Computerized Solvent Modeling

The formulation or reformulation of coatings, inks, and cleaners generally represents a considerable investment of laboratory work time and capital to achieve desired performance properties. To speed these efforts and enhance accuracy, Dow has developed the CHEMCOMP† Service.

The CHEMCOMP Service is a series of computerized solvent modeling programs:

- Evaporation Rate Program.
- Solvent Blend Program.
- VOC Program.
- Flash Point Estimator.
- Hansen Solubility Parameter Sphere Estimator.

Formulators may utilize the Evaporation Rate Program, Solvent Blend Program, VOC Program, Flash Point Estimator and Hansen Solubility Parameter Sphere Estimator with assistance from the development team for DOWANOL products.

CHEMCOMP streamlines routine calculations and laboratory work normally encountered when coatings, inks, and cleaners are formulated. The modules perform solvent matching and profiling in a fraction of the time normally required. They are interactive, offer immediate feedback, and encourage "what if ?" inquiries.

Evaporation Rate Program

The Evaporation Rate Program accurately predicts the evaporation behavior of solvent blends with up to 10 components. Using an extensive database of over 430 solvents, it accurately models the evaporation rate of an exact blend specified by the user. In effect, it simulates the results obtained with a Shell Evaporometer (ASTM D3539-76).

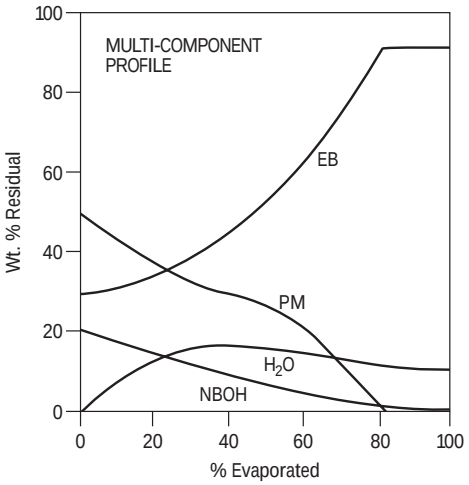
Additionally, both the relative humidity (0-99%) and the air temperature at the time of evaporation can be specified. This makes possible the simulation of actual use environments, whether at ambient conditions or in a baking oven.

Evaporation Rate Program data are displayed in a number of different plot formats (Figure 1) or in tabular form (Table 1).

The Evaporation Rate Program also calculates solvent blend densities, flash points, and solubility parameters, which should then be verified by actual lab tests.

Figure 1: Evaporation Rate Program Plot Format

CHEMCOMP: Evaporation Rate Program



† Service mark of The Dow Chemical Company

Table 1: Typical Printout of Evaporation Rate Program

Dow Chemical U.S.A. Solvent Evaporation Rate Program

Case 1 – Solvents and Compositions

		COMPOSITION		
CODE	SOLVENT NAME	MOLE %	WEIGHT %	VOLUME %
PM	DOWANOL PM GLYCOL ETHER	51.10	50.00	48.37
EB	DOWANOL EB GLYCOL ETHER	22.27	28.57	28.21
NBOH	N-BUTYL ALCOHOL	26.63	21.43	23.43
H_2O	WATER	0.00	0.00	0.00

CODE	SOLVENT NAME	T90 (SEC)	RELATIVE RATE	FP (°F)	DENS (G/CC)	COST ($/LB)
PM	DOWANOL PM GLYCOL ETHER	669.	0.699509	100.	0.916	0.00
EB	DOWANOL EB GLYCOL ETHER	6095.	0.076770	143.	0.898	0.00
NBOH	N-BUTYL ALCOHOL	1064.	0.439783	97.	0.811	0.00
H_2O	WATER	1490.	0.314038		0.997	0.00

Estimated Properties for the Initial Blend

DENSITY AT 25°C, G/CC	0.888
CLOSED CUP FLASH POINT, °F	103.
SOLUBILITY PARAMETER, SQRT (CAL/CC)	10.4
HYDROGEN BONDING, RELATIVE TO ISOOCTANE = 0	16.4
DIPOLE MOMENT, DEBYE	1.7
90% EVAPORATION TIME, SECONDS	3910.42
RATE RELATIVE TO NBAC AT 90% EVAPORATED	0.119657

Data Summary - Initial and Air Temp = 25.00°C, Rel Humidity = 60.00%

0.35% of Solvent Lost During Sample Injection Time of 8.00 Seconds

% EVAP	0.0	15.0	30.0	45.0	60.0	75.0	90.0
SECONDS	0.	264.	635.	1046.	1522.	2226.	3910.
REL RATE	0.00	0.30	0.25	0.22	0.20	0.18	0.12
FP (F)	104.	125.	134.	142.	150.	161.	165.
WT% PM	49.69	39.75	34.43	29.34	21.12	5.21	0.00
WT% EB	28.65	32.69	38.46	47.08	60.89	83.44	89.97
WT% NBOH	21.33	16.40	11.84	7.67	3.63	0.35	0.00
WT% H_2O	0.33	11.16	15.26	15.92	14.36	10.99	10.03

Select Plot Option
1 = No more plots 2 = Line printer plots 3 = Pen plots

Solvent Blend Program

The Solvent Blend Program matches the solvency characteristics of a target solvent or blend with the same data base as the Evaporation Rate Program. Solubility parameters, hydrogen bonding criteria, and dipole moment are matched to the standards specified in the target. Hansen parameters can also be used. When the program finds a match, it saves the information and looks for additional matches.

The blend program offers a variety of selection options, including:

- Forward calculation which provides solubility parameters when given a known solvent blend.
- Reverse calculation that provides multi-component blends when given the solubility parameters.
- Data for solvent substitutions, such as EB glycol ether or methylene chloride replacements.
- Selectivity that can include/exclude solvents from the blend search.
- Data refined with evaporation and flashpoint characteristics.

A typical run may involve several thousand searches. The program lists all the "hits" it finds (Table 2). The user must then determine which is the most practical blend for his or her application.

Table 2: Typical Printout of Solvent Blend Program

The calculated values for this solvent blend are:

- Solubility Parameter 8.74
- Hydrogen Bonding Parameter 5.62
- Dipole Moment 1.08

Limits chosen for search are as follows:

- Solubility Parameter . . . . . 8.60 to 8.88
- Hydrogen Bonding Parameter . . 5.50 to 5.80
- Dipole Moment . . . . . 0.95 to 1.50

You have specified 111 solvents to be included in the search for a blend containing 3 components, one of which is PMA.

Blend #	Sol. Param.	H_2 Bond.	Dipole Moment	Solv. #1 Wt%	Solv. #2 Wt%	Solv. #3 Wt%
1	8.79	5.56	1.12	PMA 60	ACET 5	CHEX 35
2	8.70	5.53	1.42	PMA 45	ACET 25	HEPT 30
3	8.65	5.59	1.35	PMA 50	ACET 20	HEPT 30
4	8.60	5.65	1.29	PMA 55	ACET 15	HEPT 30
5	8.61	5.62	1.44	PMA 45	ACET 25	ISOE 30
6	8.67	5.70	1.46	PMA 45	ACET 25	ISOG 30
7	8.62	5.76	1.40	PMA 50	ACET 20	ISOG 30
8	8.64	5.73	1.47	PMA 45	ACET 25	ISOH 30

Found 100 blends that meet limits out of 119,308 checked.

VOC Program

This program enables the user to determine the amount of volatile organic compounds in a specific formulation.

The VOC Program data base includes dozens of commonly used components – solvents, resins, pigments, and additives. Formulation components not already in the database can easily be added.

Table 3: Typical Printout of VOC Program Calculations

VOC Calculations

FORMULATION: Epoxy Modified Acrylic

COMMENTS: Bake Schedule: 350°F, 10 min.

TYPE OF CALCULATIONS: Dispersion

Material	Density Lb/Gal	Formula		Solids		VOC	
		Lb	Gal	Lb	Gal	Lb	Gal
Titanium Dioxide	34.72	95.5	2.75	95.5	2.75	—	—
Acryloid[1] AT-400	8.60	—	—	—	—	—	—
Methyl Amyl Ketone	6.77	15.8	2.33	—	—	15.8	2.33
Resin Solid	9.45	47.4	5.02	47.4	5.02	—	—
DER* 661 Epoxy Resin	9.90	—	—	—	—	—	—
Resin Solid	9.90	15.5	1.57	15.5	1.57	—	—
DOWANOL PM	7.56	28.0	3.70	—	—	28.0	3.70
DOWANOL DPM	7.91	6.7	0.85	—	—	6.7	0.85
CYMEL[2] 370	9.80	—	—	—	—	—	—
Iso-Butanol	6.68	4.6	0.68	—	—	4.6	0.68
Resin Solid	10.47	33.5	3.20	33.5	3.20	—	—
Totals	12.29	247.0	20.10	191.9	12.53	55.1	7.57

VOC = 2.74 Lb/Gal 328.25 G/L

* Trademark of The Dow Chemical Company
[1] Trademark of Rohm & Haas Company
[2] Trademark of American Cyanamid Company

Flash Point Estimator

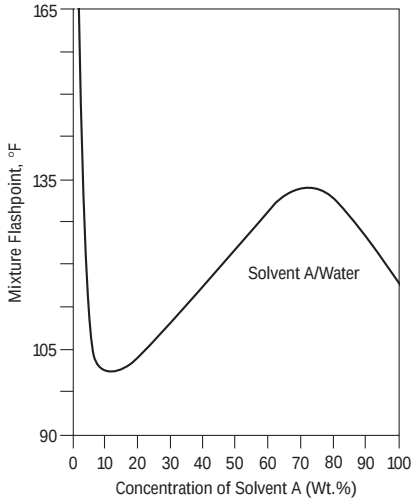
The Flash Point Estimator uses sophisticated algorithms to calculate the flash points of solvents or blends. It produces profiles of binary solvent systems that are much more detailed than those resulting from a few measurements (Figure 2).

The Flash Point Estimator is an efficient way to predetermine the effect of water or a higher boiling solvent on the flash point of a solvent system. All data obtained from the Flash Point Estimator should then be verified by actual lab tests.

Figure 2: Typical Printout from Flash Point Estimator

CHEMCOMP: Flashpoint Estimator

Binary Flash Point Curve



Hansen Solubility Parameter Sphere Estimator

Total cohesive energy arises from the combination of three distinct solubility parameters: Non-polar interaction (δ_d), a polar value (δ_p), and a hydrogen bonding (δ_h) component. To express this relationship, Hansen developed the following equation:

$$\text{Solubility Parameter Total} = [\delta_d^2 + \delta_p^2 + \delta_h^2]^{1/2}$$

The distance in space between two sets of parameters or spheres represents the "radius of interaction" (^{ij}R). If a solvent's three solubility parameters produce a point within the resin's radius of interaction, the solvent will dissolve the resin. The radius of interaction is expressed by the following equation:

$$^{ij}R = [4(i\delta_d - j\delta_d)^2 + (i\delta_p - j\delta_p)^2 + (i\delta_h - j\delta_h)^2]^{1/2}$$

In this equation, "i" represents the parameters of the resin and "j" represents the parameters of the solvent. Solubility occurs when the radius of interaction of a solvent/resin combination is less than the radius of interaction of the resin.

A simpler method for determining if a solvent will dissolve a resin is the RED value. A solvent will dissolve a resin if RED <1.0. The RED value is represented by the following equation:

$$\text{RED value} = \frac{^{ij}R}{R_{resin}}$$

The Hansen Solubility Parameter Sphere Estimator, as part of the complete CHEMCOMP service, offers:

- A complete database of solubility parameters and radius of interaction for resins.
- Solubility evaluations for various solvents of different polarity.
- Solubility predictions for up to 430 solvents.

Solubility Paramater Evaluation of Acrylic Resin

As an example of the capabilities of the Hansen Solubility Parameter Sphere Estimator, solvent-based acrylic resin was evaluated against 20 solvents at 10% by weight. Lab data entered into the sphere was calculated using the following parameters in Joules/cc: D = 17.1, P = 6.1, H = 9.9, R = 11.3, FIT = 1.0, and NC = 20. Sixteen of the possible 430 results are shown in Table 4.

Table 4: Typical Output from Sphere (Calculated Solubility Sphere for Solvent-based Acrylic Resin)

No.	Solvent	D	P	H	Solub.	RED	MV
1	Acetaldehyde	14.7	8.0	11.3		0.473	57.1
2	Acetic acid	14.5	8.0	13.5		0.584	57.1
3	Acetic anhydride	16.0	11.7	10.2		0.533	94.5
4	Acetone	15.5	10.4	7.0		0.539	74.0
5	Acetonitrile	15.3	18.0	6.1	0*	1.150	52.6
6	Acetophenone	19.6	8.6	3.7		0.739	117.4
7	Acrylonitrile	16.4	17.4	6.8		1.044	67.1
8	Allyl alcohol	16.2	10.8	16.8		0.756	68.4
9	Amyl acetate	15.3	3.1	7.0		0.488	148.0
10	Aniline	19.4	5.1	10.2		0.417	91.5
11	Anisole	17.8	4.1	6.7		0.356	119.1
12	Aromatic 100	17.2	1.0	3.1		0.752	0.0
13	Benzene	18.4	0.0	2.0		0.913	89.4
14	Benzaldehyde	19.4	7.4	5.3		0.587	101.5
15	Benzoic acid	18.2	6.9	9.8		0.207	100.0
16	Benzonitrile	17.4	9.0	3.3		0.640	102.6

*Used in test.

Using the Hansen Solubility Parameter Theory

One key element in reformulating solvent-based coatings is selecting a suitable replacement for the existing solvent. This selection process can be simplified by using the Hansen solubility parameter theory. Through a three dimensional display of the three solubility parameters for a resin and several solvents, one can determine whether or not a solvent is suitable to take into the lab to test, eliminating guesswork and trial-and-error testing. Appropriate blend mixtures can also be determined with this method.

Understanding Solubility Parameter Theory

The solubility parameter theory is one of the best methods for explaining solute (resin)/solvent interactions. This theory has been applied in a wide variety of technologies, including coatings and polymer science. Every compound, both solvent and polymeric resin, has characteristic solubility parameters that are determined by its structure. Hansen pioneered the concept that the total solubility parameter δ_t arises from a nonpolar interaction δ_d a polar interaction δ_p, and a hydrogen bonding component δ_h. The three partial solubility parameters are related by Equation 1.

(1) $\delta_t = [\delta_d^2 + \delta p^2 + \delta_h^2]^{1/2}$

While it is not unusual to think of the total solubility parameter as one distinct number, it is more useful to consider the set of three distinct partial solubility parameters that each influence the total solubility parameter.
The solubility parameters of a great number of solvents are known and the values from some of the common resin solvents are listed in Table 5. Solubility parameters of solvent blends can be calculated from Equation 2 where Ø is the volume fraction of the component.

(2) $\delta_{mixture} = Ø_1\delta_1 + Ø_2\,\delta_2 + \ldots$

Table 5: Hansen Solubility Parameters for Propylene Oxide Derivatives and Selected Solvents

SOLVENT	d_d (NON-POLAR)	d_p (POLAR)	d_h (HYDROGEN BONDING)
DOWANOL PM	15.6	7.2	13.6
DOWANOL DPM	15.5	4.0	11.5
DOWANOL TPM	15.1	3.5	11.5
DOWANOL PnB	14.9	2.4	10.7
DOWANOL PMA	16.1	6.1	6.6
Acetone	15.5	10.4	7.0
Methyl Isobutyl Ketone	15.3	6.1	4.1
n-Butanol	16.0	5.7	15.8
Toluene	18.0	1.4	2.0
Xylene	17.6	1.0	3.1
Methanol (MeOH)	15.1	12.3	22.3
Propylene Glycol (PG)	16.8	9.4	23.3
Cyclohexanone	17.8	6.3	5.1
Methyl Ethyl Ketone (MEK)	16.0	9.0	5.1
50 Xylene/50 MeOH	16.35	6.65	12.7
50 Propylene Glycol/50 MEK	16.4	9.2	14.2
50 Propylene Glycol/ 50 Cyclohexanone	17.3	7.85	14.2

Visualizing Solubility Parameters

By plotting the three solubility parameters (δ_d, δ_p, δ_h) in a three coordinate system, a point is achieved that represents the combined effect of those parameters. Though this point doesn't represent a physical object in physical space, it allows one to visualize the similarities and differences between various solvents and resins in a coordinate system. A fundamental principal of solvency is that "like dissolves like," so the closer two materials' points are in the 3-D plot, the more likely it is that the two materials will be soluble in one another.

The question now becomes, how close is close enough for one material to be soluble in another? The radius of interaction for a resin (^iR) helps answer this question. The radius of interaction is a number that expresses the length of a radius originating at a resin's unique point in this 3-D coordinate system. The radius defines a sphere around the resin's point as in Figure 3. If a solvent's three solubility parameters produce a point within the resin's radius of interaction (point "A"), then the solvent will dissolve the resin. The closer a solvent's point is to the center of the sphere, the better the solubility. Should the solvent's point fall outside the sphere (point "B"), then the resin will be insoluble in that solvent.

A resin's radius of interaction is determined experimentally by testing it with various solvents with known solubility parameters. In practice, this process actually yields less than a perfect sphere, but the data make it possible to arrive at an average value for the radius that allows reasonable predictions about resin/solvent interactions. Table 5 lists the Hansen solubility parameters and radii of interaction for a number of resins used in solvent-based

coatings. Solubility parameters for many other polymers and resins are available in standard references like Barton's handbooks on solubility parameters.

Figure 3 - Hansen Solubility Parameter Sphere

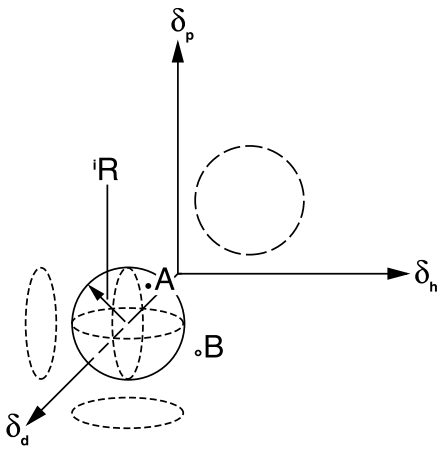


Table 6: Hansen Solubility Parameters and Radii of Interaction for Selected Resins

HANSEN VALUES				
RESIN (TRADEMARK, SUPPLIER)	d_d **NON-POLAR**	d_p **POLAR**	d_h **HYDROGEN BONDING**	^iR
Acrylonitrile-butadiene elastomer Hycar[1] 1052, Goodrich	18.6	8.8	4.2	9.6
Alkyd, long oil (66% oil length) Plexal[2] P65, Polyplex	20.4	3.4	4.6	13.7
Cellulose nitrate (1/2 sec; H-23) Hagedorn	15.4	14.7	8.8	11.5
D.E.N.[3] epoxy novolac 438	20.3	15.4	5.3	15.1
D.E.R.[3] epoxy resin 331	15.0	16.4	6.1	16.7
Melamine (Cymel[4] 300) American Cyanamid	20.4	8.5	10.6	14.7
Polyamide (Versamid[5] 930) General Mills	17.4	-1.9	14.9	9.6

[1] Trademark of B.F. Goodrich [2] Trademark of Polyplex [3] Trademark of The Dow Chemical Company
[4] Trademark of American Cyanamid [5] Trademark of General Mills

Speeding Up The Solvent Selection Process Using Mathematics

Rather than doing a time-consuming and complicated set of 3-D drawings, one simple equation can be used to get the job done faster. Equation 3 provides a method for determining the radius of interaction for a solvent/resin combination (^{ij}R).

$$(3)\ ^{ij}R = [4(^i\delta_d - {}^j\delta_d)^2 + (^i\delta_p - {}^j\delta_p)^2 + (^i\delta_h - {}^j\delta_h)^2]^{1/2}$$

In this equation the "i" terms correspond to the parameters of the resin and the "j" terms to the parameters of the solvent. Solutions to this equation let us predict whether a resin will be soluble in a given solvent. Mathematically, solubility occurs when the radius of interaction of a solvent/resin combination (^{ij}R) is less than the radius of interaction of the resin (^iR.). In visual terms, this simply means the solvent's point falls within the resin's sphere. Solubility improves as (^{ij}R) becomes increasingly smaller with respect to (^iR). Visually, the solvent's point falls closer to the center of the resin's sphere.

Manufacturers generally provide information on the solubilities of their resins in various solvents. So the real utility of using solubility parameter theory in the manner just described lies in making predictions about solvents that may not have been tested. This is particularly true when working with solvent blends.

The following example shows the calculations to determine if a solvent blend of 50 volume percent of xylene and 50 volume percent of methanol will be a possible solvent for D.E.N.* epoxy novolac 438. The epoxy resin of interest is insoluble in both pure solvents although our calculations (Table 6) suggest that a 50/50 solvent blend will demonstrate solubility for the resin.

The Hansen parameters for the 50/50 volume fraction blend are:

$^{j}\delta_d = 0.5(17.6) + 0.5(15.1) = 16.35$

$^{j}\delta_p = 0.5(1.0) + 0.5(12.3) = 6.65$

$^{j}\delta_h = 0.5(3.1) + 0.5(22.3) = 12.7$

The center point coordinates and radius of the solubility sphere for D.E.N. epoxy novolac 438 as taken from Table 2 are:

$^{i}\delta_d = 20.3 \;\; ^{i}\delta_p = 15.4 \;\; ^{i}\delta_h = 5.3 \;\; ^{i}R = 15.1$

The radius of interaction (^{ij}R) for the solvent blend of 50/50 xylene/MeOH as calculated from Equation 3 is equal to 13.9. Since this radius of interaction is less than the (^{i}R) (15.1) for the epoxy resin, the resin is expected to be soluble in the solvent blend.

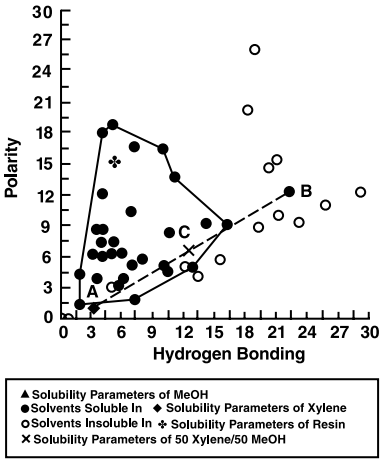
Computer Calculations Speed Initial Solvent Screening Process

Using a Lotus 1-2-3** spreadsheet, solvent/resin solubility matches can be made efficiently. As an example, each of the solvents and solvent blends listed in Table 24 was examined as a possible solvent for the resins listed in Table 7. The spreadsheet was used to screen each solvent using Equation 3 to calculate the radius of interaction ^{ii}R. The results are shown in Table 6 where the resin is listed as soluble in the solvent if the calculated ^{ij}R value is less than the resin sphere radius ^{i}R. The computer aided calculations can quickly suggest possible solvents or solvent blends to try in resin solubility studies. Table 7 suggests that a 50/50 blend of xylene/methanol will dissolve six of the seven resins although both pure solvents are not good solvents for these resins. Another example indicates that two ketones, methyl ethyl ketone (MEK) and cyclohexanone are both good solvents for the resins. Use of either ketone with propylene glycol, which is a poor solvent, would still yield several good solvent blends for resin dissolution.

Testing The Solubility Parameter Theory

An array of solvents with varying solubility parameters was used to characterize the solubility profile of the epoxy resin sample. Tests used 0.4 grams (10% solids) of resin in a vial equipped with a polyseal cap that contained 3.6 grams of test solvent. After shaking the vial for ten minutes, the samples were inspected for solubility behavior and reported as either soluble or insoluble. Areas of product solubility were then plotted (Figure 4) and the data used to calculate the partial solubility parameters for the particular resin. This laboratory method is similar to the test method used to determine the radius of interaction for a resin.

Figure 4 - Two Dimensional Solubility Profile for D.E.N. 438 Epoxy Resin



** Trademark of Lotus Development Corporation.

Table 7: Solubility of Resins in Propylene Oxide Derivatives and Other Selected Solvents and Solvent Blends

Resin soluble in listed solvent (Y = Yes. N= No)

Solvent	Hycar[1] 1052	Plexal[2] P65	Cellulose Nitrate[3]	D.E.N.[4] 438	D.E.R.[5] 331	Cymel[6] 300	Versamid[7] 930
DOWANOL PM	N	Y	Y	Y	Y	Y	N
DOWANOL DPM	N	Y	Y	N	Y	Y	Y
DOWANOL TPM	N	Y	N	N	Y	Y	Y
DOWANOL PnB	N	Y	N	N	Y	Y	Y
DOWANOL PMA	Y	Y	Y	Y	Y	Y	N
Acetone	Y	Y	Y	Y	Y	Y	N
Methyl Isobutyl Ketone	Y	Y	Y	Y	Y	Y	N
n-Butanol	N	N	Y	N	Y	Y	Y
Xylene	Y	Y	N	N	Y	Y	N
Toluene	Y	Y	N	Y	Y	Y	N
Methanol	N	N	N	N	N	N	N
Propylene Glycol (PG)	N	N	N	N	N	Y	N
MEK	Y	Y	Y	Y	Y	Y	N
Cyclohexanone	Y	Y	Y	Y	Y	Y	N
50 Xylene/50 MeOH	N	Y	Y	Y	Y	Y	Y
50 PG/50 MEK	N	N	Y	Y	Y	Y	N
50 PG/50 Cyclohexanone	N	Y	Y	Y	Y	Y	N

Notes:
[1] Hycar 1052 is an Acrylonitrile-Butadiene Elastomer, Trademark of Goodrich
[2] Plexal P65 is a long oil alkyd (66% oil length), Trademark of Polyplex
[3] The cellulose nitrate (1/2 sec; H-23) is sold by Hagedorn
[4] D.E.N. epoxy novolac 438, Trademark of The Dow Chemical Company
[5] D.E.R. epoxy resin 331, Trademark of The Dow Chemical Company
[6] Cymel 300 is a melamine resin, Trademark of American Cyanamid
[7] Versamid 930 is a polyamide resin, Trademark of General Mills

Determining Soluble Blends

The solubility envelope shown in Figure 4 was generated by plotting the solubility behavior of the D.E.N. 438 epoxy resin in a number of solvents for which the solvents' partial solubility parameters are known. The two most important solubility parameters- polarity and hydrogen bonding ability- are used to show the solvents that dissolve the D.E.N. 438 resin (filled circles) or do not dissolve the D.E.N. 438 resin (open circles). The **B** represents the resin's unique point in two-dimensional space derived from its hydrogen bonding and polar components. Because only a small number of solvents were tested, the solubility envelope does not form a sphere around the resin's unique point like the theoretical model in Figure 4.

The envelope drawn between the filled circles on the solubility plot encloses an area where solvents or solvent blends would be expected to dissolve the particular epoxy resin. The solvents and areas outside the solubility envelope represent areas of limited solubility or total insolubility for the resin. A tie line drawn between two solvent points located outside this envelope could furnish certain solvent blends capable of solubilizing if the tie line passes through the area of solubility.

An example of this behavior is shown by the tie line "A - B" representing the blend of xylene/methanol; calculations in Figure 4 show that a 50/50 blend of these two solvents should be a good solvent for the D.E.N. 438 epoxy resin. The tie line drawn between two solvent points on the solubility plot represents any number of solvent compositions of the two pure solvents, which is the graphic equivalent to Equation 2. The point "C," which is one-half the distance between the two solvent points, represents the 50/50 solvent blend. The blend of two non-solvents gives new composite solubility parameters that better match the solubility parameters of the D.E.N. 438 epoxy resin. The Hansen solubility parameters of the 50/50 blend are:

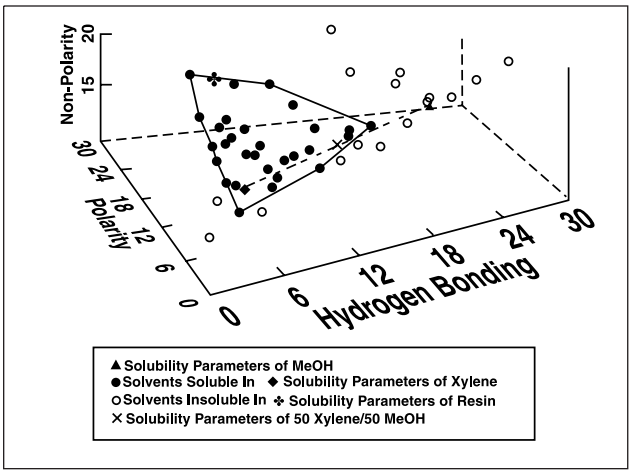
$\delta_d = 16.35$ $\delta_p = 6.65$ $\delta_h = 12.7$

which puts the hydrogen bonding/polarity point in the bottom half of the solubility envelope for the epoxy resin.

A three-dimensional representation of the D.E.N. 438 epoxy resin solubility envelope is shown in Figure 5, adding the non-polarity component of the Hansen solubility parameters to the polarity and hydrogen bonding components. Again, the tie line between the two non-solvents (xylene and methanol) is shown with the 50/50 midpoint which represents a viable solvent blend that should dissolve the epoxy resin.

To determine the best match, it is best to use all three partial solubility parameters. The contributions of the three partial solubility parameters (δ_d, δ_p and δ_h values) to the blend are based on the volume fraction of each solvent (i.e., 50/50 blend or 40/60 blend). Solubility parameters of solvent mixtures can be calculated from Equation 2 where 0 is the volume fraction of a mixture component. Or, the solubility parameters of a blend can be estimated by a graphical method using a solubility envelope similar to Figure 5.

Figure 5- 3-D Solubility Profile for D.E.N. 438 Epoxy Resin



Summary

Reformulating an existing solvent-based coating with a new solvent blend can be simplified by using the Hansen solubility parameter theory. A new solvent blend can be found by calculating the solubility parameters of the existing solvent blend and then selecting a new solvent blend that has similar solubility parameters. If the solubility parameters of the new blend fall within the radius of interaction of the resin (^iR), then the resin will be soluble (i.e., $^{ij}R < {}^iR$). Computer-aided calculations, using Lotus 1-2-3 or a similar program, can quickly provide solvents and solvent blends that would be an appropriate substitute for reformulation. Solvent substitutes can also be determined experimentally and with the results plotted based on the various solvents' solubility parameters. When plotted using all three solubility parameters, the most accurate results are found.