Lower and Upper Critical Solution Temperatures of Binary Polymeric Solutions

Abstract

The phase behavior of binary polymeric solutions such as lower and upper critical solution temperatures has an important role in many polymeric processes. For theoretical investigation on the prediction of these temperatures, a substantial number of data points on binary polymeric solutions were collected from literatures and used to present a reliable calculation routine through chemical engineering thermodynamic modeling approach. The thermodynamic model of Compressible Regular Solution was used. The minimization of errors and predefined objective function was done by applying Particle Swarm Optimization technique. An efficient and accurate empirical correlation employing some quantitative structure–property relationship concept through statistical modeling was developed. To develop the statistical model, the connectivity indices of polymer and solvent were used as the independent variables of the model. Four statistical parameters were defined as auxiliary criteria to evaluate the models and convergence of calculations. In addition, attempts were made to develop and correlate the connectivity indices (topological descriptors) of polymer and solvent to the lattice fluid theory parameters of Sanchez-Lacombe Equation of State. The reliability and accuracy of proposed approaches were discussed in-details and the results were compared to the available experimental data. Desirable agreements between calculated and experimental data were found in thermodynamic model as demonstrated by a maximum Individual Absolute Relative Deviation of 5 %. An averaged IARD of 4.3 % was obtained for the empirical model. The new correlation predicts connectivity indices of components with acceptable accuracy.

Keywords: critical solution temperature; polymeric solution; thermodynamics correlation; the quantitative structure–property relationship; connectivity indices.

1. INTRODUCTION

The lower critical solution temperature (LCST) is the temperature below which components of a mixture are completely miscible for all compositions [[1](#_ENREF_1), [2](#_ENREF_2)]. On the other side, a temperature above which the miscibility of components for all compositions will be observed is referred as upper critical solution temperature (UCST) [[3](#_ENREF_3)]. UCST and LCST can be observed in partially miscible polymeric solutions and depends on the operating pressure and solution component compositions [[2](#_ENREF_2), [4](#_ENREF_4)]. The spinodal and binodal curves [[5](#_ENREF_5)] have shared minimum (critical point) and maximum respectively at LCST and UCST.

In polymeric processes such as polymerization and membrane fabrication [[6-9](#_ENREF_6)], any knowledge on phase behaviors vs. solution composition and operating pressure is highly valuable and plays an important role. While the experimental data on LCST and UCST are available, however still accurate and reliable approach or model to correlate these critical solution temperatures (CST) data is rarely found [[6-9](#_ENREF_6)]. The research works in literatures to model and correlate LCST and/or UCST data include [[10](#_ENREF_10)]; phase equilibrium data based calculation [[11](#_ENREF_11)], empirical correlations [[12](#_ENREF_12), [13](#_ENREF_13)], the quantitative structure–property relationship (QSPR) models and etc. [[10](#_ENREF_10), [14-18](#_ENREF_14)].

To develop more accurate and predictive models for LCST and/or UCST, here, the compressible regular solution theory and lattice fluid theory were used for thermodynamic modeling. In addition, the connectivity indices of polymer and solvent were used to develop a reliable empirical model. Attempts were made to correlate the connectivity indices of selected components to the lattice fluid scaling parameters. The evolutionary based algorithm of particle swarm optimization was used for minimization of errors. The details of modeling, calculations and the obtained results are illustrated in following paragraphs.

1. Thermodynamic modeling of UCST and LCST
   1. Model development

Various miscibility behaviors can be observed in binary polymeric solutions such as showing only one LCST, only one UCST, both LCST and UCST simultaneously, cases in which the LCST and UCST regions have overlapped which are computationally more complicated. For current work, we considered systems that only show one LCST or one UCST, and other cases might be investigated in a future work. The LCST and/or UCST is the point where spinodal and binodal (coexistence) curves cross, in where there’s a shared minima for the case of LCST and a shared maximum for the later.

The binodal curve, itself, represent the local thermodynamic equilibrium of two phases at contact, thus one may write the equilibrium criteria for component "*i*" at two phases as presented by Eq. 1[[2](#_ENREF_2), [5](#_ENREF_5), [19](#_ENREF_19)], where  is the chemical potential of component *i* and superscripts *l* and *r*, refer to polymer lean and polymer rich phases respectively.

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The spinodal condition requires that the second derivative of, with respect to the composition (in terms of volume fraction), at constant temperature and pressure, to be positive as presented by Eq.2[[5](#_ENREF_5), [18](#_ENREF_18), [20](#_ENREF_20)];

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In addition, applying material balance, in the form of volume fraction of the two components, one obtains Eq. 3, which must be holding on this point (and any point).

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These set of equations must be solved simultaneously to find the corresponding temperature (LCST / UCST) in a trial and error procedure and by an initial guess, which is a kind of optimization problems that  is used as main optimizing criteria (in which=and refers to standard state of the chemical potential of component “*i*”). For optimization purpose, Particle Swarm Optimization (PSO) Technique was used [[21](#_ENREF_21), [22](#_ENREF_22)].

Chemical potential,  in Eq. 1(for )can be calculated by using activity coefficient models such as Flory-Huggins theory and its extensions (such as Lattice Cluster Theory) [[2](#_ENREF_2)]**.** These models require binary interaction parameters, which must be calculated or experimentally measured and this limits their application [[23](#_ENREF_23)]. It must be noted that using a model which needs only pure component properties, is of the much interest [[5](#_ENREF_5)]. Thus, thermodynamic model of Compressible Regular Solution theory (CRS) was considered in this paper for development of Model. The main equations of this theory for a binary solution are given by Eqs. 4-6 [[20](#_ENREF_20), [24-26](#_ENREF_24)] where accounts for molar volume of component “*i*”.

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The pure component properties are needed for the activity coefficient calculations using CRS theory, which can be obtained by group contribution methods (GCM) [[20](#_ENREF_20), [24-26](#_ENREF_24)]. Group contribution methods, themselves, can be regarded as some QSPR method for estimation and calculation of physicochemical properties of interest. The solubility parameter values at temperature  in CRS model requires the estimation of the solubility parameter at 298 K through some group contribution methods (as given by), here the van Krevelen GCM was used [[24](#_ENREF_24)]. In addition, the reduced density (hard core density) were calculated from the modified Sanchez-Lacombe Lattice Fluid model (SL-EOS) [[27](#_ENREF_27)] (given as ) using an iterative root seeking technique [[28](#_ENREF_28)] and the Constantinou and Gani group contribution method for evaluation for the scaling parameters () [[24](#_ENREF_24), [25](#_ENREF_25), [27](#_ENREF_27)]. In addition, the coefficients of thermal expansion for each component were calculated through the modified SL-EOS model [[27](#_ENREF_27)]. For calculation of in CRS model ( represents number of hard cores in lattices of volume), one might useequality, where  is the molecular weight of components (for polymer the repeating units). In this case, Eq. 2 simplifies to Eq. 8 considering  as dependent composition [[5](#_ENREF_5)];

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Using these equations, the temperature of interest, i.e. LCST and/or UCST, can be searched employing an appropriate optimization technique [[22](#_ENREF_22)].

* 1. Method of calculations

Particle Swarm Optimization (PSO) technique was used in this work for determination of temperature which satisfies the thermodynamic modeling criteria. In thermodynamic modeling, the CRS model, itself, requires no optimization and calculation as this model is straightforward [[5](#_ENREF_5)], however, finding the temperature of interest i.e. LCST and/or UCST, requires solution of a set of equations as described in previous section, which is an optimization problem. In this case, the number of variables in PSO is 1 (temperature) [[22](#_ENREF_22)], and the main objective function is the local equilibrium criteria. The parameters for initialization of PSO are listed in Table 1.

Table 1. PSO parameters

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| **Parameter** | **Symbol** | **Value** |
| Maximum Number of Iterations | MaxIt | 1200 |
| Population Size | nPop | 150 |
| Number of Decision Variables | nVar | 1 |
| Upper & Lower Bounds of Variables | VarMin  VarMax | 100  750 |
| Objective Functions | ObjFun | . |

The PSO has been considered to ensure both the higher accuracy of calculations and lower computational costs [[22](#_ENREF_22)]. The swarm intelligence based algorithm of PSO provides a precise evolution of calculations toward the best optimal solution of optimization problems as it employs the local and global optimums to control the goodness of each estimated solution [[22](#_ENREF_22), [29](#_ENREF_29), [30](#_ENREF_30)]. It is necessary to note that in the any evolutionary/swarm intelligent algorithm, the input upper and lower bounds for variables introduced are important factors [[22](#_ENREF_22)]. It should be checked whether the reported values are close to the introduced bounds or not. It is recommended that the bound should be refined to a domain that covers all current variables when the variables (particles) are very close to the bounds.

1. Empirical modeling of UCST and LCST
   1. Model development

In empirical modeling, commonly the available LCST and/or UCST data are related to physiochemical properties, such as density, critical properties, or solubility parameters [[12](#_ENREF_12), [13](#_ENREF_13), [16](#_ENREF_16)]. However, there are polymers, for those, the mentioned properties are unknown. Thus to nominate required properties, two criteria must be met; (i) the nominated property clearly differ from one polymer (solvent) to the others, and (ii) the experimental data be available in the literature or one can estimate them easily using a reliable routine. To develop the empirical model of interest, the connectivity indices (structural descriptors) of polymeric systems (polymer and solvent) were used as the independent variables of model. It must be noted that, this way, the highly predictive advantage of QSPR will be incorporated to the empirical modeling.

Such connectivity indices (i.e. structural descriptors) have been used by Lie and Zhong [[13](#_ENREF_13)] for presentation of their simple correlation. They employed eight connectivity indices, five of those were adopted to the polymer are; (i) polymer zero-order valence connectivity index (), (ii) polymer third-order valence connectivity index contributed by the chain backbone (), (iii) polymer third-order cluster connectivity index (), (iv) polymer first order connectivity index contributed by the side groups () and (v) polymer third-order connectivity index contributed by the side groups (). Using chain backbone and side group indices, the local structure of individual different polymers can be determined, and one can assure that no similar values for different system would be obtained. Hence, the chain backbone and side group indices of polymer (as mentioned in paragraph above) together with the third, fourth and fifth-order connectivity indices of solvent (e.g. ,  and ) were selected as independent variables to develop the model. The calculation procedure to estimate the connectivity indices is simple and can be found elsewhere in details [[31](#_ENREF_31)].

To obtain the empirical model of interest, one can express LCST and/or UCST, the dependent variable indicated by, as a function of the selected independent variables, by Eq. 17;

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The defined independent variables in Eq. 17can be divided to the following main groups as indicated by subscripts 1 and 2:

1: Polymer variable ()

2: Solvent variables ()

Mathematically, every algebraic function () can be approximated by a new function () as presented by Eq. 18, which represents the relationship between the approximated dependent variable, , and independent variables,[[32](#_ENREF_32), [33](#_ENREF_33)].

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In which, shows the number of independent variables.

As shown by Eq. 19, the approximated dependent variable can be expressed in the form of Volterra Functional Series for  independent variables [[32](#_ENREF_32)];

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In which,,,,,  and  are constant coefficients.

Applying Eq. 19 to Eq. 17for two main variables of and, one would obtain Eq. 20, where, - are constant coefficients which must be determined by using the available data.

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This equation (Eq. 20) can be rewritten in matrix form as shown by Eq. 13 where the superscript  refers to the transpose of the matrix. Such matrix formulation would be beneficiated from its easy implementation in calculation routines such as MathWorks MATLAB [[34](#_ENREF_34)] and etc.

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Applying Eq. 19, onecan obtain also the corresponding approximations for  and, as shown byEqs. 14-15in matrix form**.**

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Eqs. 13-15 show the ***most*** generalized approximation of the LCST and/or UCST, in which,,,,,  and are model constants. The optimum values of the model constants can be calculated by implementation of an efficient algorithm by regression of model to the available experimental data [[22](#_ENREF_22)]. It is necessary to note that, by assuming some of these constants equal to zero, one would find more simple equations and reduce this model to the simple correlations (as of [[15](#_ENREF_15)]).

In any empirical study, to evaluate the agreement between the real (experimental) and calculated data, statistical methods and function are required. Here, four statistical parameters including sum of squares due to error of the fit (SSE), square of the correlation (R2), adjusted R-square (R2-adj) and standard error of the regression (RMSE) were implemented based on Refs. [[34](#_ENREF_34)] as summarized in Table 2. The model that satisfies all these parameters can be accepted.

Considering the presented statistical parameters, one can use the following rules of thumb to evaluate the model parameters [[34](#_ENREF_34), [35](#_ENREF_35)]; (1) SSE; value closer to zero indicates a good fitness, which has a smaller random error component, (2) R-sq.; value closer to **1** indicates that a greater proportion of variance is accounted for the model, (3) Adj R-sq.; value closer to **1** indicates a good fitness, however it can take on any value less than or equal to **1** and (4) RMSE; value closer to **0** indicates a fitness that it is more useful for prediction.

Table 2. Statistical Parameters used in this study

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| **Parameter** | **Equation** |
| sum of squares due to error of the fit |  |
| square of the correlation |  |
| adjusted R-square |  |
| standard error of the regression |  |
| **Note:** *n* is number of data and *m* is number of coefficient in the models. | |

The standard error of the regression (RMSE) relationship, given as, indicates that in any established empirical model of interest, the number of coefficients in the models must be lower than the number of data points () as  is a non-negative value. Mathematically, for a problem of interest where the number of known variables (data) is lower than that of unknown variables (coefficients), an underdetermined system of equations would be obtained, which requires special iterative regression methods to find the optimal solution. An overdetermined systems of equations is obtained whenever, the number of unknown variables (coefficients) is lower than that of known variables (data).

This implication draws the correct method of application of the presented generalized model for the employed database of experimental CST data in any individual research. In other words, the large number of unknown variables -, -,- and all,, , and  can be reduced and updated according to the number of available experimental data in any research this way. On the other hand, the RMSE relationship and its subsequent implications and the relationship for adjusted R-square clearly show that using a large number of data points in training step of any proposed model, essentially, will not result in reliable and robust solution of unknown constants. In fact, and with no doubt, a large training dataset increases the coverage domain of model, as larger fraction of known data are being used, but significantly reduces the goodness of the model. The best training dataset is the one in which the maximum and minimum data are included and intervals of high fluctuation are sampled concisely. It is interesting that such reduction of an empirical model has the advantage of a reduction in computational costs and enhances consistency of model.

To reduce the number of model coefficients and provide a simpler but still general model, the coefficients indicated by,,, and  were eliminated from the model equation and only coefficients of first kind , and  were considered in present paper and the obtained relationship is given as presented in Eq. 16, which alternatively can be obtained using the Volterra Functional Series up to second term for the functional variables  and .

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The final expression for proposed empirical model of LCST and/or UCST is simple as it requires a limited number of coefficients to be regressed to the data, and it is general as it provides all possible crosslinking of considered independent variables of system in its formulation, in other words, all possible binary crosslinking of , , , , , ,  and are considered and included in the model.

* 1. Method of calculation

Here, PSO technique was used for determination of model coefficients. In this case, the number of variables in PSO is 16 [[22](#_ENREF_22)], and the main objective functions are the prescribed statistical parameters. The parameters for initialization of PSO are listed in Table 3.

Table 3. PSO parameters

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| **Parameter** | **Symbol** | **Value** |
| Maximum Number of Iterations | MaxIt | 100 |
| Population Size | nPop | 250 |
| Number of Decision Variables | nVar | 16 |
| Upper & Lower Bounds of Variables | VarMin  VarMax | -500  1000 |
| Objective Functions | ObjFun | *Statistical parameters.* |

1. New group contribution based correlation
   1. Correlating topological indices with lattice fluid parameters

In QSPR modeling works [[10](#_ENREF_10), [17](#_ENREF_17)], the determination and calculation of topological indices of molecules requires the application of commercial software packages and needs a considerable computational cost and time [[10](#_ENREF_10), [14-18](#_ENREF_14)]. The optimization of molecules geometry to approach the most stable geometry which has the lowest internal energy needs a number of module selection and applications. On the other side, the lattice fluid parameters such as the scaling parameters of modified SL-EOS () are well-known or can be calculated and determined using some well-established methods, such as the Constantinou and Gani group contribution method [[24](#_ENREF_24), [25](#_ENREF_25), [27](#_ENREF_27)]. Thus here, having the available topological indices and the scaling parameters of modified SL-EOS, attempts were made to establish reliable correlations which relate each topological index to the scaling parameters of modified SL-EOS.

Eight connectivity indices were investigated among which five parameters were adopted to the polymer (as listed below) (i) polymer zero-order valence connectivity index (), (ii) polymer third-order valence connectivity index contributed by the chain backbone (), (iii) polymer third-order cluster connectivity index (), (iv) polymer first order connectivity index contributed by the side groups () and (v) polymer third-order connectivity index contributed by the side groups (), and the third, fourth and fifth-order connectivity indices (,  and ) were set for solvent respectively as 3 remaining parameters. The calculation procedure to estimate the connectivity indices can be found elsewhere in details [[31](#_ENREF_31)]. On the other hand, the Constantinou and Gani group contribution method was used for evaluation of the scaling parameters () [[24](#_ENREF_24), [25](#_ENREF_25), [27](#_ENREF_27)].

A linear discrete form of Volterra functional series [[32](#_ENREF_32), [33](#_ENREF_33), [36](#_ENREF_36)] was used to relate the connectivity indices (dependent variables) to the modified SL-EOS parameters (independent variables). To obtain the expressions of interest, one can express connectivity indices, the dependent variable indicated by, as a function of the selected independent variables (modified SL-EOS parameters), by Eq. 17;

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Mathematically, algebraic function  can be approximated by a new function () as presented by Eq. 18, which represents the relationship between the approximated dependent variable, , and independent variables,[[32](#_ENREF_32), [33](#_ENREF_33)] where shows the number of independent variables.

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Eq. 19 shows a linear discrete form of Volterra functional series [[32](#_ENREF_32), [33](#_ENREF_33), [36](#_ENREF_36)] in which is the approximated dependent variable and, , , ,  and  are constant coefficients.

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Applying Eq. 19 to Eq. 17,after rearrangement and simplification, one would obtain Eq. 20, where, - are constant coefficients which must be determined by using the available data.

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Eq. 20 is the reduced form of Eq. 19 up to the third term which is known as Kolmogorov-Gabor polynomials [[32](#_ENREF_32), [33](#_ENREF_33), [37](#_ENREF_37)]. The coefficients  are unknown constants that must be determined using the available connectivity indices (dependent variables) and modified SL-EOS parameters (independent variables).

* 1. Method of calculation

For each connectivity index of interest, a system of equations can be constructed by substituting available data in Eq. 20 as illustrated in Eq. 21 where  is number of data points.

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The solution for system of equations presented in Eq. 21 can be given by Eq. 22;

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Here  indicate the matrix of coefficients,  is the matrix of known dependent data (connectivity indices) and  is the matrix of coefficients constructed using available/calculated modified SL-EOS parameters. The superscripts  and respectively indicates the transpose and invers of matrix.

1. Results and discussion
   1. Required data

The experimental data of LCST and UCST were collected from literature [[14](#_ENREF_14), [16](#_ENREF_16)] and listed in appendixes (**Table 9** and Table 10 respectively). The structural descriptors of binary polymeric solution are calculated and checked against the available data in Refs. [[13](#_ENREF_13), [31](#_ENREF_31)] and summarized in appendixes (Table 11 and Table 12 for polymers and solvents respectively). The lattice fluid parameters of modified SL-EOS () were calculated and listed in appendixes (Table 13 and Table 14 for polymers and solvents respectively).

* 1. Thermodynamic model

For each binary polymeric system listed in **Table 9** and Table 10, minimization of the predefined objective function (here, the local equilibrium criteria) was performed using the PSO technique. As illustrated in Table 1, a population of 150 particles is initially produced in PSO as the initial guess of LCST/UCST (dimension) which upper and lower bounds of variables were set within range 100-750. Over iterations, the PSO checks the best local and global guesses and move around to find the final optimal dimension according to the introduced Objective Function. The PSO successfully approaches to the final value of LCST/UCST in each system after 23 iterations in average. The evaluation of objective function and iterations using PSO technique is illustrated in Fig. 1.

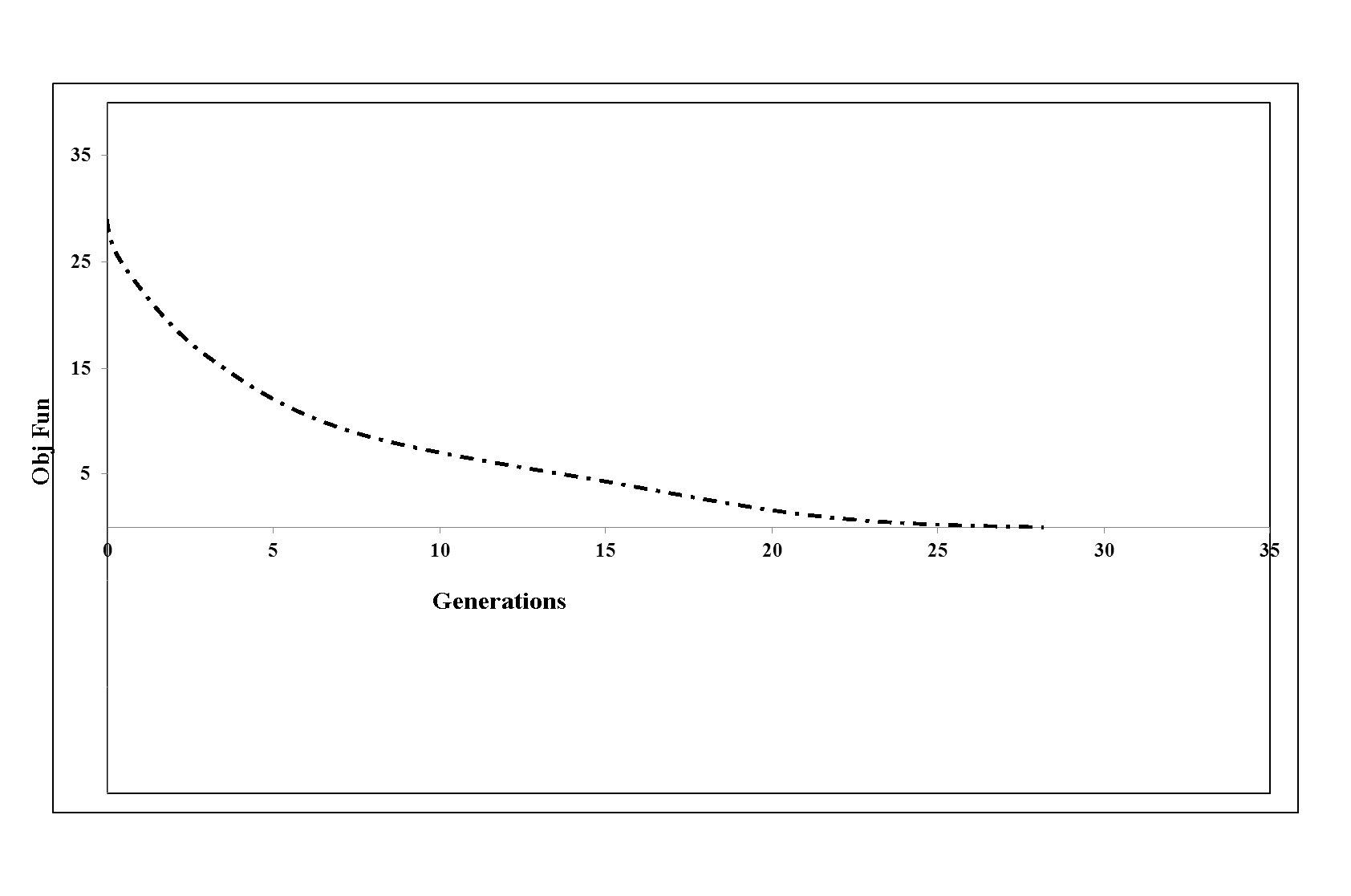


Fig. 1. The average convergence of PSO

The deviation of calculated LCST/UCST data was compared to the experimental data listed in **Table 9** and Table 10. For each binary system, the Individual Absolute Relative Deviation (IARD) between calculated and experimental data was used to present the accuracy of calculations as defined in Eq. 23 where temperatures are in Kelvin.

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The correlation results of thermodynamic model are depicted in Fig. 2 and Fig. 3 respectively for LCST and UCST binary systems.

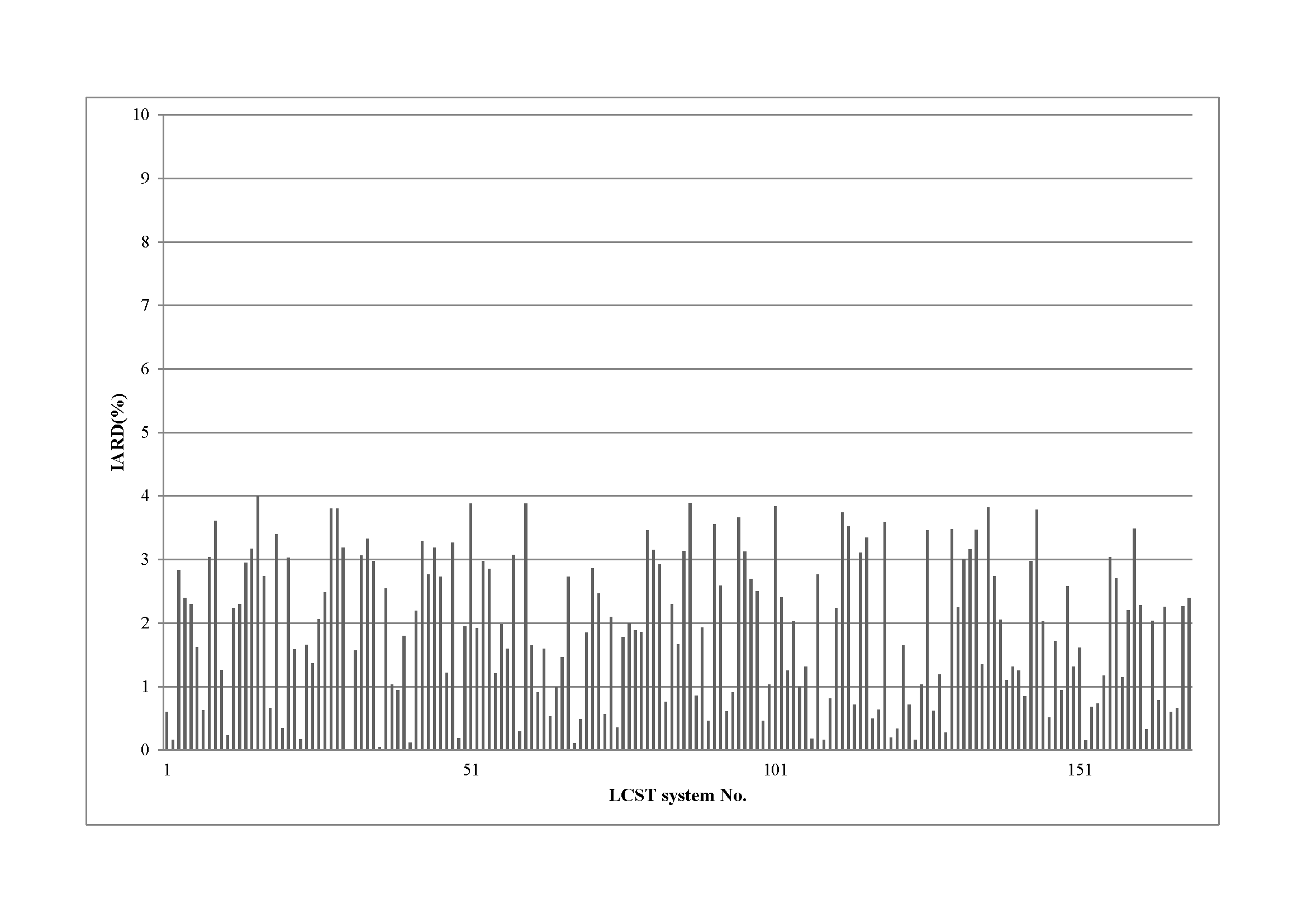


Fig. 2. The Individual Absolute Relative Deviation (IARD) between calculated and experimental LCST data

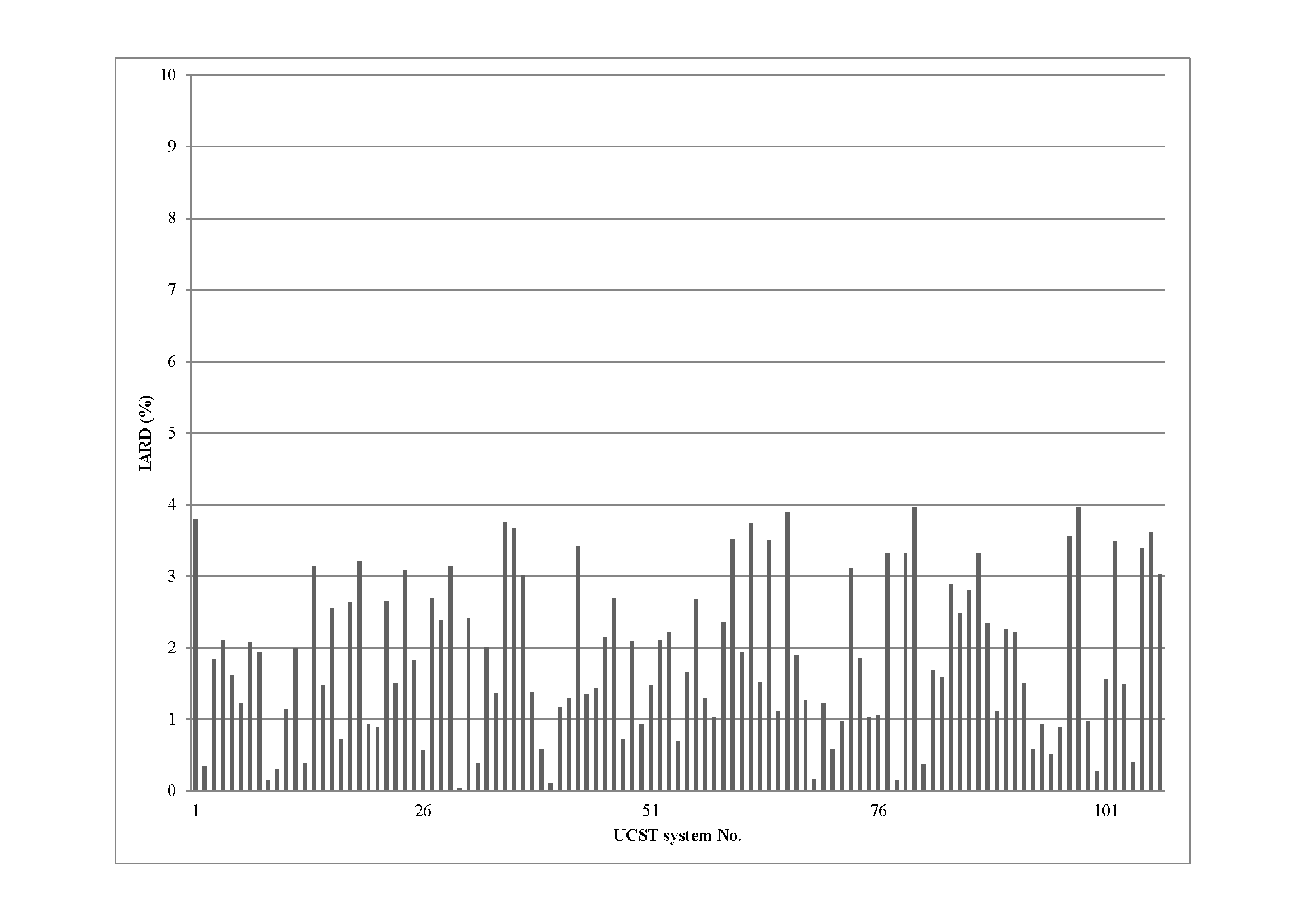


Fig. 3. The Individual Absolute Relative Deviation (IARD) between calculated and experimental UCST data

Desirable agreements between calculated and experimental data were found in the presented thermodynamic model as demonstrated by a maximum IARD of 5 %. Beside the reliable optimization technique which provides fast convergence to the final solution, the CRS thermodynamic model demonstrates confident predictions for polymeric solutions as also reported elsewhere [[5](#_ENREF_5), [38](#_ENREF_38)]. The required input data of CRS model are the scaling parameters of lattice fluid theory of Sanchez and Lacombe which are known for a substantial number of materials and in the case of unavailability can be simply calculated using some group contribution method. The computational cost of model application is low and the final solution can be obtained by just a few iterations as demonstrated in Fig. 1. The accuracy of model together with fast convergence of computation routine reveals the high potential of proposed method for further applications.

* 1. Empirical model

The statistical parameters values are summarized in Table 4.

Table 4. Statistical parameters for the obtained LCST / UCST equations

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| **Parameter** | **Value** | |
| **for LCST** | **for LCST** |
| SSE | 0.0617 | 0.1591 |
| R-sq. | 0.8919 | 0.9091 |
| adjusted R-sq. | 0.8925 | 0.9096 |
| RMSE | 0.2199 | 0.3517 |

The obtained optimal coefficients of developed statistical model, i.e. - - and - in Eq. 16, for LCST and UCST are listed in Table 5.

Table 5. Optimal coefficients of statistical model obtained for LCST and UCST data

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| --- | --- | --- | --- | --- | --- | --- |
|  | **Optimal coefficients of LCST model** | | | | | |
|  |  |  |  |  |  |
|  | 485.3 | 8.633 | 47.04 | -7.221 | 3.262 | -1.733 |
|  | 0 | -0.3127 | 1.0393 | -0.1165 | 1.0266 | -1.3911 |
|  | 0 | 1.2373 | 1.1458 | 1.1040 | - | - |
| ***Recommendation:*** *(i) connectivity indices of polymer should be normalized by mean 2.176 and std 0.7416; (ii) connectivity indices of solvent should be normalized by mean 2.955 and std 1.283* | | | | | | |
|  | **Optimal coefficients of UCST model** | | | | | |
|  |  |  |  |  |  |
|  | 316.8 | 43.29 | 16.22 | 8.266 | 11.42 | -1.56 |
|  | 0 | 4.0885 | 15.4705 | -3.9651 | 195.5912 | -164.3854 |
|  | 0 | 48.3833 | -9.7024 | -9.3262 | - | - |
| ***Recommendation:*** *(i) connectivity indices of polymer should be normalized by mean -82.29 and std 132; (ii) connectivity indices of solvent should be normalized by mean 7.248 and std 19.17* | | | | | | |

The correlation results of obtained models of LCST and UCST are illustrated in Fig. 4 and Fig. 5 respectively.

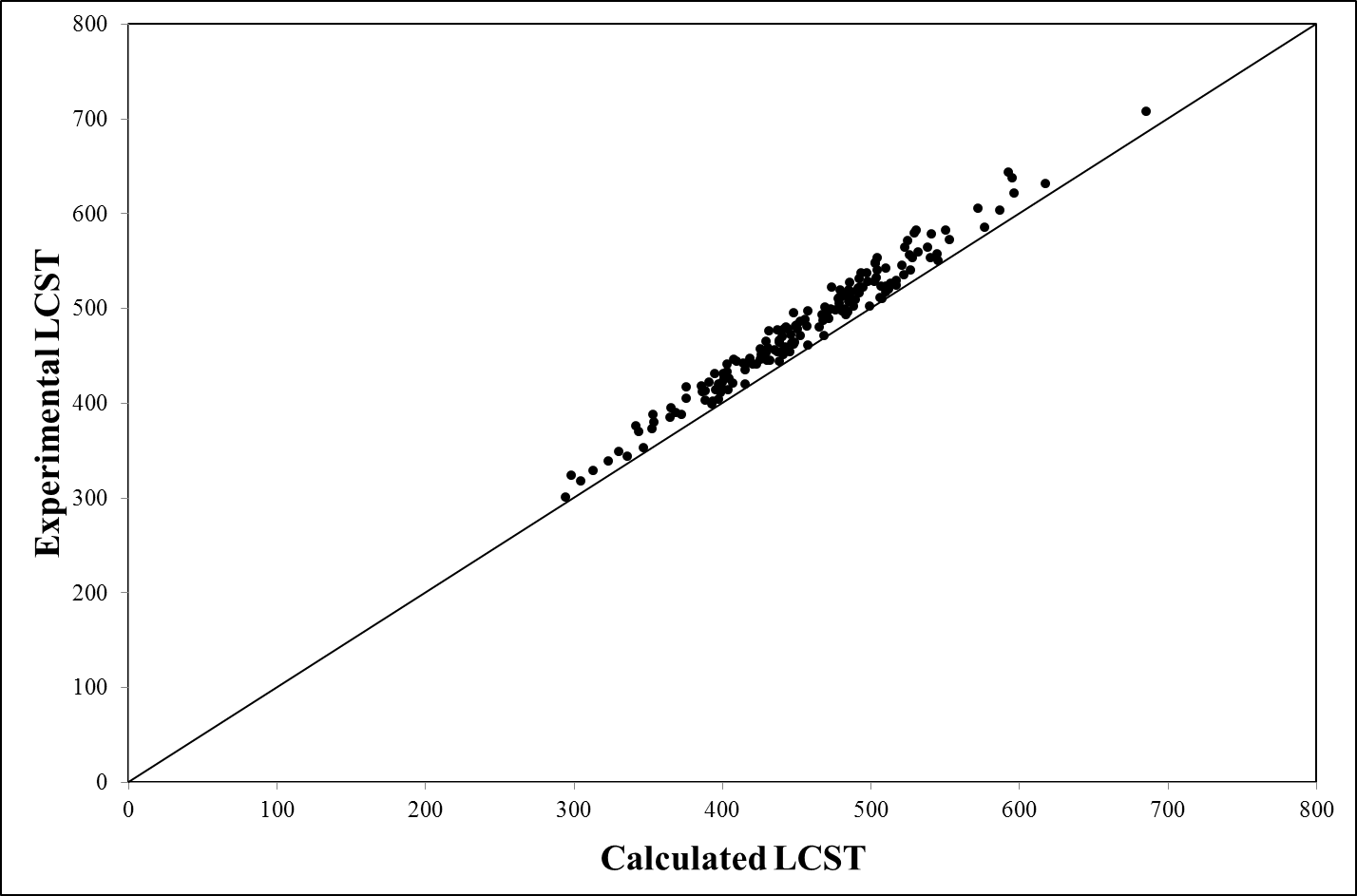


Fig. 4. The correlation results of obtained models of LCST

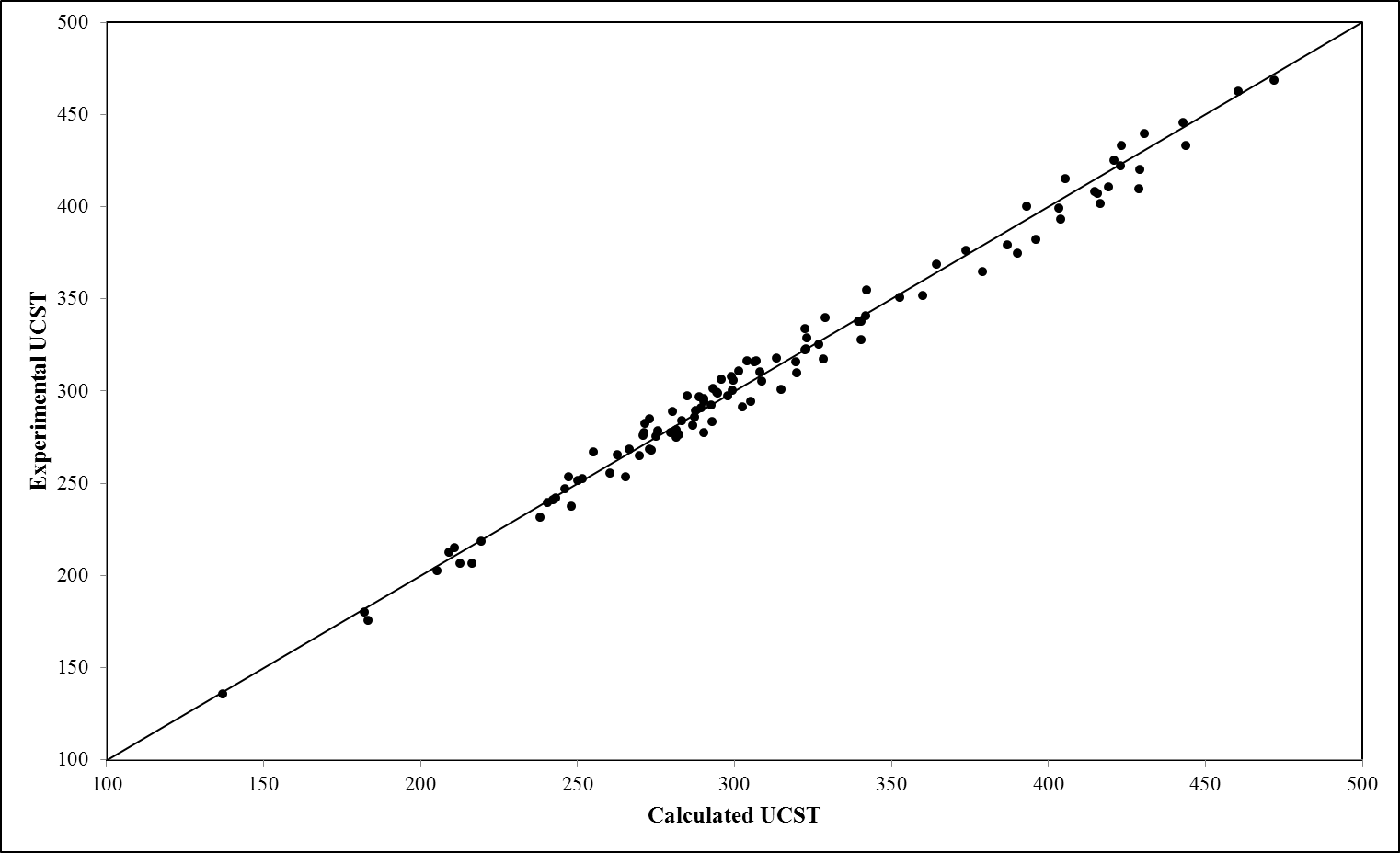


Fig. 5. The correlation results of obtained models of UCST

Based on the obtained statistical parameters listed in Table 4, both the models are desirable and result in considerable accuracy in predictions. The increase in adjusted R-sq. value suggests that the addition of additional constant and coefficients to the model equations may increase the correlation and accuracy of predictions. This can be simply justified as the model equation (Eq. 16) was developed based on some simplification applied to the general form presented in Eqs. 13-15. According to the correlations shown in Fig. 4 and Fig. 5, the agreement between the experimental data and model predications are desirable.

* 1. New group contribution based correlation

For each connectivity index of interest, the aforementioned system of equations (Eq. 21) was constructed and solved. The coefficients of each model then were calculated using Eq. 22 as listed in Table 6.

Table 6. Obtained model coefficients

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |  |
| *a0* | -3.90332 | 1.03859 | -9.80256×10-2 | -7.15071 | -4.30298 | 3.38060 | 2.47805 | 1.68207 |
| *a1* | -4.02362×10-3 | -2.70222×10-3 | 1.55240×10-3 | 3.61805×10-3 | 3.92652×10-3 | 2.47410×10-4 | -1.77303×10-4 | -2.29583×10-4 |
| *a2* | -4.15914×10-2 | -2.12398×10-3 | -3.59079×10-3 | -2.46037×10-2 | -9.16374×10-3 | -3.71859×10-3 | -2.32192×10-3 | -1.15389×10-3 |
| *a3* | 2.91502×10-2 | 1.63677×10-3 | 1.76236×10-3 | 1.97301×10-2 | 8.40892×10-3 | -2.26346×10-3 | -1.78076×10-3 | -1.45682×10-3 |
| *a4* | 9.90248×10-6 | 1.24268×10-6 | 1.30665×10-7 | 4.56275×10-6 | 1.14879×10-6 | 1.88472×10-6 | 1.45618×10-6 | 1.08607×10-6 |
| *a5* | 1.03818×10-5 | 9.98853×10-7 | 7.95056×10-8 | 5.21157×10-6 | 1.74858×10-6 | -5.25702×10-6 | -4.51324×10-6 | -4.03907×10-6 |
| *a6* | -1.82260×10-6 | -3.55109×10-7 | 4.56412×10-7 | -1.12049×10-6 | 4.07587×10-7 | 2.18997×10-6 | 1.78060×10-6 | 1.55828×10-6 |
| *a7* | 1.54025×10-5 | 7.95713×10-7 | 1.53662×10-6 | 9.07445×10-6 | 4.32482×10-6 | -2.05887×10-6 | -1.18385×10-6 | -2.15246×10-7 |
| *a8* | 2.00724×10-5 | 1.05835×10-6 | 1.36691×10-6 | 1.26978×10-5 | 4.64858×10-6 | 6.98349×10-6 | 5.42834×10-6 | 3.96362×10-6 |
| *a9* | -3.28928×10-5 | -1.36473×10-6 | -3.30425×10-6 | -2.15038×10-5 | -1.05731×10-5 | -3.27922×10-6 | -2.99776×10-6 | -2.98750×10-6 |

Using the model coefficients listed in Table 6, the connectivity indices were back-calculated and the deviations were obtained in terms of AARD (accumulative averaged relative deviation which equals average of IARD values) as listed in Table 7.

Table 7. Obtained correlation for developed group contribution of connectivity indices

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |  |
| AARD (%) | 28.88 | 28.27 | 7.67 | 48.15 | 43.70 | 31.81 | 41.09 | 41.22 |

The correlation of model predictions and the calculated connectivity indices are shown in Fig. 6-Fig. 13 for each eight studied connectivity indices.

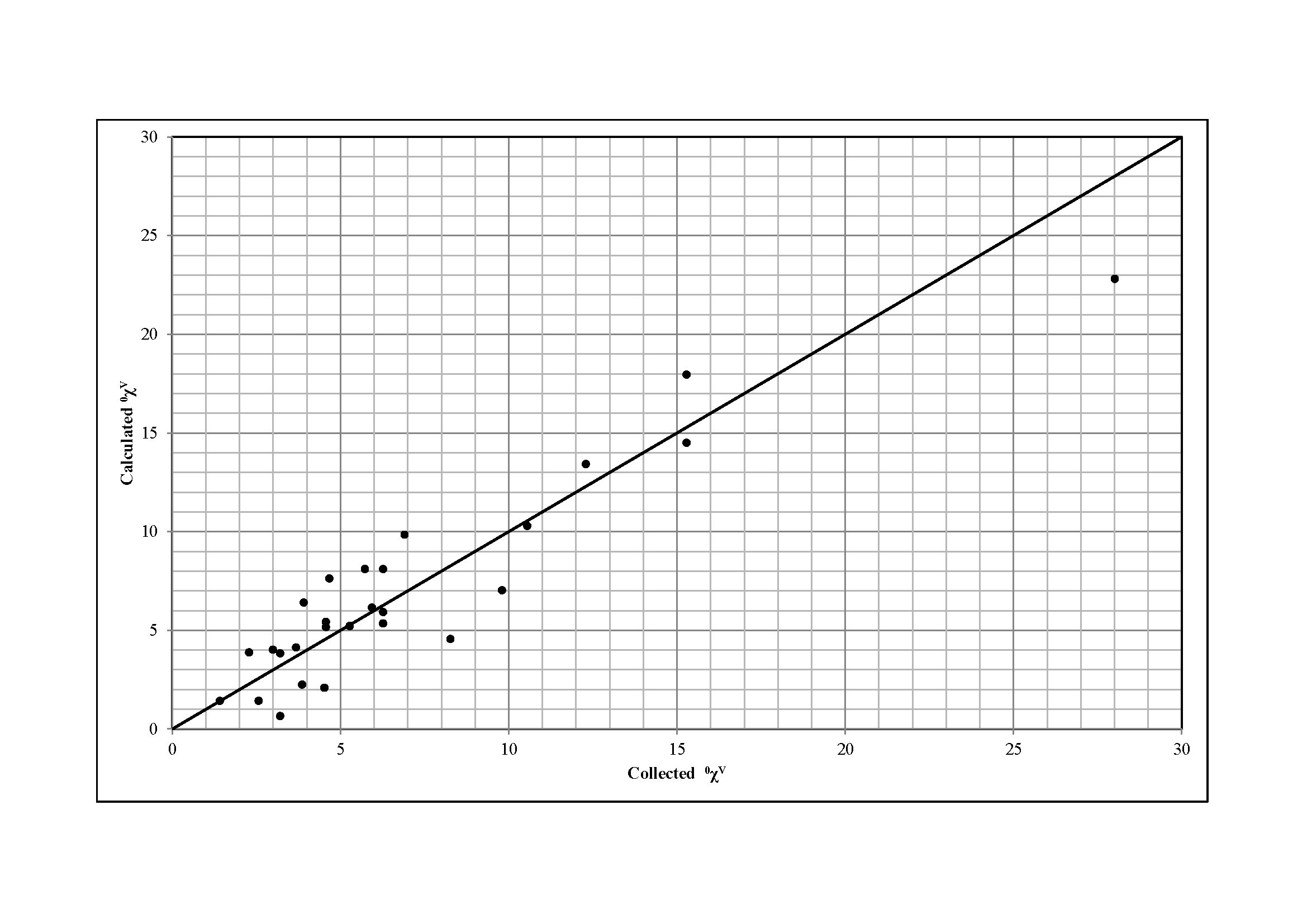


Fig. 6. The correlation results of 

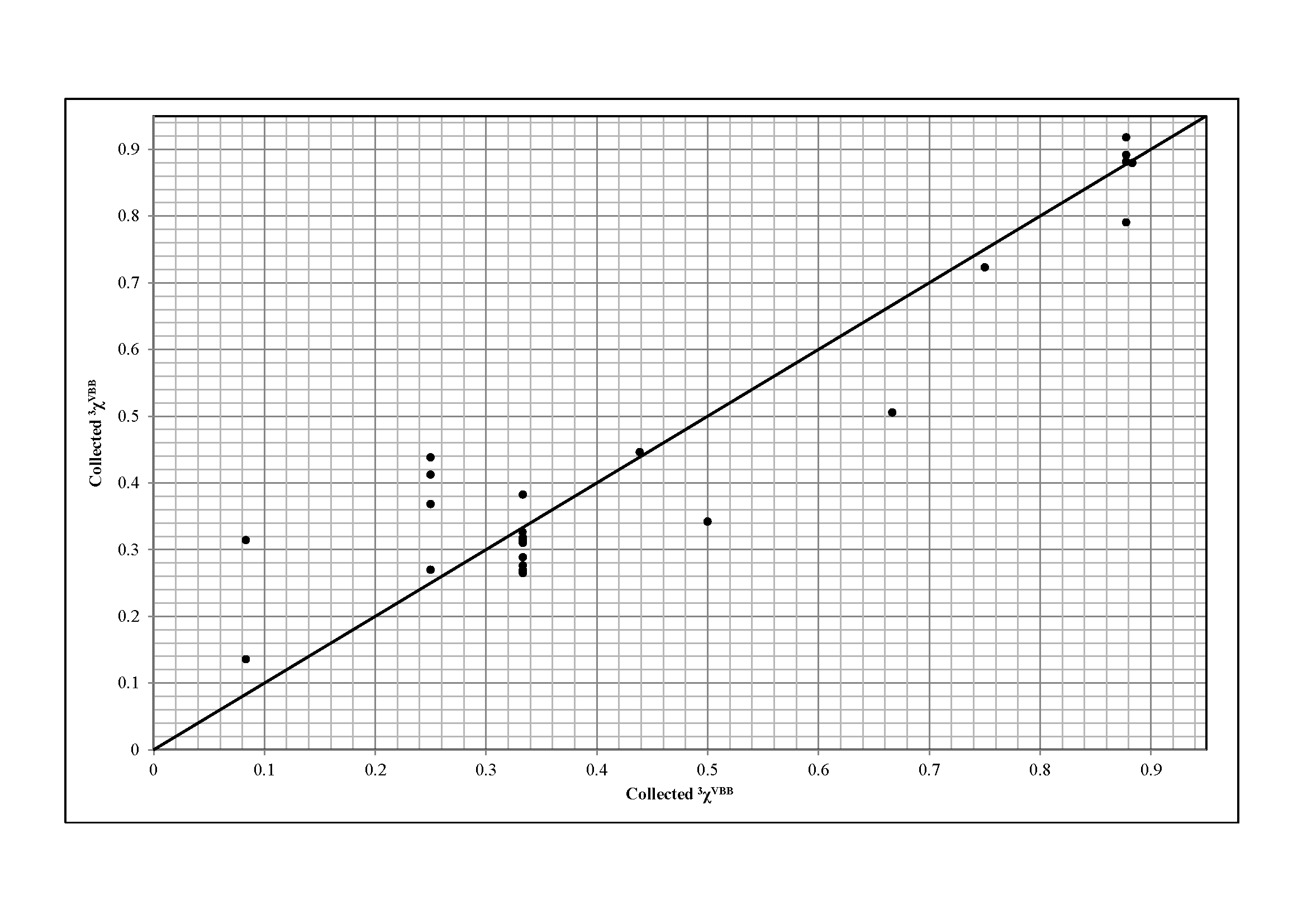


Fig. 7. The correlation results of 

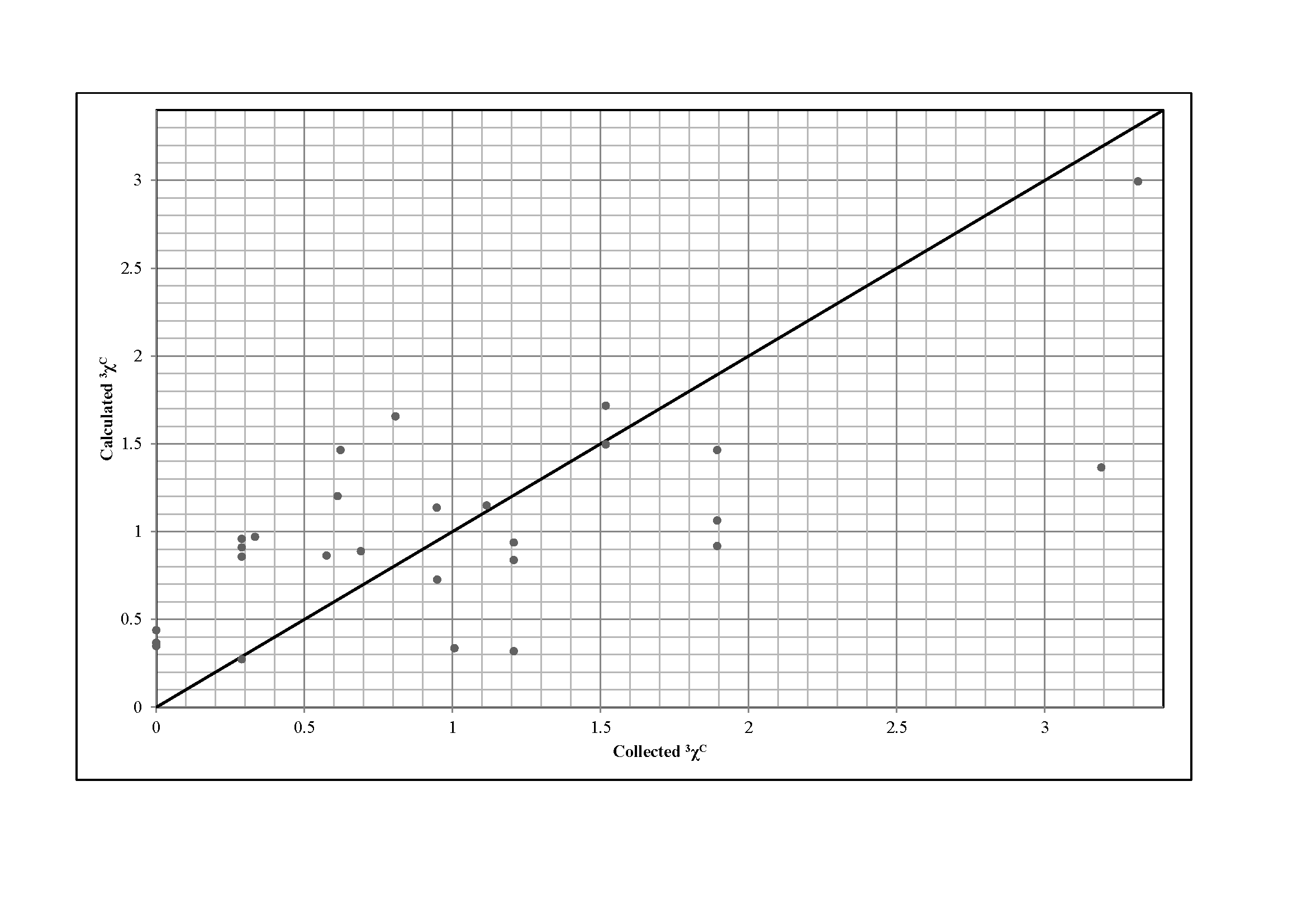


Fig. 8. The correlation results of 

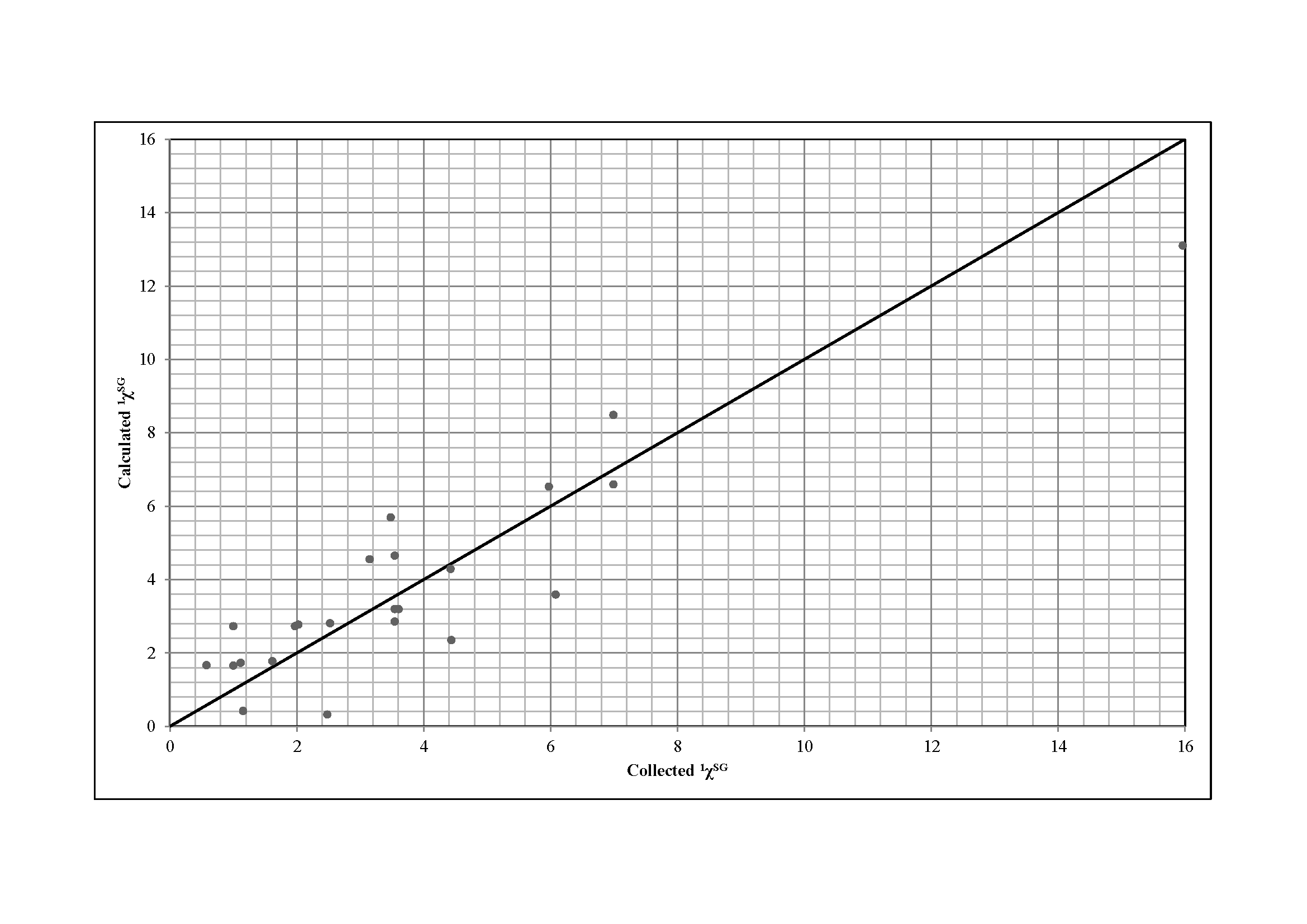


Fig. 9. The correlation results of 

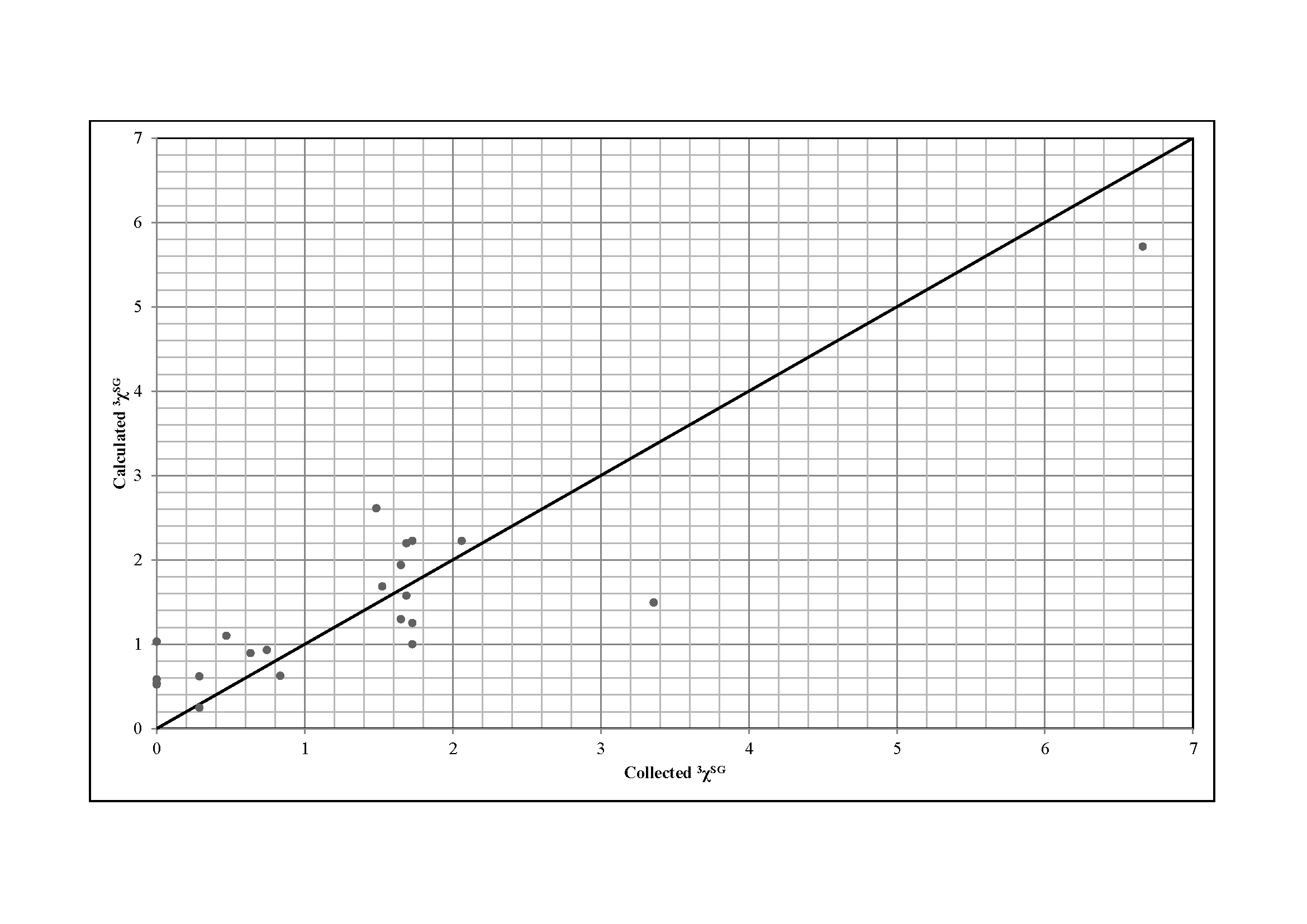


Fig. 10. The correlation results of 

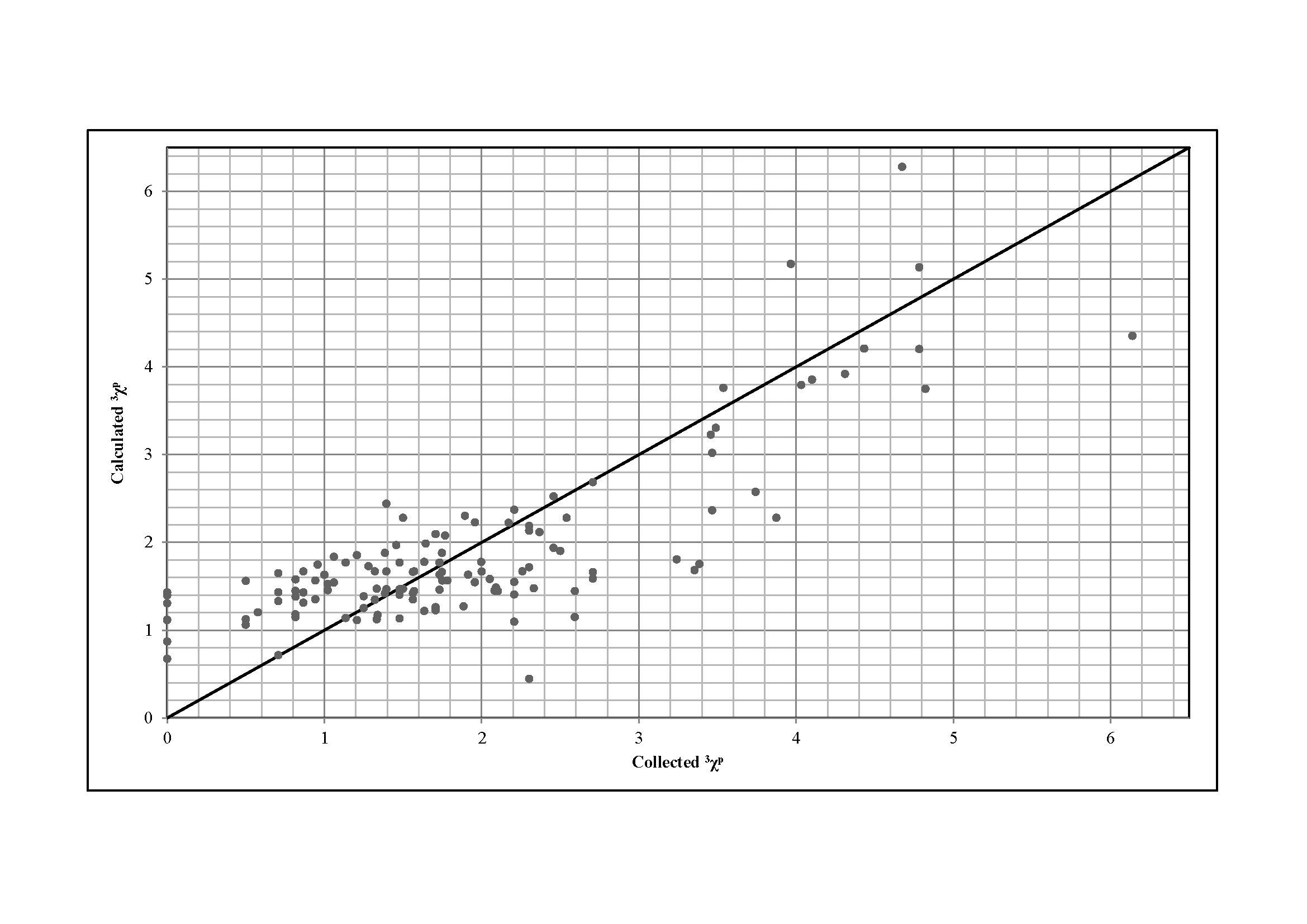


Fig. 11. The correlation results of 

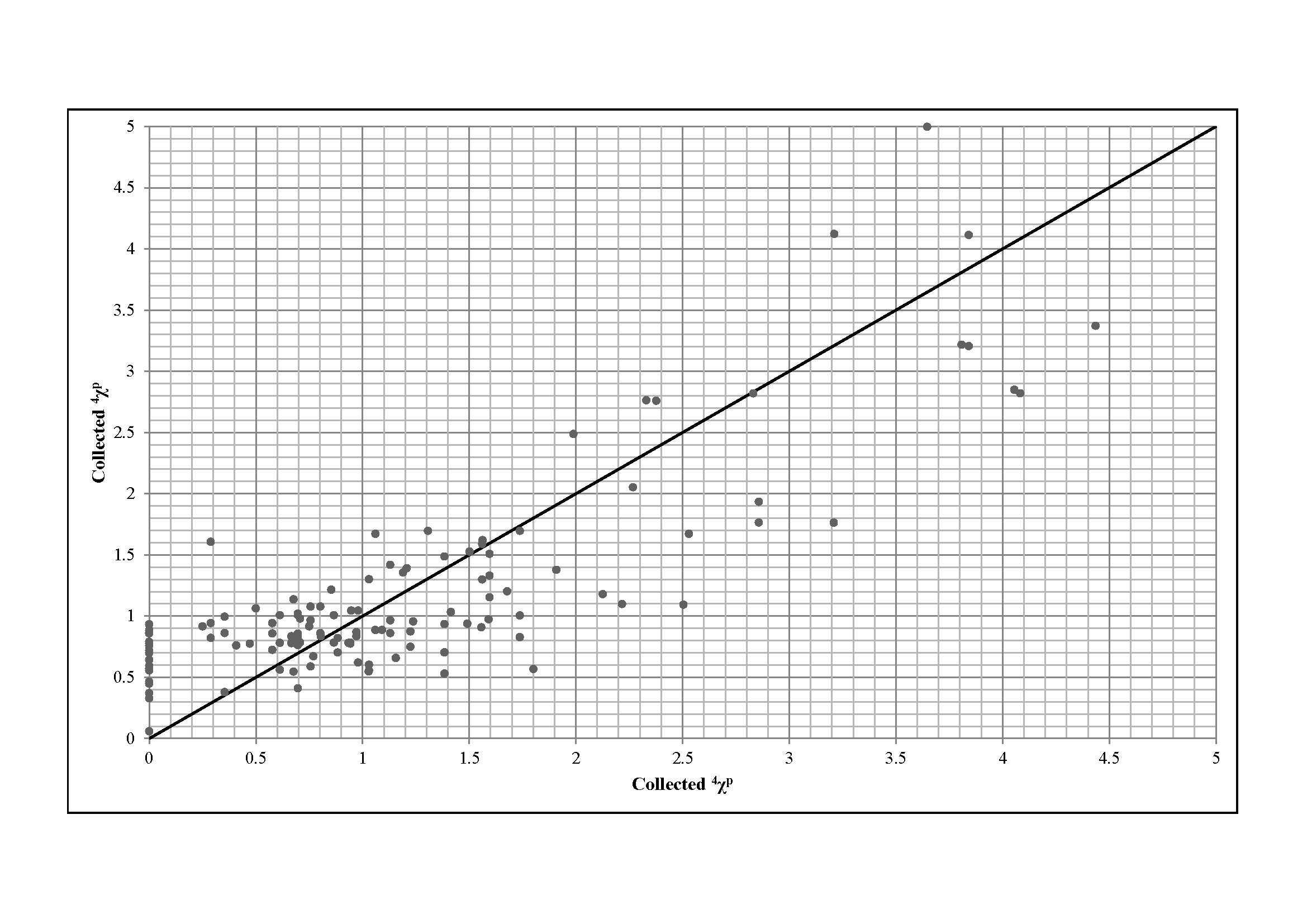


Fig. 12. The correlation results of 

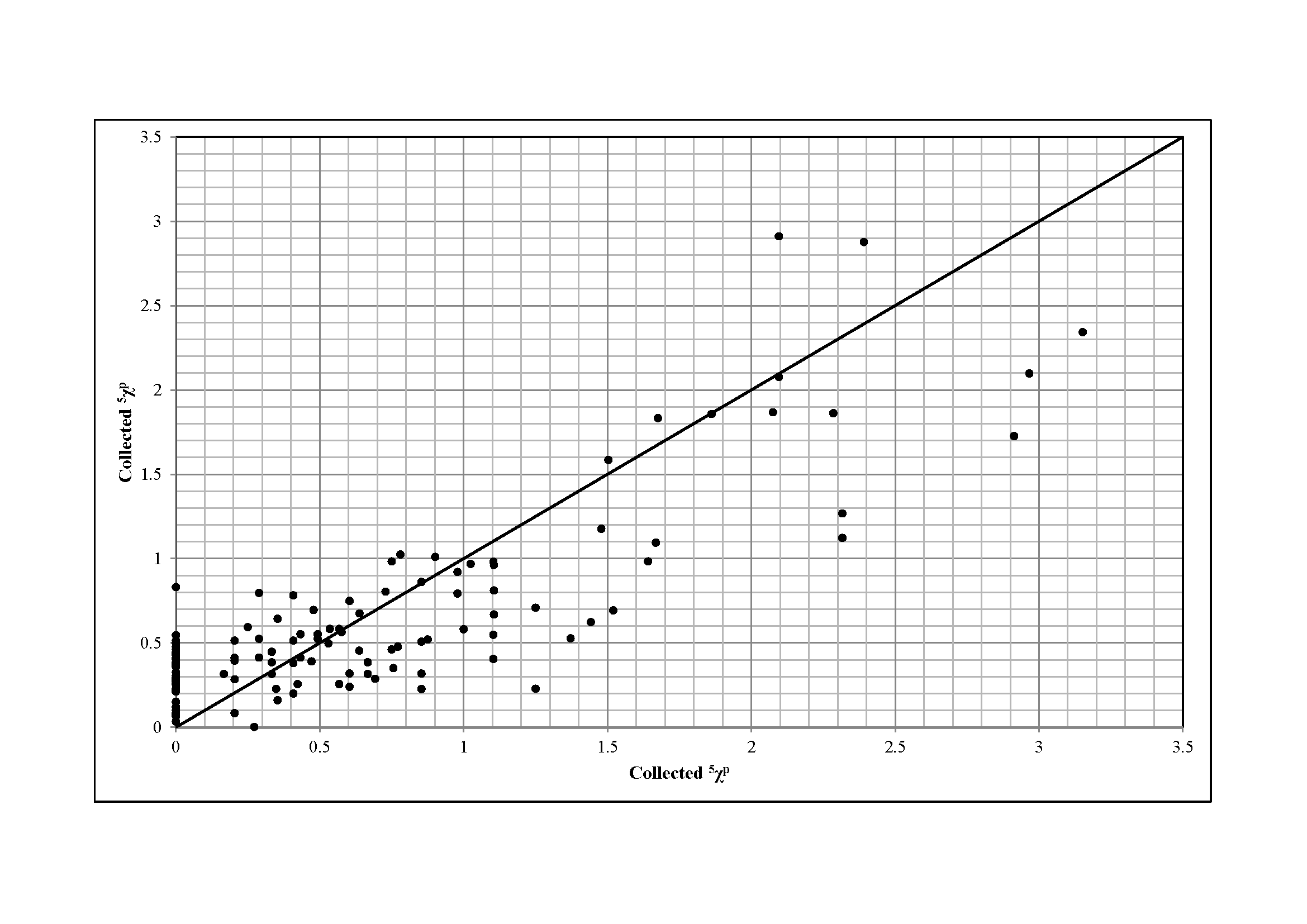


Fig. 13. The correlation results of 

Having the obtained correlations of these connectivity indices, the application of QSPR models, as reported elsewhere [[10](#_ENREF_10), [17](#_ENREF_17)] could be coupled to the chemical thermodynamic models and approaches. So, the necessity of the utilization of commercial geometry optimization software packages for components topology determination could be removed and molecule descriptors can be substituted by the parameters such as scaling parameters of modified SL-EOS for which well-established calculation and interpretation approaches have been developed. The illustrated correlation results in Fig. 6-Fig. 13 show the desirable accuracy in estimation of connectivity indices using lattice fluid theory parameters as inputs.

The R2 of developed models in this work and models available in literature are compared as listed in Table 8. According to the results, both modeling for both LCST and UCST are of superiority over available models. Imre et al. [[12](#_ENREF_12)] and Liu et al. [[15](#_ENREF_15)] have developed their correlations for a limited number of systems which fails to be extended to other systems. The neural network (NN) developed by Xu et al. [[16](#_ENREF_16)] demonstrated great reliability in fitting of experimental data as it is expected from NN which pattern recognition tools, however, they did not provide the details about the structure of NN and the optimal weights and biases which are mandatory if one aims to reproduce the data or to use their model.

Table 8. Comparison of R2 of developed models in this work and models available in literature

|  |  |  |
| --- | --- | --- |
| **Ref.** | **LCST / UCST** | **R2** |
| Xu et al. [[17](#_ENREF_17)] | LCST | 0.8874 |
| Melagraki et al. [[10](#_ENREF_10)] | LCST | 0.8860 |
| Liu et al. [[13](#_ENREF_13)] | LCST | 0.7700 |
| Gharagheizi et al. [[14](#_ENREF_14)] | UCST | 0.8824 |
| Xu et al. (NN) [[16](#_ENREF_16)] | LCST | 0.9625 |
| Xu et al. (MLRA) [[16](#_ENREF_16)] | LCST | 0.8739 |
| Liu et al. [[15](#_ENREF_15)] | LCST | 0.9009 |
| Imre et al. (Eq. 3) [[12](#_ENREF_12)] | LCST | 0.8897 |
| Imre et al. (Eq. 7) [[12](#_ENREF_12)] | LCST | 0.8979 |
| This work (CRS) | LCST | ***0.9619*** |
| This work (CRS) | UCST | ***0.9618*** |
| This work (Empirical) | LCST | ***0.8919*** |
| This work (Empirical) | UCST | ***0.9091*** |

1. Conclusion

A thermodynamic model was developed and examined for estimation of upper critical solution temperature (UCST) and lower critical solution temperature (LCST) of binary polymeric solutions focusing on the systems which are used in membranes fabrication. The compressible regular solution theory of Mayes together with the Sanchez-Lacombe lattice fluid theory equation of state was employed. The application of thermodynamic model requires the application of an optimization technique to obtain the temperature of interest. The particle swarm optimization technique was used for minimization of predefined constrains. The accuracy and reliability of model was demonstrated by an Individual Absolute Relative Deviation (IARD) of about 5 % and convergence of 30 iterations. In addition, a statistical model was developed using the connectivity indices of polymer and solvent as the independent variables of the model for which an averaged IARD of 4.3 % was obtained. To improve the QSPR models and remove the necessity of commercial molecular geometry optimizers, some simple correlations were developed to relate the lattice fluid theory scaling parameters to eight connectivity indices. The correlation results show an IARD (%) value of about 5 which is desirable. All presented models and correlations can be used for rapid and accurate prediction of LCST and UCST data.

1. Appendix

Table 9. The experimental data of Lower Critical Solution Temperature (LCST) [[16](#_ENREF_16)]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Polymer** | **Solvent** | **LCST [K]** | |
| Exp. | Cal. |
| 1 | Poly(4-methylpent-1-ene) | Butane | 388 | 365 |
| 2 |  | Pentane | 441 | 431 |
| 3 |  | Heptane | 522 | 499 |
| 4 |  | Octane | 553 | 507 |
| 5 |  | 2-Methylbutane | 431 | 415 |
| 6 |  | 2,2-Dimethylbutane | 462 | 456 |
| 7 |  | 2,2-Dimethylpentane | 499 | 486 |
| 8 |  | 2,2,3-Trimethylbutane | 521 | 517 |
| 9 |  | Cyclopentane | 505 | 469 |
| 10 |  | Hexane | 487 | 447 |
| 11 |  | Nonane | 579 | 551 |
| 12 |  | 2,4-Dimethylpentane | 499 | 481 |
| 13 |  | 3-Ethylpentane | 532 | 511 |
| 14 | Polybut-1-ene | Pentane | 421 | 397 |
| 15 |  | Heptane | 509 | 480 |
| 16 |  | Octane | 540 | 510 |
| 17 |  | 2-Methylbutane | 416 | 407 |
| 18 |  | 2,2-Dimethylbutane | 444 | 424 |
| 19 |  | 2,2,3-Trimethylbutane | 507 | 478 |
| 20 |  | 2,5-Dimethylhexane | 519 | 491 |
| 21 |  | 3-Ethylpentane | 523 | 496 |
| 22 |  | 3,4-Dimethylhexane | 559 | 535 |
| 23 |  | Hexane | 464 | 454 |
| 24 |  | Nonane | 564 | 545 |
| 25 |  | 2,4-Dimethylpentane | 480 | 474 |
| 26 |  | 2,3-Dimethylpentane | 517 | 487 |
| 27 |  | Cyclopentane | 498 | 466 |
| 28 | poly(cis-1,4-butadiene) | Hexane | 373 | 355 |
| 29 |  | 2,2,3-Trimethylbutane | 414 | 404 |
| 30 |  | Octane | 390 | 368 |
| 31 |  | Hexan-3-one | 510 | 475 |
| 32 |  | Pentan-3-one | 481 | 453 |
| 33 |  | 2-Methylhexane | 370 | 351 |
| 34 |  | 2,2,4-Trimethylpentane | 388 | 357 |
| 35 |  | Propylene oxide | 414 | 407 |
| 36 | Poly(dimethyl siloxane) | Pentane | 453 | 413 |
| 37 |  | Heptane | 528 | 499 |
| 38 |  | Octane | 553 | 510 |
| 39 |  | Dodecane | 643 | 616 |
| 40 |  | Cetane | 708 | 667 |
| 41 |  | Hexane | 493 | 451 |
| 42 |  | Decane | 603 | 563 |
| 43 | Polyethylene | Hexane | 411 | 382 |
| 44 |  | Heptane | 459 | 444 |
| 45 |  | Nonane | 531 | 508 |
| 46 |  | Decane | 557.55 | 537 |
| 47 |  | Dodecane | 605.55 | 574 |
| 48 |  | Tridecane | 631.55 | 597 |
| 49 |  | 2,2-Dimethylpentane | 399 | 367 |
| 50 |  | 2,2,3-Trimethylbutane | 444 | 431 |
| 51 |  | 2,3-Dimethylpentane | 463 | 442 |
| 52 |  | 3-Ethylpentane | 471 | 440 |
| 53 |  | 2,2,4,4-Tetramethylpentane | 513 | 492 |
| 54 |  | 2,3,4-Trimethylhexane | 545 | 516 |
| 55 |  | Methylcyclopentane | 488 | 454 |
| 56 |  | Methylcyclohexane | 537 | 490 |
| 57 |  | Octan-1-ol | 621 | 608 |
| 58 |  | Pentyl acetate | 528 | 503 |
| 59 |  | Pentane | 353 | 331 |
| 60 |  | Octane | 496 | 470 |
| 61 |  | Undecane | 581.75 | 536 |
| 62 |  | 2,4-Dimethylpentane | 395 | 377 |
| 63 |  | 2,2,4-Trimethylpentane | 495 | 476 |
| 64 |  | 3,4-Dimethylhexane | 515 | 475 |
| 65 |  | Cyclopentane | 472 | 447 |
| 66 |  | Cyclohexane | 518 | 493 |
| 67 |  | Butyl acetate | 490 | 463 |
| 68 | Polyisobutene | Cyclopentane | 461 | 433 |
| 69 |  | Cyclohexane | 516 | 485 |
| 70 |  | Cycloheptane | 572 | 540 |
| 71 |  | Cyclooctane | 637 | 588 |
| 72 |  | Heptane | 442 | 404 |
| 73 |  | Octane | 477 | 450 |
| 74 |  | Dodecane | 582 | 567 |
| 75 |  | 2-Methylbutane | 318 | 303 |
| 76 |  | 2-Methylpentane | 376 | 354 |
| 77 |  | 3-Methylpentane | 405 | 384 |
| 78 |  | 3-Methylhexane | 446 | 421 |
| 79 |  | 3-Ethylpentane | 458 | 418 |
| 80 |  | 2,3-Dimethylpentane | 451 | 439 |
| 81 |  | 2,4-Dimethylpentane | 403 | 386 |
| 82 |  | 2,2,3-Trimethylbutane | 445 | 420 |
| 83 |  | Ethylcyclopentane | 524 | 494 |
| 84 |  | 3-Methylheptane | 478 | 437 |
| 85 |  | 2,2-Dimethylhexane | 454 | 423 |
| 86 |  | 2,5-Dimethylhexane | 446 | 416 |
| 87 |  | 3.4-Dimethylhexane | 497 | 474 |
| 88 |  | Propylcyclopentane | 547 | 529 |
| 89 |  | Pentane | 344 | 327 |
| 90 |  | Hexane | 402 | 389 |
| 91 |  | Methylcyclopentane | 478 | 451 |
| 92 |  | 2-Methylhexane | 426 | 413 |
| 93 |  | 2,2-Dimethylpentane | 404 | 386 |
| 94 |  | 3,3-Dimethylpentane | 451 | 429 |
| 95 |  | Methylcyclohexane | 526 | 508 |
| 96 |  | 2-Methylheptane | 466 | 430 |
| 97 |  | 2,4-Dimethylhexane | 458 | 435 |
| 98 |  | 2,2,4-Trimethylpentane | 435 | 409 |
| 99 |  | Decane | 535 | 509 |
| 100 | Poly(isotactic methyl methacrylate) | Methyl acetate | 441 | 428 |
| 101 |  | Ethyl acetate | 478 | 447 |
| 102 |  | Hexan-3-one | 511 | 476 |
| 103 |  | Pentan-3-one | 497 | 486 |
| 104 |  | Butyl chloride | 454 | 416 |
| 105 |  | Heptan-4-one | 522 | 519 |
| 106 |  | Butan-2-one | 464 | 426 |
| 107 |  | Tetrahydrofuran (THF) | 519.5 | 483 |
| 108 | Poly(a-methylstyrene) | Cyclopentane | 417.6 | 409 |
| 109 |  | Cyclohexane | 456 | 427 |
| 110 |  | Butyl chloride | 412 | 391 |
| 111 |  | Butyl acetate | 446.9 | 416 |
| 112 |  | Hexyl acetate | 500.9 | 479 |
| 113 |  | Methyl cyclohexane | 431 | 407 |
| 114 |  | Pentyl acetate | 475.8 | 455 |
| 115 | Poly(propylene) | Pentane | 422 | 400 |
| 116 |  | Hexane | 470 | 433 |
| 117 |  | Octane | 542 | 496 |
| 118 |  | Nonane | 571 | 538 |
| 119 |  | 2,2-Dimethylbutane | 441 | 412 |
| 120 |  | 2,3-Dimethylbutane | 465 | 457 |
| 121 |  | 2,2-Dimethylpentane | 489 | 483 |
| 122 |  | 2,2,3-Trimethylbutane | 511 | 478 |
| 123 |  | 2,3-Dimethylpentane | 513 | 492 |
| 124 |  | 3-Ethylpentane | 520 | 501 |
| 125 |  | 2,2,4,4-Tetramethylpentane | 548 | 505 |
| 126 |  | 2,3,4-Trimethylhexane | 585 | 537 |
| 127 |  | Methylcyclopentane | 518 | 477 |
| 128 |  | Methylcyclohexane | 564 | 560 |
| 129 |  | Diethyl ether | 420 | 410 |
| 130 |  | Heptane | 511 | 496 |
| 131 |  | 2-Methylbutane | 413 | 374 |
| 132 |  | 2,4-Dimethylpentane | 481 | 462 |
| 133 |  | 2,2,4-Trimethylpentane | 510 | 497 |
| 134 |  | 3,4-Dimethylhexane | 553 | 550 |
| 135 |  | Cyclopentane | 495 | 491 |
| 136 |  | Cyclohexane | 540 | 522 |
| 137 | Polypent-1-ene | Pentane | 433 | 423 |
| 138 |  | Hexane | 482 | 456 |
| 139 |  | Octane | 556 | 542 |
| 140 |  | 2-Methylbutane | 422 | 395 |
| 141 |  | 2,4-Dimethylpentane | 493 | 482 |
| 142 |  | 2,2-Dimethylpentane | 502 | 475 |
| 143 |  | 2,3-Dimethylpentane | 529 | 499 |
| 144 |  | 3-Methylheptane | 537 | 521 |
| 145 |  | Heptane | 522 | 497 |
| 146 |  | 2,2-Dimethylbutane | 457 | 442 |
| 147 |  | 2,2,4-Trimethylpentane | 527 | 482 |
| 148 |  | Cyclopentane | 502 | 470 |
| 149 | Poly(pchlorostyrene) | Isobutyl acetate | 348.5 | 317 |
| 150 |  | Ethyl carbitol | 300.8 | 291 |
| 151 |  | Butyl carbitol | 323.1 | 294 |
| 152 |  | tert-Butyl acetate | 338.4 | 331 |
| 153 | Polystyrene | Cyclopentane | 427 | 411 |
| 154 |  | Cyclohexane | 486 | 463 |
| 155 |  | Methylcyclopentane | 417 | 401 |
| 156 |  | Methylcyclohexane | 480 | 448 |
| 157 |  | Benzene | 523 | 502 |
| 158 |  | Toluene | 550 | 498 |
| 159 |  | Ethyl acetate | 412 | 395 |
| 160 |  | Propyl acetate | 451 | 424 |
| 161 |  | i-Propyl acetate | 380 | 353 |
| 162 |  | Ethyl butyrate | 471 | 456 |
| 163 |  | Isobutyl acetate | 445 | 432 |
| 164 |  | sec-Butyl acetate | 442 | 422 |
| 165 |  | tert-Butyl acetate | 329 | 321 |
| 166 |  | Diethyl malonate | 578 | 548 |
| 167 |  | i-Amyl acetate | 493 | 488 |
| 168 |  | Methyl acetate | 384.5 | 364 |
| 169 |  | Butan-2-one | 420 | 396 |

Table 10. The experimental data of Upper Critical Solution Temperature (UCST) [[14](#_ENREF_14)]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Polymer** | **Solvent** | **UCST [K]** | |
| Exp. | Cal. |
| 1 | cellulose diacetate | 2-butanone | 310 | 296 |
| 2 |  | 2-propanone | 280 | 269 |
| 3 | cellulose tricaprylate | N,N-dimethylformamide | 413 | 390 |
| 4 | cellulose triacetate | benzyl alcohol | 341 | 324 |
| 5 |  | 2-propanone | 300 | 294 |
| 6 | hydroxypropylcellulose | water | 343.85 | 336 |
| 7 | methylcellulose | water | 332.65 | 308 |
| 8 | poly(1-butene) (isotactic) | anisole | 362.3 | 343 |
| 9 | poly(butyl methacrylate) | 2-propanol | 297.3 | 284 |
| 10 | poly(4-chlorostyrene) | benzene | 274 | 263 |
| 11 |  | ethylbenzene | 258.45 | 244 |
| 12 |  | ethyl chloroacetate | 271.35 | 253 |
| 13 |  | isopropylbenzene | 332.15 | 319 |
| 14 |  | isopropyl chloroacetate | 264.95 | 249 |
| 15 |  | methyl chloroacetate | 337.75 | 315 |
| 16 |  | tetrachloroethene | 317.55 | 308 |
| 17 |  | tetrachloromethane | 323.85 | 302 |
| 18 | poly(ethyl acrylate) | 1-butanol | 318.05 | 298 |
| 19 |  | ethanol | 310.55 | 292 |
| 20 |  | methanol | 293.65 | 266 |
| 21 |  | 1-propanol | 312.65 | 296 |
| 22 | polyethylene (linear) | anisole | 426.65 | 410 |
| 23 |  | benzyl phenyl ether | 462.65 | 429 |
| 24 |  | biphenyl | 400.65 | 379 |
| 25 |  | 1-decanol | 426.45 | 404 |
| 26 |  | diphenyl ether | 437.05 | 419 |
| 27 |  | diphenylmethane | 415.35 | 388 |
| 28 |  | 1-dodecanol | 410.15 | 383 |
| 29 |  | 4-nonylphenol | 435.55 | 417 |
| 30 |  | 1-octanol | 453.25 | 442 |
| 31 |  | 4-octylphenol | 447.65 | 425 |
| 32 |  | pentyl acetate | 434 | 423 |
| 33 |  | 4-tert-pentylphenol | 463.35 | 426 |
| 34 | poly(p-hexylstyrene) | 2-butanone | 302.6 | 291 |
| 35 | poly(2-hydroxyethyl methacrylate) | 1-propanol | 326.5 | 308 |
| 36 | polyisobutylene | diphenyl ether | 306 | 291 |
| 37 |  | ethylbenzene | 249 | 231 |
| 38 |  | ethyl heptanoate | 306 | 292 |
| 39 |  | ethyl hexanoate | 330 | 320 |
| 40 |  | toluene | 260 | 251 |
| 41 | poly(dl-lactide) | dibutyl phthalate | 358.8 | 349 |
| 42 |  | dipentyl phthalate | 415.8 | 402 |
| 43 | poly(methyl methacrylate) | acetonitrile | 314 | 294 |
| 44 |  | 1-chlorobutane | 320 | 305 |
| 45 |  | 2,2-dimethyl-3-pentanone | 308.15 | 292 |
| 46 |  | 2,4-dimethyl-3-pentanone | 319.15 | 315 |
| 47 |  | 2-ethylbutanal | 295.15 | 276 |
| 48 |  | 3-heptanone | 307.7 | 306 |
| 49 |  | 4-heptanone | 309 | 298 |
| 50 |  | 2-octanone | 325.15 | 297 |
| 51 |  | 3-octanone | 346.85 | 331 |
| 52 |  | acetonitrile | 301 | 283 |
| 53 |  | 1-chlorobutane | 309 | 295 |
| 54 |  | 4-heptanone | 319 | 303 |
| 55 |  | 3-hexanone | 279 | 272 |
| 56 | poly(4-methyl-1-pentene) (isotactic) | biphenyl | 467.8 | 463 |
| 57 |  | diphenyl ether | 483.2 | 460 |
| 58 |  | diphenylmethane | 449.8 | 416 |
| 59 | poly(R-methylstyrene) | methylcyclohexane | 357 | 342 |
| 60 | poly(2-methyl-5-vinylpyridine) | butyl acetate | 294.95 | 289 |
| 61 |  | ethyl butyrate | 323.15 | 310 |
| 62 |  | ethyl propionate | 298.55 | 273 |
| 63 |  | 3-methylbutyl acetate | 322.15 | 299 |
| 64 |  | 2-methylpropyl acetate | 326.15 | 310 |
| 65 |  | pentyl acetate | 321.35 | 305 |
| 66 | poly(2-methyl-5-vinylpyridine) | propionitrile | 269.55 | 261 |
| 67 |  | propyl acetate | 292.45 | 270 |
| 68 |  | propyl propionate | 331.15 | 327 |
| 69 |  | tetrahydronaphthalene | 322.65 | 301 |
| 70 | polypropylene (isotactic) | benzyl phenyl ether | 455 | 434 |
| 71 |  | benzyl propionate | 430.7 | 395 |
| 72 |  | biphenyl | 398.3 | 390 |
| 73 |  | 4-tert-butylphenol | 439.2 | 406 |
| 74 |  | dibenzyl ether | 456.4 | 425 |
| 75 |  | diphenyl ether | 416 | 382 |
| 76 |  | 4-tert-pentylphenol | 414 | 396 |
| 77 | polystyrene | 1-chloro-n-decane | 279.7 | 274 |
| 78 |  | 1-chloro-n-dodecane | 331.7 | 312 |
| 79 |  | 1-chloro-n-undecane | 305.9 | 280 |
| 80 |  | 1-nitopropane | 272 | 251 |
| 81 |  | 2,5-dimethyl furan | 145 | 142 |
| 82 |  | 2-methylpropyl acetate | 227 | 216 |
| 83 |  | 2-propyl acetate | 250 | 235 |
| 84 |  | 3-methylbutyl acetate | 224 | 208 |
| 85 |  | cyclodecane | 289 | 270 |
| 86 |  | cycloheptane | 290 | 278 |
| 87 |  | cyclohexane | 306.51 | 297 |
| 88 |  | cyclooctane | 286 | 282 |
| 89 |  | cyclopentane | 293 | 277 |
| 90 |  | diethyl malonate | 309 | 291 |
| 91 |  | dl-menthol | 388.1 | 361 |
| 92 |  | dl-terpineol | 351.6 | 332 |
| 93 |  | dodecadeuterocyclohexane | 312.5 | 293 |
| 94 |  | dodecyl acetate | 285.2 | 273 |
| 95 |  | ethyl acetate | 229 | 212 |
| 96 |  | ethyl chloroacetate | 255 | 237 |
| 97 |  | ethylcyclohexane | 342.95 | 312 |
| 98 |  | hexyl-m-xylene | 285.5 | 275 |
| 99 |  | isoamyl acetate | 224 | 218 |
| 100 |  | isobutyl acetate | 227 | 219 |
| 101 |  | isopropyl acetate | 246 | 231 |
| 102 |  | methylcyclopentane | 348 | 331 |
| 103 |  | n-butyl formate | 264 | 250 |
| 104 |  | n-propyl acetate | 193 | 185 |
| 105 |  | o-dichlorobenzen | 220 | 214 |
| 106 |  | propyl acetate | 193 | 186 |
| 107 |  | trans-decahydronaphthalene | 293 | 279 |

Table 11. Connectivity Indices of selected polymers

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Polymer** |  |  |  |  |  |
| 1 | cellulose diacetate | 12.2925 | 0.8777 | 1.1154 | 5.9733 | 1.5236 |
| 2 | cellulose triacetate | 15.2841 | 0.8777 | 1.5177 | 6.9909 | 1.6868 |
| 3 | cellulose tricaprylate | 28.0120 | 0.8777 | 3.3148 | 15.9667 | 6.6615 |
| 4 | hydroxypropyl cellulose | 15.2841 | 0.8777 | 1.5177 | 6.9909 | 1.6868 |
| 5 | methylcellulose | 10.5520 | 0.8833 | 0.2887 | 4.4234 | 0.2887 |
| 6 | poly(2-hydroxyethyl methacrylate) | 6.9058 | 0.25 | 0.8077 | 3.4814 | 1.4835 |
| 7 | poly(2-methyl-5-vinylpyridine) | 6.2676 | 0.3333 | 1.8938 | 3.5437 | 1.7272 |
| 8 | poly(4-chlorostyrene) | 6.2676 | 0.3333 | 1.8938 | 3.5437 | 1.7272 |
| 9 | poly(4-methylpent-1-ene) | 4.5689 | 0.3333 | 0.6124 | 1.9712 | 0.4714 |
| 10 | poly(a-methylstyrene) | 5.939 | 0.25 | 0.9469 | 3.6052 | 1.6498 |
| 11 | poly(butyl methacrylate) | 8.2676 | 0.3333 | 0.9484 | 4.4367 | 0.8347 |
| 12 | poly(cis-1,4-butadiene) | 2.5689 | 0.6667 | 0 | 0 | 0 |
| 13 | poly(dimethyl siloxane) | 3.9083 | 0.7501 | 1.2071 | 1 | 0 |
| 14 | poly(dl-lactide) | 3.8618 | 0.4388 | 0 | 1.1547 | 0 |
| 15 | poly(ethyl acrylate) | 5.2760 | 0.3333 | 0.6910 | 2.5260 | 0.7440 |
| 16 | poly(isotactic methyl methacrylate) | 4.5236 | 0.25 | 1.0067 | 2.4814 | 0.6124 |
| 17 | poly(methyl methacrylate) | 4.5689 | 0.3333 | 0.5749 | 2.0260 | 0.6339 |
| 18 | poly(p-hexylstyrene) | 9.8031 | 0.3333 | 3.1907 | 6.0817 | 3.3573 |
| 19 | poly(pchlorostyrene) | 5.7273 | 0.25 | 0.622 | 3.5437 | 2.0605 |
| 20 | poly(propylene) | 2.2845 | 0.3333 | 0.2887 | 0.5774 | 0 |
| 21 | poly(R-methylstyrene) | 6.2676 | 0.3333 | 1.8938 | 3.5437 | 1.7272 |
| 22 | polybut-1-ene | 2.9916 | 0.3333 | 0.2887 | 1.1154 | 0 |
| 23 | polyethylene | 1.4142 | 0.5 | 0 | 0 | 0 |
| 24 | polyisobutene | 3.2071 | 0.0833 | 1.2071 | 1 | 0 |
| 25 | polyisobutylene | 3.2071 | 0.0833 | 1.2071 | 1 | 0 |
| 26 | polypent-1-ene | 3.6787 | 0.3333 | 0.2887 | 1.6154 | 0.2887 |
| 27 | Polystyrene | 4.6712 | 0.333 | 0.3333 | 3.1498 | 1.6498 |

Table 12. Connectivity Indices of selected solvents

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Solvent** |  |  |  |
| 1 | 1-butanol | 0.7071 | 0.3536 | 0 |
| 2 | 1-chlorobutane | 0.7071 | 0.3536 | 0 |
| 3 | 1-chloro-n-decane | 2.2071 | 1.3839 | 0.8536 |
| 4 | 1-chloro-n-dodecane | 2.7071 | 1.7374 | 1.1035 |
| 5 | 1-chloro-n-undecane | 2.4571 | 1.5607 | 0.9786 |
| 6 | 1-decanol | 2.2071 | 1.3839 | 0.8536 |
| 7 | 1-dodecanol | 2.7071 | 1.7374 | 1.1035 |
| 8 | 1-nitopropane | 0.8660 | 0.5773 | 0 |
| 9 | 1-octanol | 1.7071 | 1.0303 | 0.6036 |
| 10 | 1-propanol | 0.5 | 0 | 0 |
| 11 | 2,2,3-trimethylbutane | 1.7321 | 0 | 0 |
| 12 | 2,2,4,4-tetramethylpentane | 1.0607 | 1.591 | 0 |
| 13 | 2,2,4-trimethylpentane | 1.0206 | 1.2247 | 0 |
| 14 | 2,2-dimethyl-3-pentanone | 2.0908 | 0.6124 | 0 |
| 15 | 2,2-dimethylbutane | 1.0607 | 0 | 0 |
| 16 | 2,2-dimethylhexane | 1.2803 | 0.7071 | 0.5303 |
| 17 | 2,2-dimethylpentane | 1 | 0.75 | 0 |
| 18 | 2,3,4-trimethylhexane | 2.5931 | 1.0289 | 0.2722 |
| 19 | 2,3-dimethylbutane | 1.3333 | 0 | 0 |
| 20 | 2,3-dimethylpentane | 1.782 | 0.4714 | 0 |
| 21 | 2,4-dimethylhexane | 1.5707 | 0.9714 | 0.3333 |
| 22 | 2,4-dimethylpentane | 0.9428 | 0.9428 | 0 |
| 23 | 2,4-dimethyl-3-pentanone | 2.1031 | 0.7698 | 0 |
| 24 | 2,5-dimethyl furan | 1.9570 | 1.4916 | 0.7559 |
| 25 | 2,5-dimethylhexane | 1.3214 | 0.6667 | 0.6667 |
| 26 | 2-butanone | 0.8164 | 0 | 0 |
| 27 | 2-ethylbutanal | 1.7320 | 0.8660 | 0 |
| 28 | 2-methylbutane | 0.8165 | 0 | 0 |
| 29 | 2-methylheptane | 1.385 | 0.8026 | 0.433 |
| 30 | 2-methylhexane | 1.135 | 0.6124 | 0.4082 |
| 31 | 2-methylpentane | 0.866 | 0.5774 | 0 |
| 32 | 2-methylpropyl acetate | 1.3214 | 0.6667 | 0.3333 |
| 33 | 2-octanone | 1.6350 | 0.9794 | 0.5675 |
| 34 | 2-propanol | 0 | 0 | 0 |
| 35 | 2-propanone | 0 | 0 | 0 |
| 36 | 2-propyl acetate | 0.9428 | 0.7071 | 0 |
| 37 | 3,3-dimethylpentane | 1.9142 | 0.25 | 0 |
| 38 | 3,4-dimethylhexane | 2.2593 | 0.8047 | 0.1667 |
| 39 | 3-ethylpentane | 1.7321 | 0.866 | 0 |
| 40 | 3-heptanone | 1.7474 | 0.7567 | 0.4928 |
| 41 | 3-hexanone | 1.4784 | 0.6969 | 0.2041 |
| 42 | 3-methylbutyl acetate | 1.5629 | 0.9343 | 0.4714 |
| 43 | 3-methylheptane | 1.7474 | 0.7567 | 0.4928 |
| 44 | 3-methylhexane | 1.4784 | 0.6969 | 0.2041 |
| 45 | 3-methylpentane | 1.3938 | 0.2887 | 0 |
| 46 | 3-octanone | 1.9974 | 0.9469 | 0.5350 |
| 47 | 4-heptanone | 1.5629 | 1.1299 | 0.2887 |
| 48 | 4-nonylphenol | 4.3111 | 4.0550 | 2.2852 |
| 49 | 4-octylphenol | 4.1014 | 2.8311 | 2.0752 |
| 50 | 4-tert-butylphenol | 3.5370 | 2.3769 | 1.8619 |
| 51 | 4-tert-pentylphenol | 4.0323 | 2.3302 | 1.6755 |
| 52 | acetonitrile | 0 | 0 | 0 |
| 53 | anisole | 2.3021 | 1.5954 | 1.1052 |
| 54 | benzene | 1.5 | 1.0607 | 0.75 |
| 55 | benzyl alcohol | 2.3021 | 1.5954 | 1.1052 |
| 56 | benzyl phenyl ether | 4.4327 | 3.8079 | 2.9663 |
| 57 | benzyl propionate | 3.4894 | 1.9888 | 1.5034 |
| 58 | biphenyl | 3.9663 | 3.2111 | 2.3914 |
| 59 | butyl acetate | 1.3850 | 0.8026 | 0.4330 |
| 60 | butylchloride | 0.7071 | 0.3536 | 0 |
| 61 | cyclodecane | 2.5 | 1.6778 | 1.25 |
| 62 | cycloheptane | 1.75 | 1.2374 | 0.875 |
| 63 | cyclohexane | 1.5 | 1.0607 | 0.75 |
| 64 | cyclooctane | 2 | 1.4142 | 1 |
| 65 | cyclopentane | 1.25 | 0.8839 | 0 |
| 66 | dibenzyl ether | 4.6742 | 3.6468 | 2.5412 |
| 67 | dibutyl phthalate | 4.8224 | 4.0827 | 2.9137 |
| 68 | diethyl ether | 0.7071 | 0.4082 | 0 |
| 69 | diethyl ketone | 1.3938 | 0.2887 | 0 |
| 70 | diethylmalonate | 2.3677 | 1.9082 | 0.6381 |
| 71 | dipentyl phthalate | 6.1389 | 4.4362 | 3.1522 |
| 72 | diphenyl ether | 4.7828 | 3.8415 | 2.0956 |
| 73 | diphenylmethane | 4.7828 | 3.8415 | 2.0956 |
| 74 | dipropylketone | 1.5629 | 1.1299 | 0.2887 |
| 75 | dl-menthol | 3.3542 | 2.5044 | 1.3717 |
| 76 | dl-terpineol | 3.2406 | 2.1261 | 1.5202 |
| 77 | dodecadeuterocyclohexane | 3.8742 | 2.5302 | 1.6412 |
| 78 | dodecyl acetate | 3.3850 | 2.2168 | 1.4425 |
| 79 | ethanol | 0 | 0 | 0 |
| 80 | ethylacetate | 0.866 | 0.5774 | 0 |
| 81 | ethylbenzene | 2.3021 | 1.5954 | 1.1052 |
| 82 | ethylbutyrate | 1.5629 | 1.1299 | 0.2887 |
| 83 | ethylcarbitol | 1.7071 | 1.0303 | 0.6036 |
| 84 | ethylchloroacetate | 1.4784 | 0.6969 | 0.2041 |
| 85 | ethylcyclohexane | 2.3021 | 1.5954 | 1.1052 |
| 86 | ethylcyclopentane | 2.0521 | 0.6969 | 0.5761 |
| 87 | ethylheptanoate | 2.3319 | 1.5567 | 0.7716 |
| 88 | ethylhexanoate | 2.0819 | 1.0913 | 0.6371 |
| 89 | ethylpropionate | 1.4784 | 0.6969 | 0.2041 |
| 90 | ethylpropyl | 1.4784 | 0.6969 | 0.2041 |
| 91 | hexyl-m-xylene | 3.7421 | 3.2091 | 1.6684 |
| 92 | i-amylacetate | 1.5629 | 0.9343 | 0.4714 |
| 93 | i-propylacetate | 0.9428 | 0.9428 | 0.4082 |
| 94 | isopropylbenzene | 2.5926 | 1.8008 | 1.2504 |
| 95 | i-propyl chloroacetate | 1.7671 | 1.1897 | 0.4082 |
| 96 | isobutylacetate | 1.3214 | 0.6667 | 0.6667 |
| 97 | methanol | 0 | 0 | 0 |
| 98 | methylacetate | 0.8165 | 0 | 0 |
| 99 | methyl chloroacetate | 1.3938 | 0.2887 | 0 |
| 100 | methylcyclohexane | 1.8938 | 1.3067 | 0.901 |
| 101 | methylcyclopentane | 1.6438 | 1.1299 | 0.2887 |
| 102 | methylethyl | 0.8165 | 0 | 0 |
| 103 | N,N-dimethylformamide | 0.8165 | 0 | 0 |
| 104 | n-butane | 0.5 | 0 | 0 |
| 105 | n-butylacetate | 1.385 | 0.8026 | 0.433 |
| 106 | n-butylcarbitol | 2.2071 | 1.3838 | 0.8536 |
| 107 | n-butyl formate | 1.2071 | 0.6768 | 0.3536 |
| 108 | n-cetane | 3.4571 | 2.2678 | 1.4786 |
| 109 | n-decane | 1.9571 | 1.2071 | 0.7286 |
| 110 | n-dodecane | 2.4571 | 1.5607 | 0.9786 |
| 111 | n-heptane | 1.2071 | 0.6768 | 0.3536 |
| 112 | n-hexane | 0.9571 | 0.5 | 0.25 |
| 113 | n-hexylacetate | 1.885 | 1.1561 | 0.6925 |
| 114 | n-nonane | 1.7071 | 1.0303 | 0.6036 |
| 115 | n-octane | 1.4571 | 0.8536 | 0.4786 |
| 116 | n-pentane | 0.7071 | 0.3536 | 0 |
| 117 | n-pentylacetate | 1.635 | 0.9794 | 0.5675 |
| 118 | n-propylacetate | 1.135 | 0.6124 | 0.4082 |
| 119 | n-propylcyclopentane | 2.1717 | 1.5629 | 0.7803 |
| 120 | n-tridecane | 2.7071 | 1.7375 | 1.1036 |
| 121 | n-undecane | 2.2071 | 1.3839 | 0.8536 |
| 122 | o-dichlorobenzen | 2.5403 | 1.5017 | 1.0244 |
| 123 | pentyl acetate | 1.6350 | 0.9794 | 0.4232 |
| 124 | propionitrile | 0.5 | 0 | 0 |
| 125 | propyl acetate | 1.1350 | 0.6124 | 0.4082 |
| 126 | propyleneoxide | 0.5774 | 0 | 0 |
| 127 | propyl propionate | 1.3391 | 0.7567 | 0.3485 |
| 128 | sec-butylacetate | 1.5707 | 0.9714 | 0.3333 |
| 129 | tert-butylacetate | 1.0206 | 1.2247 | 0 |
| 130 | tetrachloroethene | 1.3333 | 0 | 0 |
| 131 | tetrachloromethane | 0 | 0 | 0 |
| 132 | tetrahydrofuran (THF) | 1.25 | 0.8839 | 0 |
| 133 | tetrahydronaphthalene | 3.4663 | 2.8576 | 2.3165 |
| 134 | toluene | 1.8938 | 1.3067 | 0.901 |
| 135 | trans-decahydronaphthalene | 3.4663 | 2.8576 | 2.3165 |
| 136 | water | 0 | 0 | 0 |

Table 13. Scaling parameters of selected polymers

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | Polymer |  |  |  |
| 1 | cellulose diacetate | 2532.55 | -787.35 | 702.03 |
| 2 | cellulose triacetate | 2221.92 | 125.66 | 1805.38 |
| 3 | cellulose tricaprylate | 1341.64 | -932.89 | 659.85 |
| 4 | hydroxypropyl cellulose | 1546.36 | -1416.1 | 118.08 |
| 5 | methylcellulose | 3638.53 | -1727.74 | -2104.69 |
| 6 | poly(2-hydroxyethyl methacrylate) | 809.2 | 160.47 | 1132.86 |
| 7 | poly(2-methyl-5-vinylpyridine) | 884.68 | 409.33 | 1202.69 |
| 8 | poly(4-chlorostyrene) | 935.72 | 344.21 | 1613.17 |
| 9 | poly(4-methylpent-1-ene) | 756.29 | 183.01 | 741.73 |
| 10 | poly(a-methylstyrene) | 741.04 | 268.07 | 1002.76 |
| 11 | poly(butyl methacrylate) | 928.77 | 478.88 | 1169.34 |
| 12 | poly(cis-1,4-butadiene) | 522.01 | 424.01 | 990.01 |
| 13 | poly(dimethyl siloxane) | 476.01 | 302.01 | 1104 |
| 14 | poly(dl-lactide) | 642.89 | 516.72 | 1299.15 |
| 15 | poly(ethyl acrylate) | 917.06 | 419.7 | 1142.98 |
| 16 | poly(isotactic methyl methacrylate) | 651.82 | 529.83 | 1318.12 |
| 17 | poly(methyl methacrylate) | 925.99 | 432.81 | 1161.95 |
| 18 | poly(p-hexylstyrene) | 702.79 | 119.72 | 769.51 |
| 19 | poly(pchlorostyrene) | 935.72 | 344.21 | 1613.17 |
| 20 | poly(propylene) | 711.62 | 318.09 | 889.07 |
| 21 | poly(R-methylstyrene) | 829.52 | 337.19 | 1120.39 |
| 22 | polybut-1-ene | 703.97 | 288.42 | 842.42 |
| 23 | polyethylene | 651.65 | 430.12 | 926.17 |
| 24 | polyisobutene | 720.55 | 331.2 | 908.04 |
| 25 | polyisobutylene | 908.04 | 720.55 | 436.61 |
| 26 | polypent-1-ene | 696.32 | 258.75 | 795.77 |
| 27 | Polystyrene | 1103.45 | 759.12 | 373.48 |

Table 14. Scaling parameters of selected solvent

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | Solvent |  |  |  |
| 1 | 1-butanol | 1136.41 | 1052.29 | 443.67 |
| 2 | 1-chlorobutane | 557.36 | 322.65 | 1083.23 |
| 3 | 1-chloro-n-decane | 511.46 | 144.63 | 803.33 |
| 4 | 1-chloro-n-dodecane | 496.16 | 85.29 | 710.03 |
| 5 | 1-chloro-n-undecane | 305.63 | 114.96 | 756.68 |
| 6 | 1-decanol | 1006.39 | 265.65 | 856.51 |
| 7 | 1-dodecanol | 991.09 | 206.31 | 763.21 |
| 8 | 1-nitropropane | 775.64 | 366.48 | 863.6 |
| 9 | 1-octanol | 1021.69 | 324.99 | 949.81 |
| 10 | 1-propanol | 1059.94 | 473.34 | 1183.06 |
| 11 | 2,2,3-trimethylbutane | 708.2 | -202.47 | 468.18 |
| 12 | 2,2,4,4-tetramethylpentane | 648.23 | -90.44 | 505.28 |
| 13 | 2,2,4-trimethylpentane | 736.71 | -21.32 | 622.91 |
| 14 | 2,2-dimethyl-3-pentanone | 897.97 | 214.1 | 777.73 |
| 15 | 2,2-dimethylbutane | 684.39 | 120.38 | 706.66 |
| 16 | 2,2-dimethylhexane | 669.09 | 61.04 | 613.36 |
| 17 | 2,2-dimethylpentane | 676.74 | 90.71 | 660.01 |
| 18 | 2,3,4-trimethylhexane | 780.1 | -176.13 | 520.19 |
| 19 | 2,3-dimethylbutane | 735.43 | -4.76 | 650.59 |
| 20 | 2,3-dimethylpentane | 727.78 | -34.43 | 603.94 |
| 21 | 2,4-dimethylhexane | 720.13 | -64.1 | 557.29 |
| 22 | 2,4-dimethylpentane | 727.78 | -34.43 | 603.94 |
| 23 | 2,4-dimethyl-3-pentanone | 949.01 | 88.96 | 721.66 |
| 24 | 2,5-dimethyl furan | 488.41 | 526.66 | 1238.52 |
| 25 | 2,5-dimethylhexane | 720.13 | -64.1 | 557.29 |
| 26 | 2-butanone | 836.72 | 342.69 | 842.51 |
| 27 | 2-ethylbutanal | 899.47 | 276.73 | 812.8 |
| 28 | 2-methylbutane | 675.46 | 107.27 | 687.69 |
| 29 | 2-methylheptane | 652.51 | 18.26 | 547.74 |
| 30 | 2-methylhexane | 660.16 | 47.93 | 594.39 |
| 31 | 2-methylpentane | 667.81 | 77.6 | 641.04 |
| 32 | 2-methylpropyl acetate | 599.08 | 276.23 | 1051.12 |
| 33 | 2-octanone | 806.12 | 224.01 | 655.91 |
| 34 | 2-propanol | 573.97 | -105.73 | 751.9 |
| 35 | 2-propanone | 844.37 | 372.36 | 889.16 |
| 36 | 2-propyl acetate | 606.73 | 305.9 | 1097.77 |
| 37 | 3,3-dimethylpentane | 676.74 | 90.71 | 660.01 |
| 38 | 3,4-dimethylhexane | 720.13 | -64.1 | 557.29 |
| 39 | 3-ethylpentane | 660.16 | 47.93 | 594.39 |
| 40 | 3-heptanone | 813.77 | 253.68 | 702.56 |
| 41 | 3-hexanone | 829.07 | 313.02 | 795.86 |
| 42 | 3-methylbutyl acetate | 591.43 | 246.56 | 1004.47 |
| 43 | 3-methylheptane | 652.51 | 18.26 | 547.74 |
| 44 | 3-methylhexane | 660.16 | 47.93 | 594.39 |
| 45 | 3-methylpentane | 667.81 | 77.6 | 641.04 |
| 46 | 3-octanone | 806.12 | 224.01 | 655.91 |
| 47 | 4-heptanone | 813.77 | 253.68 | 702.56 |
| 48 | 4-nonylphenol | -228.89 | -306.45 | 351.27 |
| 49 | 4-octylphenol | -221.24 | -276.78 | 397.92 |
| 50 | 4-tert-butylphenol | -203.85 | -279.91 | 523.09 |
| 51 | 4-tert-pentylphenol | -211.5 | -309.58 | 476.44 |
| 52 | acetonitrile | 772.18 | 496.56 | 1159.03 |
| 53 | anisole | 1312.35 | 333.72 | 1342.53 |
| 54 | benzene | -22.39 | 384.4 | 908.29 |
| 55 | benzyl alcohol | 215.88 | 44.18 | 766.16 |
| 56 | benzyl phenyl ether | -300.59 | 416.03 | 1131.75 |
| 57 | benzyl propionate | -132.15 | 388.61 | 1077.73 |
| 58 | biphenyl | -711.73 | 279.34 | 797.11 |
| 59 | butyl acetate | 531.46 | 358.59 | 1041.57 |
| 60 | butylchloride | 557.36 | 322.65 | 1083.23 |
| 61 | cyclodecane | 590.45 | 192.76 | 552.97 |
| 62 | cycloheptane | 613.4 | 281.77 | 692.92 |
| 63 | cyclohexane | 621.05 | 311.44 | 739.57 |
| 64 | cyclooctane | 605.75 | 252.1 | 646.27 |
| 65 | cyclopentane | 628.7 | 341.11 | 786.22 |
| 66 | dibenzyl ether | -727.52 | 257.56 | 933.3 |
| 67 | dibutyl phthalate | -257.21 | 484.96 | 1153.87 |
| 68 | diethyl ether | 615 | 256.86 | 954.28 |
| 69 | diethyl ketone | 829.07 | 313.02 | 795.86 |
| 70 | diethylmalonate | 455.08 | 527.55 | 1405 |
| 71 | dipentyl phthalate | -272.51 | 274.14 | 1060.57 |
| 72 | diphenyl ether | -285.36 | 427.97 | 1154.69 |
| 73 | diphenylmethane | -727.03 | 220 | 703.81 |
| 74 | dipropylketone | 813.77 | 253.68 | 702.56 |
| 75 | dl-menthol | 381.03 | 444.02 | 1125.92 |
| 76 | dl-terpineol | 386.27 | 158.26 | 683.82 |
| 77 | dodecadeuterocyclohexane | -22.39 | 384.4 | 908.29 |
| 78 | dodecyl acetate | 470.26 | 121.23 | 668.37 |
| 79 | ethanol | 514 | 6.3 | 789 |
| 80 | ethylacetate | 546.76 | 417.93 | 1134.87 |
| 81 | ethylbenzene | 818.57 | 237.88 | 546.89 |
| 82 | ethylbutyrate | 531.46 | 358.59 | 1041.57 |
| 83 | ethylcarbitol | 1141.64 | 421.92 | 2033.51 |
| 84 | ethylchloroacetate | 778.1 | 483.6 | 1430.44 |
| 85 | ethylcyclohexane | 317.37 | 257.18 | 701.95 |
| 86 | ethylcyclopentane | 432.26 | 274.69 | 720.48 |
| 87 | ethylheptanoate | 508.51 | 269.58 | 901.62 |
| 88 | ethylhexanoate | 516.16 | 299.25 | 948.27 |
| 89 | ethylpropionate | 539.11 | 388.26 | 1088.22 |
| 90 | ethylpropyl | 1174.87 | 203.03 | 929.54 |
| 91 | hexyl-m-xylene | 191.71 | -39.02 | 400.31 |
| 92 | i-amylacetate | 591.43 | 246.56 | 1004.47 |
| 93 | i-propylacetate | 606.73 | 305.9 | 1097.77 |
| 94 | isopropylbenzene | 730.61 | 192.33 | 948.72 |
| 95 | i-propyl chloroacetate | 548.6 | 409.25 | 1456.21 |
| 96 | isobutylacetate | 599.08 | 276.23 | 1051.12 |
| 97 | methanol | 521.65 | 35.97 | 835.65 |
| 98 | methylacetate | 554.41 | 447.6 | 1181.52 |
| 99 | methyl chloroacetate | 496.28 | 550.95 | 1539.96 |
| 100 | methylcyclohexane | -37.62 | 372.46 | 885.35 |
| 101 | methylcyclopentane | 77.27 | 389.97 | 903.88 |
| 102 | methylethyl | 730.61 | 192.33 | 948.72 |
| 103 | N,N-dimethylformamide | 870.27 | 402.64 | 992.81 |
| 104 | n-butane | 615.49 | 219.3 | 724.79 |
| 105 | n-butylacetate | 531.46 | 358.59 | 1041.57 |
| 106 | n-butylcarbitol | 467.12 | -96.6 | 968.08 |
| 107 | n-butyl formate | 839.01 | 426.32 | 1079.39 |
| 108 | n-cetane | 523.69 | -136.74 | 164.99 |
| 109 | n-decane | 569.59 | 41.28 | 444.89 |
| 110 | n-dodecane | 554.29 | -18.06 | 351.59 |
| 111 | n-heptane | 592.54 | 130.29 | 584.84 |
| 112 | n-hexane | 600.19 | 159.96 | 631.49 |
| 113 | n-hexylacetate | 805.63 | 261.57 | 885.4 |
| 114 | n-nonane | 577.24 | 70.95 | 491.54 |
| 115 | n-octane | 584.89 | 100.62 | 538.19 |
| 116 | n-pentane | 607.84 | 189.63 | 678.14 |
| 117 | n-pentylacetate | 813.28 | 291.24 | 932.05 |
| 118 | n-propylacetate | 828.58 | 350.58 | 1025.35 |
| 119 | n-propylcyclopentane | 59.12 | 237.16 | 732.83 |
| 120 | n-tridecane | 546.64 | -47.73 | 304.94 |
| 121 | n-undecane | 561.94 | 11.61 | 398.24 |
| 122 | o-dichlorobenzen | 545.39 | 357.42 | 1533.35 |
| 123 | pentyl acetate | 813.28 | 291.24 | 932.05 |
| 124 | propionitrile | 764.53 | 466.89 | 1112.38 |
| 125 | propyl acetate | 828.58 | 350.58 | 1025.35 |
| 126 | propyleneoxide | 711.13 | 355.65 | 1118.56 |
| 127 | propyl propionate | 820.93 | 320.91 | 978.7 |
| 128 | sec-butylacetate | 553.85 | 298.18 | 1081.62 |
| 129 | tert-butylacetate | 570.43 | 340.96 | 1147.24 |
| 130 | tetrachloroethene | 1537.77 | 529.92 | 2468.67 |
| 131 | tetrachloromethane | 1440.36 | 447.69 | 2332.07 |
| 132 | tetrahydrofuran (THF) | 635.86 | 408.34 | 1062.36 |
| 133 | tetrahydronaphthalene | -52.99 | 265.72 | 721.69 |
| 134 | toluene | -37.62 | 372.46 | 885.35 |
| 135 | trans-decahydronaphthalene | 1106.95 | 232.8 | 491.21 |
| 136 | water | 647 | 22.1 | 1000 |

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