et al. (2010)
$[C_4mPyr][FAP]$	293-353	7	1.09	Ge et al. (2007)
[TBPh][SER]	298.15-353.15	7	0.07	Gardas et al. (2009)
[TBPh][LYS]	298.15-353.15	7	0.07	Gardas et al. (2009)
[TBPh][CYS]	298.15-353.15	7	0.08	Gardas et al. (2009)
[TBPh][PRO]	298.15-353.15	7	2.10	Gardas et al. (2009)
[TBPh][TAU]	298.15-353.15	7	2.01	Gardas et al. (2009)
[TBPh][THR]	298.15-353.15	7	0.21	Gardas et al. (2009)
[TBPh][VAL]	313.15-353.15	5	0.02	Gardas et al. (2009)
Total	273.15-390.00	237	1.16	

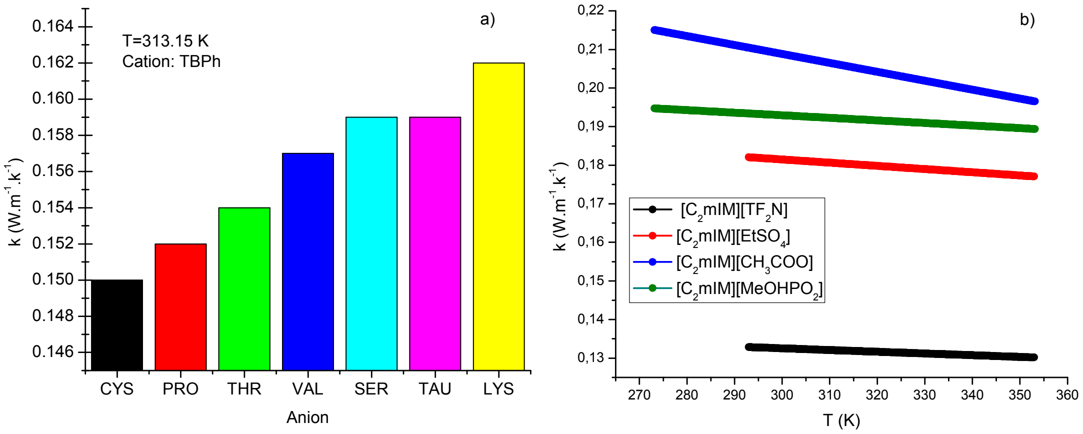

Figure 1: a) Thermal conductivity variation with different anions for tetrabutyl phosphonium (TBPh) cation at T=313.15 K. b) Thermal conductivity variation with temperature for 1-ethyl-3-methylimidazolium (C_2mIM) cation.

The modified model of this work was better to predict all of IL analyzed than the authors (Table 4). The RD for all ILs was 6.18 % in this work, against 7.13 % of Gardas and Coutinho (2009) model. For both models, using a new data set, the maximum and minimum deviation was almost 13 % and 2.45 %, respectively. Therefore, the modified model in this work can predict k for more ILs in a simple and precise way.

Table 4: Thermal conductivity prediction using models proposed by Gardas and Coutinho (2009) and in this work for five new data set of pure ionic liquids at 1 atm.

Ionic liquid	Temperature range (K)	Data points	RD - Gardas and Coutinho (2009) (%)	RD - This work (%)	Reference
[C$_6$mIm][PF$_6$]	294.7-334.9	7	4.32	2.57	Nieto de Castro et al. (2010)
[C$_4$mIm][BF$_4$]	293-353	3	13.15	12.58	Tomida et al. (2007a)
[C$_2$mIm][EtSO$_4$]	283.11-352.82	8	2.46	2.45	Chen et al. (2013)
[C$_2$mIm][CF$_3$SO$_3$]	300-375	2	9.87	9.19	Tenney et al. (2014)
[C$_4$mPyr][TF$_2$N]	293-333	5	5.84	4.11	Nieto de Castro et al. (2010)
Total	283.11-375.00	25	7.13	6.18	

4. Conclusions

From the work of literature, we expanded the applicability range of the model for thermal conductivity (k) prediction for pure ionic liquids, including the group contribution parameters of C(CN$_3$)$^-$, B(CN)$_4^-$, DCA$^-$, CH$_3$COO$^-$, HOPO$_2^-$, SER$^-$, LIS$^-$, CYS$^-$, PRO$^-$, TAU$^-$, THR$^-$, VAL$^-$ and FAP$^-$. The model proposed in this work obtained a relative average deviation of 1.16 % and is promising due to superior results in all cases analyzed when comparing with the literature model for a new data set of ILs.

Notation

ILs	Ionic liquids
k	Thermal conductivity
RD	Relative average deviation
GC	Group contribution

Abbreviation of ILs	Full name	CAS number
[C$_4$mIm][PF$_6$]	1-butyl-3-methylimidazolium hexafluorophosphate	174501-64-5
[C$_6$mIm][PF$_6$]	1-hexyl-3-methylimidazolium hexafluorophosphate	304680-35-1
[C$_8$mIm][PF$_6$]	1-octyl-3-methylimidazolium hexafluorophosphate	304680-36-2
[C$_2$mIm][BF$_4$]	1-ethyl-3-methylimidazolium tetrafluoroborate	143314-16-3
[C$_4$mIm][BF$_4$]	1-butyl-3-methylimidazolium tetrafluoroborate	174501-65-6
[C$_2$mIm][TF$_2$N]	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	174899-82-2
[C$_4$mIm][TF$_2$N]	1-butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	174899-83-3
[C$_6$mIm][TF$_2$N]	1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	382150-50-7
[C$_8$mIm][TF$_2$N]	1-octyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	178631-04-4
[C$_{10}$mIm][TF$_2$N]	1-decyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	433337-23-6
[C$_3$mmIm][TF$_2$N]	1,2-dimethyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]imide	169051-76-7
[C$_2$mIm][EtSO$_4$]	1-ethyl-3-methylimidazolium ethyl sulfate	342573-75-5
[C$_2$mIm][CF$_3$SO$_3$]	1-ethyl-3-methylimidazolium trifluoromethanesulfonate	145022-44-2
[C$_4$mIm][CF$_3$SO$_3$]	1-butyl-3-methylimidazolium trifluoromethanesulfonate	174899-66-2
[THTDPh][TF$_2$N]	Trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide	460092-03-9
[THTDPh][Cl]	Trihexyl(tetradecyl)phosphonium chloride	258864-54-9
[C$_4$mPyr][TF$_2$N]	1-butyl-1-methylpyrrolidinium bis[(trifluoromethyl)sulfonyl]imide	223437-11-4
[C$_4$mIm][DCA]	1-butyl-3-methylimidazolium dicyanamide	448245-52-1
[C$_4$mIm][C(CN)$_3$]	1-butyl-3-methylimidazolium tricyanomethane	878027-73-7
[C$_8$mIm][C(CN)$_3$]	1-methyl-3-octylimidazolium tricyanomethanide	1203710-60-4
[C$_{10}$mIm][C(CN)$_3$]	3-decyl-1-methylimidazolium tricyanomethanide	1203710-61-5
[C$_6$mIm][B(CN)$_4$]	1-hexyl-3-methylimidazolium tetracyanoborate	1240857-50-4
[C$_{10}$mIm][B(CN)$_4$]	1-decyl-3-methylimidazolium tetracyanoborate	1201894-90-7
[C$_2$mIm][CH$_3$COO]	1-ethyl-3-methylimidazolium acetate	143314-17-4
[C$_2$mIm][MeOHPO$_2$]	1-ethyl-3-methylimidazolium methyl phosphonate	81994-80-1
[C$_4$mPyr][DCA]	1-butyl-1-methylpyrrolidinium dicyanamide	370865-80-8
[C$_4$mPyr][FAP]	1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	851856-47-8
[TBPh][SER]	Tetrabutylphosphonium L-serinate	899795-70-1
[TBPh][LYS]	Tetrabutylphosphonium L-lysinate	899795-74-5
[TBPh][CYS]	Tetrabutylphosphonium L-cysteinate	899795-83-6
[TBPh][PRO]	Tetrabutylphosphonium L-prolinate	899795-76-7
[TBPh][TAU]	Tetrabutylphosphonium 2-aminoethanesulfonate	945415-32-7
[TBPh][THR]	Tetrabutylphosphonium L-threoninate	899795-77-8
[TBPh][VAL]	Tetrabutylphosphonium L-valinate	899795-72-3

Acknowledgments

The authors acknowledge the financial support from CNPq (Grant Number 167869/2018-3).

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