Determination of the Hansen solubility parameters with a novel optimization method

Ming Weng[1,2]

[1]College of Materials and Textiles, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, People's Republic of China
[2]National and Local Joint Engineering Laboratory for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, People's Republic of China
Correspondence to: M. Weng (E-mail: mweng@zstu.edu.cn)

ABSTRACT: The Hansen solubility parameters (HSPs) are useful for predicting solvent–solute affinity. In this study, the HSPs and the sphere radii (*Ro*'s) of poly(ether sulfone), bitumen, and lignin were determined by a novel optimization method. A hybrid algorithm, which could locate multiple optima, was developed and used to solve optimization problems for maximizing the fitness (*F*) and minimizing both *Ro* and the numbers of good solvent and total outliers. For most selected samples, improved results with higher *F* and reduced *Ro* and number of outliers were obtained. The results clarify the correlations among three criteria for an optimal solubility sphere, namely, the smallest *Ro*, highest *F*, and lowest number of outliers. They can be satisfied simultaneously only when outliers are avoided; otherwise, a reduction in *Ro* decreases *F* but can retain the same outliers. Thereby, defining the solubility sphere as the one having the smallest *Ro* and the lowest number of outliers is more reasonable according to the physical significance in both cases. © 2015 Wiley Periodicals, Inc. J. Appl. Polym. Sci. **2016**, *133*, 43328.

INTRODUCTION

Hansen Solubility Parameters (HSPs)

The solubility parameter (SP) is of practical significance in material design and processing. It has been applied to predict the polymer compatibility, chemical resistance, and permeation rate and to characterize the surface properties of pigments, fillers, and fibers.[1]

SP was first defined by Hildebrand as the square root of the cohesive energy density[2]:

$$\delta = \sqrt{\frac{E}{V}} \qquad (1)$$

where E is the measured latent heat of vaporization of the pure solvent and V is its molar volume.

The Hildebrand SP is limited to regular solutions or nonpolar systems exclusively involving van der Waals interactions. For systems containing polar molecules or specific interactions, the use of multicomponent SPs, such as three-dimensional HSPs, is required.[1,3] The Hansen dispersion, polar, and hydrogen-bonding solubility parameters (δ_d, δ_p, and δ_h, respectively) are defined as follows[4]:

$$\delta_d = \sqrt{\frac{E_d}{V}}, \delta_p = \sqrt{\frac{E_p}{V}}, \delta_h = \sqrt{\frac{E_h}{V}} \qquad (2)$$

where E_d, E_p, and E_h are the cohesive energy components induced by dispersion, polar, and hydrogen-bonding interactions, respectively. This is based on the assumption that $E = E_d + E_p + E_h$.

The sum of the squares of three HSPs is equal to the square of the Hildebrand SP:

$$\delta^2 = \delta_d^2 + \delta_p^2 + \delta_h^2 \qquad (3)$$

In Hansen's system, the solubility of a solvent is represented by a point in the $\delta_d \times \delta_p \times \delta_h$ space, whereas the solubility of a solute is represented by a volume. In principle, the solubility volume includes all good solvents and excludes all bad ones. A good or bad solvent refers to a solvent whose solute affinity is higher or lower, respectively, than a critical level. In terms of a large number of experimental data and HSP evaluations, Hansen found that in a modified $2\delta_d \times \delta_p \times \delta_h$ space (Figure 1), the solubility volume could be simplified into a sphere identified by four parameters: the coordinate of the sphere center ($2\delta_{d2}$, δ_{p2}, δ_{h2}) and the sphere radius (*Ro*), where δ_{d2}, δ_{p2}, and δ_{h2} are the respective HSPs of the solute.[1,3,4] In the modified space, the
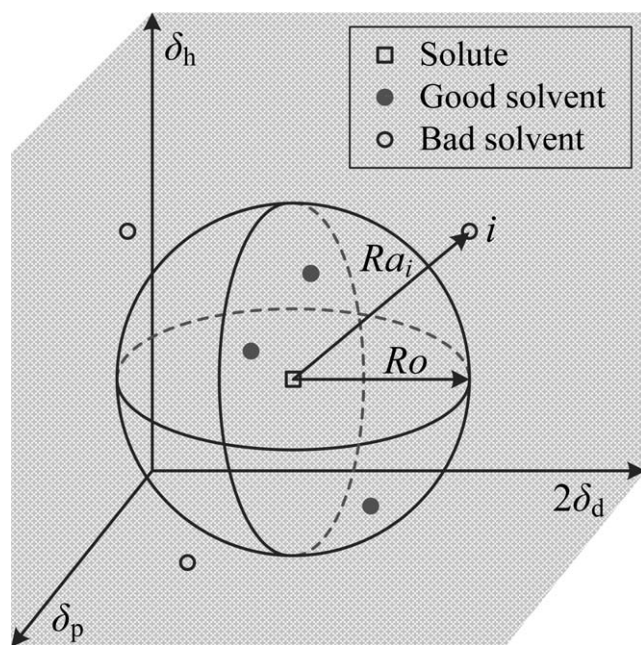
Figure 1. Hansen's solubility system in the modified $2\delta_d \times \delta_p \times \delta_h$ space.

strength of a specific solvent–solute interaction is reflected by two parameters: the distance in HSPs (Ra) and the relative energy difference (RED) between the two substances:

$$Ra = \sqrt{4(\delta_{d1}-\delta_{d2})^2 + (\delta_{p1}-\delta_{p2})^2 + (\delta_{h1}-\delta_{h2})^2} \quad (4)$$

$$RED = \frac{Ra}{Ro} \quad (5)$$

where δ_{d1}, δ_{p1}, and δ_{h1} are the respective HSPs of the solvent.

An RED of less than 1 suggests a high solvent–solute affinity, an RED of greater than 1 suggests a low affinity, and an RED of 1 suggests the boundary condition.

The solubility sphere in the $2\delta_d \times \delta_p \times \delta_h$ space is by far the most widely used model because of its simple formulas, easy illustration, and abundant reported data. Therefore, it was considered in this study.

Analysis of the Current Optimization Methods for Determining the HSPs

One can effectively determine the solubility sphere of a solute by measuring the solubility, swelling, surface attack, and so on of the solute in a series of solvents with known and diverse HSPs and then fitting the solubility sphere to the experimental data by solving optimization problems for independent variable vector $\mathbf{x} = (\delta_d, \delta_p, \delta_h, Ro)$, where δ_d, $Ro > 0$ and δ_p, $\delta_h \geq 0$.[5]

In these methods, various optimization problems and solution algorithms have been involved.[1,3,6–8] All of the algorithms have one thing in common: The fitness (F) of an estimate to the experimental data is evaluated by a data-fit function, which takes the form

$$F(\mathbf{x}) = \left(\prod_{i=1}^{N} f_i(\mathbf{x}) \right)^{\frac{1}{N}} \quad (6a)$$

where N is the number of solvents and the term $f_i(\mathbf{x})$ is calculated by

$$f_i(\mathbf{x}) = \begin{cases} e^{(Ro-Ra_i)}, & \alpha_i=1 \text{ and } Ra_i > Ro \\ e^{(Ra_i-Ro)}, & \alpha_i=0 \text{ and } Ra_i < Ro \\ 1, & \text{otherwise} \end{cases} \quad (6b)$$

where Ra_i and α_i are the distance and indicator of the interaction strength between the solute and the ith solvent, respectively. An α_i of 1 denotes a good solvent, and an α_i of 0 denotes a bad one.

All of the methods can be divided into two types with respect to their optimization objectives. The first type maximizes F. The study from Gharagheizi[6] belongs to this type. He used a Nelder–Mead simplex search method to solve the problem of $\min|1 - F(\mathbf{x})|$. The second type maximizes F and minimizes Ro. For instance, Hansen[1,3] developed an algorithm that evaluates the F values of eight vertexes of a cube with variant Ro and compares them with that of the current best position, namely, the cubic center. If a higher F is found, the center is replaced with the new best position. The refinement of the cubic size is used to ensure accuracy. Recently, Ma and Zhou[7] used a goal attainment algorithm to solve the multiobjective optimization problem with respect to $\min 1-F(x)$ and $\min Ro$, whereas Vebber et al.[8] used a genetic algorithm to solve the problem of $\max F(\mathbf{x})Ro^{-1/m}$, where $Ro^{-1/m}$ ($m \approx 20$) is a size factor. As compared with the classical Hansen's method, the other methods improved the results in at least one of the aspects: a smaller Ro, a higher F, and fewer outliers.[6–8] An outlier is a good solvent that falls outside the sphere or a bad solvent that falls inside the sphere. The numbers of total, good solvent, and bad solvent outliers are denoted as n_t, n_g, and n_b, respectively, where $n_t = n_g + n_b$.

Three criteria for an optimal solubility sphere, which have been mentioned by Hansen[1,9] and other authors,[6–8] were the smallest Ro, highest F, and lowest number of outliers. To date, consistency among the three criteria, which is a prerequisite for simultaneous satisfaction of all of the criteria, has not been investigated; moreover, the lowest number of outliers as a quality criterion for an estimate has been mentioned in the studies of Hansen[9] and Vebber et al.[8] but has not yet been directly considered as an optimization objective like the other two criteria.

DESCRIPTION OF THE NOVEL OPTIMIZATION METHOD FOR DETERMINING HSPs

In this section, a novel optimization method is proposed to determine the HSPs and Ro of a solute. It differs from the current methods in both the objective function and solution algorithm, as elaborated later.

Because no theoretical proof is available on the uniqueness of the global optimum and recording local optima is desired in the new method, a hybrid global–local search algorithm with the capability of locating multiple global or global–local optima during the optimization process was developed. In this algorithm, the global search is performed until a solution is found whose objective function value is below a threshold, and then, a local search is made in the neighborhood of the solution. The resulting local optimum is recorded. After a predefined number of solutions have been found, the global optimum (optima) is determined from the records.

A restartable particle swarm optimization method[10] based on that proposed by Eberhart and Kennedy[11] was used for global

search. The particle swarm optimization method is a stochastic method that solves problems by mimicking the behavior of bird flocking. It starts with a group of particles located randomly in a hyperspace (the position of each particle is a potential solution) and searches for the optimum by updating the position and velocity of each particle according to the best position that the particle has achieved so far and that among the overall population. The best position is the one having the best objective function value. A restartable particle swarm optimization method has global convergence. The simplex search method proposed by Nelder and Mead[12] was used for the local search. The Nelder–Mead method is a direct search method which deals with a simplex having $D + 1$ vertexes in a D-dimensional space, where the position of each vertex is a potential solution. It searches for an optimum by rescaling the simplex with four procedures: reflection, expansion, contraction, and shrinkage. It converges quickly but readily toward a local optimum. The combination of local search with a global search tends to prevent the algorithm from being trapped in a local optimum. The pseudo code of the hybrid optimization algorithm for solving constrained minimization problems is given in the Appendix.

Two optimization problems are considered here. The first problem (problem I) aims to find the optimal sphere having the highest F. It is expressed by

$$\min 1 - F(\mathbf{x}) \tag{7a}$$

The objective functions are defined as follows:

$$g_G(\mathbf{x}) = g_L(\mathbf{x}) = 1 - F(\mathbf{x}) \tag{7b}$$

where g_G and g_L are the functions used for the global and local searches, respectively.

This problem is the same as that being considered in ref. 6 but will be applied to more solutes in addition to the one concerned therein. The results of this problem are used to check the global convergence and accuracy of the hybrid algorithm.

The second problem (problem II) aims to find the smallest sphere encompassing the maximum number of good solvents and having the lowest n_t. One fulfills this by locating the local optima for all possible outlier sets (n_t, n_g, n_b) and then figuring out the results for the sets having the lowest n_g and, subsequently, the result (results) for the set (sets) having the lowest n_t. The optimization problem is represented by

$$\min Ro \text{ s.t. } \min n_g, \min n_t \tag{8a}$$

where n_g and n_t are both considered to ensure the uniqueness of the resulting outlier set (n_t, n_g, n_b) and optimal solubility sphere. The inclusion of n_g is necessary because the exclusion of all good solvents and their effects may happen when the number of bad solvents is larger than n. min n_g is arbitrarily chosen, which is similar but not equivalent to the consideration in Hansen's SPHERE1 program.[1]

The objective functions are defined as follows:

$$g_G(\mathbf{x}) = 1 - F(\mathbf{x}), \ g_L(\mathbf{x}) = Ro + n_g + n_t \tag{8b}$$

This is the new optimization problem designed by concerning the number of outliers instead of F in the objective function. The reasons are as follows. According to eq. (6a), F is a function of Ro

when at least one outlier is involved. In this case, a sphere having the smallest Ro and the highest F exists if and only if the smallest sphere is exactly the one giving the highest F. However, this condition was hardly met, as indicated by the results of this study. By contrast, one must be able to find a sphere encompassing the maximum number of good solvents and having the lowest n_t and then minimize the sphere while retaining the same outliers.

The results of both problems were used to check the correctness of the new optimization problem defined by eqs. (8a) and (8b), or, eq. (8) and the consistencies among the three criteria for an optimal solubility sphere under circumstances where outliers do or do not exist.

In both problems, the data-fit function was used for global search. The reasons were twofold. First, the data-fit function is a continuous function and converges more quickly than discrete functions such as eq. (8b). Second, with an F threshold before, the local search could filter out solutions having a large number of outliers because a relatively high F corresponded to a relatively small number of outliers, as shown by the reported results. Both helped to improve the computational efficiency.

COMPUTER SIMULATIONS

The simulations started from the average HSPs of good solvents and half of the average distance between all of the good solvent pairs. They were carried out with the following parameters. For the particle swarm global search, the inertial weight was 0.729, and the position and velocity update coefficients were both 1.494. For the Nelder–Mead local search, the step length in generating a simplex was 0.1, and the reflection, expansion, contraction, and shrinking coefficients were 1, 2, 0.5, and 0.5, respectively. The F threshold was below unity and was selected on the basis of prior tests. A total number of 2×10^4 solutions were recorded for each simulation.

The input data of the simulations were the HSPs of the solvents (δ_{di}, δ_{pi}, and δ_{hi}) and the solvent–solute interaction factors (α_i, where $i = 1, 2, \ldots, N$). The experimental data of α_i were taken from the literature. The output data were the HSPs and Ro values of the solute and the corresponding F, n_t, n_g, n_b, and RED values of each solvent–solute pair.

RESULTS AND DISCUSSION

Case 1: All Good Solvents Lie Inside and All Bad Solvents Lie Outside the Solubility Sphere

With poly(ether sulfone) used as an illustration, HSPs and Ro values of poly(ether sulfone) obtained herein and reported in the literature are listed in Table I. For both problem I and problem II, the highest F reached unity, and simultaneously, the lowest number of outliers was reduced to zero. This was the same as the best results[6–8] given in Table I and thereby verified the validity and global convergence of the hybrid algorithm.

From problem I, many optima (infinite optima in a continuous space) were found, so a range of each variable is given in Table I. Table I also shows that a single optimum was derived from the same optimization problem with the Nelder–Mead simplex search method[6], and all of the reported HSPs and Ro's[6–8,13] were within the ranges obtained here. Both revealed the global search ability of the hybrid algorithm.

Table I. Calculated and Reported HSPs and *Ro* Values for Poly(ether sulfone)

Problem	δ_d (MPa$^{1/2}$)	δ_p (MPa$^{1/2}$)	δ_h (MPa$^{1/2}$)	*Ro* (MPa$^{1/2}$)	n_t	n_g	n_b	F	Reference
I	18.810–20.106	10.624–11.352	7.854–9.585	5.387–6.736	0	0	0	1	This study
II	18.810	11.245	7.854	5.387	0	0	0	1	This study
—	19.6	10.8	9.2	6.2	1	0	1	0.999	13
—	20.0902	10.6302	9.5715	6.7162	0	0	0	1	6
—	18.8	11.2	7.9	5.4	0	0	0	1	7
—	18.84	11.22	7.95	5.42	0	0	0	1	8

The global optimum for problem II was found to be the same as the specific solution for problem I having the smallest *Ro*. This validated the correctness of the optimization problem defined by eq. (7a). The resulting HSPs for PES were as follows: $\delta_d = 18.810$ MPa$^{1/2}$, $\delta_p = 11.245$ MPa$^{1/2}$, and $\delta_h = 7.854$ MPa$^{1/2}$. The *Ro* of 5.387 MPa$^{1/2}$ was lower than all of the data[6–8,13] reported elsewhere.

The results from both problems show that in the case under consideration, a sphere having the highest *F* must be the one having the lowest n_g and n_t; the correspondence was not affected by the minimization of *Ro* as long as outliers were avoided. This could be explained by eqs. (6a) and (6b), or, eq. (6), where *F* is 1 if and only if $n_t = n_g = n_b = 0$, and *F* is independent of *Ro* when $n_t = n_g = n_b = 0$. Herein, defining the solubility sphere as the one having the smallest *Ro* and highest *F* is exactly the same as defining it as the one having the smallest *Ro* and lowest n_g and n_t. An optimal solubility sphere could be determined that simultaneously satisfied the three criteria mentioned by Hansen[9] and Vebber *et al.*[8]

The *RED* values for each poly(ether sulfone)–solvent pair, both calculated from the global optimum for problem II and reported in literature, are listed in Table I-SI (Supporting Information).

Case 2: At Least One Good Solvent Falls Outside or One Bad Solvent Falls Inside the Solubility Sphere
Here, we use bitumen 1, bitumen 2, and lignin as illustrations. The optimal HSPs and *Ro* values of the three materials obtained

herein and reported in the literature are listed in Table II. The HSPs and *Ro* values having the smallest *Ro* for various (n_t, n_g, n_b) sets obtained from problem II are listed in Table III. For both problem I and problem II, the highest *F* was below 1, and at least one outlier existed.

From problem I, the highest *F* values obtained for bitumen 1, bitumen 2, and lignin were 0.980, 0.980, and 0.991, respectively; these were the highest values among all of the reported data[8,9,14,15] in Table II. As compared with the results in ref. 8, the improvements in *F* were less than 10^{-3} for the two bitumens but up to 0.001 for lignin. This again validated the global convergence and accuracy of the hybrid algorithm. Table III also shows that the optimal sphere having the highest *F* may not have had the lowest number of outliers.

From problem II, except for the *Ro* of bitumen 1, all of the *Ro* values and numbers of outliers obtained for the three materials were the lowest compared with the other reported data[8,9,14,15] in Table II. The n_t values for bitumen 1, bitumen 2, and lignin were reduced to 1, 2, and 1, respectively; these values were remarkably less than the 3, 6, and 3 values determined from the classical method. The only exception was that the *Ro* for bitumen 1 (5.881 MPa$^{1/2}$) was larger than the value of 5.76 MPa$^{1/2}$ given in ref. 14. This was because the two spheres had different numbers of outliers. As shown in Table III, the smallest *Ro*'s differed from each other for different (n_t, n_g, n_b) sets. For the same number of outliers, however, the reported *Ro* values could be further reduced for all three materials. In particular, for

Table II. Calculated and Reported HSPs and *Ro* Values for Bitumen 1, Bitumen 2, and Lignin

Material	Problem	δ_d (MPa$^{1/2}$)	δ_p (MPa$^{1/2}$)	δ_h (MPa$^{1/2}$)	*Ro* (MPa$^{1/2}$)	n_t	n_g	n_b	F	Reference
Bitumen 1	I	18.712	4.608	3.404	6.078	2	1	1	0.989	This study
	II	18.616	4.728	3.478	5.881	1	0	1	0.989	This study
	—	18.4	3.9	3.6	5.76	3	1	2	0.980	14
	—	18.66	4.79	3.45	5.94	2	1	1	0.989	8
Bitumen 2	I	18.342	3.954	3.443	5.745	4	2	2	0.980	This study
	II	18.323	4.008	3.492	5.700	2	0	2	0.980	This study
	—	18.6	3.0	3.4	6.3	6	3	3	0.977	9
	—	18.33	3.99	3.49	5.71	3	1	2	0.980	8
Lignin	I	21.917	14.303	16.859	13.826	3	2	1	0.991	This study
	II	21.553	13.852	16.932	13.164	1	0	1	0.989	This study
	—	21.9	14.1	16.9	13.7	3	2	1	0.990	15
	—	21.71	14.18	16.93	13.45	2	1	1	0.990	8

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Table III. HSPs and *Ro* Values of Bitumen 1, Bitumen 2, and Lignin at Various (n_t, n_g, n_b) Sets Calculated from Problem II

Material	δ_d (MPa$^{1/2}$)	δ_p (MPa$^{1/2}$)	δ_h (MPa$^{1/2}$)	Ro (MPa$^{1/2}$)	n_t	n_g	n_b	F
Bitumen 1	18.616	4.728	3.478	5.881	1	0	1	0.989
	18.457	4.033	2.670	5.740	1	1	0	0.984
	18.328	4.023	3.491	5.700	2	0	2	0.980
	18.471	3.939	3.895	5.579	2	1	1	0.981
	18.399	4.645	2.498	5.335	2	2	0	0.959
	18.316	4.027	3.582	5.704	3	0	3	0.977
	18.405	4.042	3.756	5.574	3	1	2	0.981
	18.528	4.142	4.234	5.344	3	2	1	0.964
	18.337	5.076	2.615	5.068	3	3	0	0.932
Bitumen 2	18.323	4.008	3.492	5.700	2	0	2	0.980
	18.322	4.029	3.544	5.702	3	0	3	0.979
	18.340	3.974	3.825	5.592	3	1	2	0.976
	18.462	3.842	3.955	5.555	3	2	1	0.976
	18.614	3.945	3.715	5.431	3	3	0	0.960
Lignin	21.553	13.852	16.932	13.164	1	0	1	0.989
	21.505	13.648	16.935	13.053	2	0	2	0.988
	19.693	12.925	14.792	9.943	2	1	1	0.955
	20.500	12.133	15.151	10.281	2	2	0	0.961
	20.674	14.223	16.511	12.427	3	0	3	0.971
	19.675	12.702	14.807	9.817	3	1	2	0.954
	19.598	12.429	14.574	9.478	3	2	1	0.948
	20.025	11.791	15.213	9.468	3	3	0	0.954

lignin, the *Ro*'s could be reduced from 13.7 MPa$^{1/2}$ [15] and 13.45 MPa$^{1/2}$ [8] to 9.48 and 9.94 MPa$^{1/2}$ for (n_t, n_g, n_b) = (3, 2, 1) and (2, 1, 1), respectively. This suggested that there was a larger space to accommodate a sphere containing the same number of outliers for lignin than for the two bitumens. Table II also shows that the *F* values obtained from problem II were comparable with the data reported elsewhere. For each material, the highest *F* was obtained for the solution having the lowest number of outliers (Table III).

In a comparison of the data in Tables II and III, two things are noticeable:

1. The sphere having the highest *F* may not have the lowest n_t. This can be explained by eqs. (6a) and (6b), or eq. (6). When at least one outlier exists, *F* is a function of *Ro*, and the highest *F* is reached if and only if the total distance from each outlier to the solubility sphere surface decreases to the minimum but not necessarily when the number of outliers decreases to the lowest value.

2. All of the *F* values obtained from problem II and refs. 8,9,14, and 15 were lower than those obtained from problem I; this suggested that a reduction in *Ro* generally decreases *F* and may change n_g and n_t. This can also be explained by eqs. (6a) and (6b), or eq. (6). As long as the smallest sphere is not the optimal one that gives the highest *F*, any change in *Ro* moves the sphere surface away from its optimal position and, hence, increases the total distance between each

outlier and the sphere surface, reduces *F*, and may simultaneously alter n_t.

To summarize, in the case under consideration, there was not such a sphere that simultaneously had the smallest *Ro* and highest *F*, whereas a smallest sphere did exist that had the lowest n_g and n_t. Herein, defining a solubility sphere as the one having the smallest *Ro* and lowest n_g and n_t rather than the one having the smallest *Ro* and highest *F* is more reasonable according to its physical significance.

The *RED* values for each solvent–solute pair for bitumen 1, bitumen 2, and lignin are listed in Tables II-SI, III-SI, and IV-SI (Supporting Information), respectively.

CONCLUSIONS

A novel optimization method was presented for determining the δs and *Ro*'s of poly(ether sulfone), bitumen, and lignin. A hybrid algorithm featured with the capability of locating multiple optimal solutions was developed and was used to solve two optimization problems: the first maximized *F*, and the second minimized both *Ro* and n_g and n_t. The latter was the new optimization problem proposed concerning the number of outliers instead of *F* in the objective function.

The global convergence and accuracy of the hybrid algorithm were validated by the results obtained from the first problem for their improved *F*s. With the new optimization objective function and hybrid algorithm, the greatest numbers of outliers

and Ro's of the three materials were reduced, and the F values were comparable to data reported in the literature.

The results obtained in this study clarify the consistencies and correlations among the three criteria for an optimal solubility sphere, namely, the smallest Ro, highest F, and lowest number of outliers. Only when outliers are avoided can the three criteria be satisfied simultaneously. When outliers are inevitable, however, a reduction in Ro generally decreases F, but the same number of outliers may be retained. As a result, defining a solubility sphere as the smallest sphere encompassing the maximum number of good solvents and having the lowest n_t rather than the one having the smallest Ro and highest F is more general and reasonable according to the physical significance when both cases are concerned.

ACKNOWLEDGMENTS

APPENDIX

The pseudo code of the hybrid global–local search optimization algorithm for solving constrained minimization problems is given next. Let $\mathbf{x}_i$ and $\mathbf{v}_i$ be the position and velocity of the ith paticle; $\mathbf{x}_{InfLim}$ and $\mathbf{x}_{SupLim}$ are inferior and supreme limits for $\mathbf{x}_i$, $\mathbf{v}_{InfLim}$ and $\mathbf{v}_{SupLim}$ are those for $\mathbf{v}_i$. Then $\mathbf{x}_i$ and $\mathbf{v}_i$ are in the ranges of $[\mathbf{x}_{InfLim}, \mathbf{x}_{SupLim}]$ an $[\mathbf{v}_{InfLim}, \mathbf{v}_{SupLim}]$, respectively, where i=1,2,...,M.

Step 1. Initialize M particles by randomly generating particle positions $\mathbf{x}_i$ and velocities $\mathbf{v}_i$.
Step 2. Evaluate the functional values of each $\mathbf{x}_i$ $[g_G(\mathbf{x}_i^t)]$, update the best position each particle has achieved ($\mathbf{y}_i^t$),
$$\mathbf{y}_i^t = \begin{cases} \mathbf{y}_i^{t-1} & g_G(\mathbf{x}_i^t) \geq g_G(\mathbf{y}_i^{t-1}) \\ \mathbf{x}_i^t & g_G(\mathbf{x}_i^t) < g_G(\mathbf{y}_i^{t-1}) \end{cases}$$ and determine the best position among the overall particle population (y^t), $\hat{\mathbf{y}}^t = \arg\min_{\mathbf{y}_i} \{g_G(\mathbf{y}_i^t)\}$.
Step 3. If the g_G value of y^t $g_G(\hat{\mathbf{y}}^t)$ is lower than a predefined critical functional value (g_G^*), isolate the particle, and go to step 4. Otherwise, go to step 5.
Step 4. Generate a simplex whose five vertexes are located at $\mathbf{x}_i^t$ and $\mathbf{x}_i^t + e_j\, dx_j$ (where $j = 1$, 2, 3, or 4), respectively, where e_j is the jth row of a 5×5 identity matrix and dx_j is the length step in the jth dimension. Perform a Nelder–Mead local search with an objective function g_L. If local optimum is found, record it,

randomly initialize the position and velocity of the global best particle, update $\mathbf{y}_i^t$ and $\hat{\mathbf{y}}^t$, and go to step 5.
Step 5. If maximum record or iteration number is met, stop. Otherwise, if the particle swarm algorithm converges, restart it, and go to step 1. Otherwise, go to step 6.
Step 6. Update the velocities and positions of M particles with the following equations and go to step 2:

$$\mathbf{v}_i^{t+1} = w\mathbf{v}_i^t + c_1\mathbf{r}_1^t(\hat{\mathbf{y}}_i^t - \mathbf{x}_i^t) + c_2\mathbf{r}_2^t(\mathbf{y}_i^t - \mathbf{x}_i^t)$$

$$\mathbf{x}_i^{t+1} = \mathbf{x}_i^t + \mathbf{v}_i^{t+1}$$

where w is the inertial weight, c_1 and c_2 are the positive constants used for accelerating the particle position and velocity, respectively; and $\mathbf{r}_1$ and $\mathbf{r}_2$ are vectors composed of random numbers in the range [0,1].

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