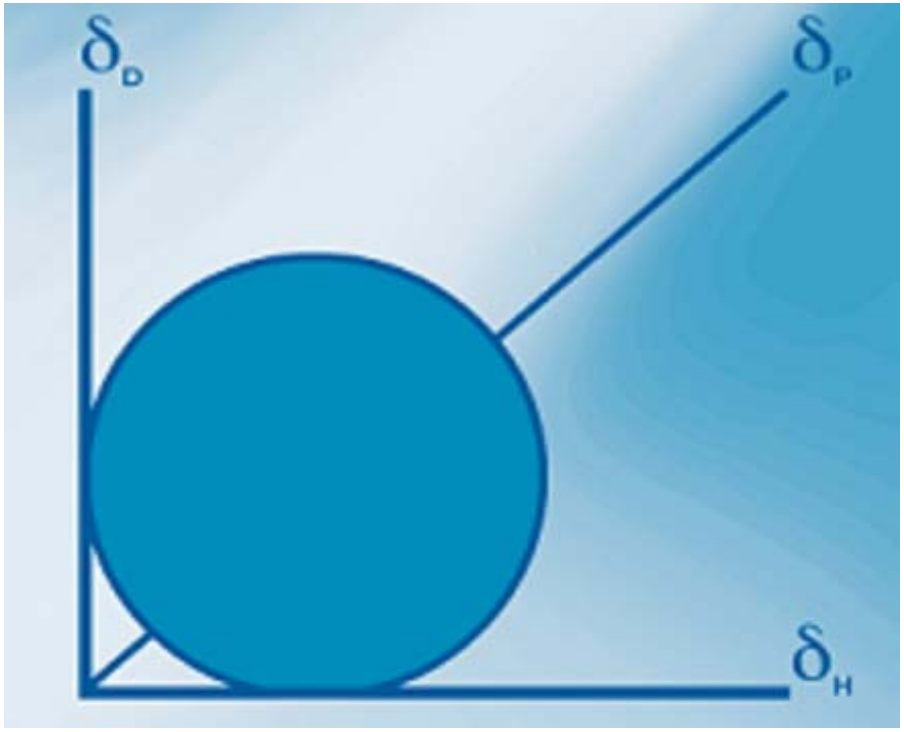
HANSEN SOLUBILITY PARAMETERS

CHARLES M. HANSEN



WHY KEEP GOING?

”Even if you’re on the right track, you’ll get run over if you just sit there.”

- Will Rogers

- To me this means help develop the
- Hansen Solubility Parameters in Practice
- (HSPiP) eBook/software

WHOLE EQUALS SUM OF PARTS

E = COHESION ENERGY = ΔE_{vap}

- $E = E_D + E_P + E_H$
- D - Dispersion (Hydrocarbon)
- P - Polar (Dipolar)
- H - Hydrogen Bonds (Electron Interchange)
- V - Molar Volume
- $E/V = E_D/V + E_P/V + E_H/V$

$$\delta^2 = \delta^2_D + \delta^2_P + \delta^2_H$$

HANSEN SOLUBILITY PARAMETERS (HSP)

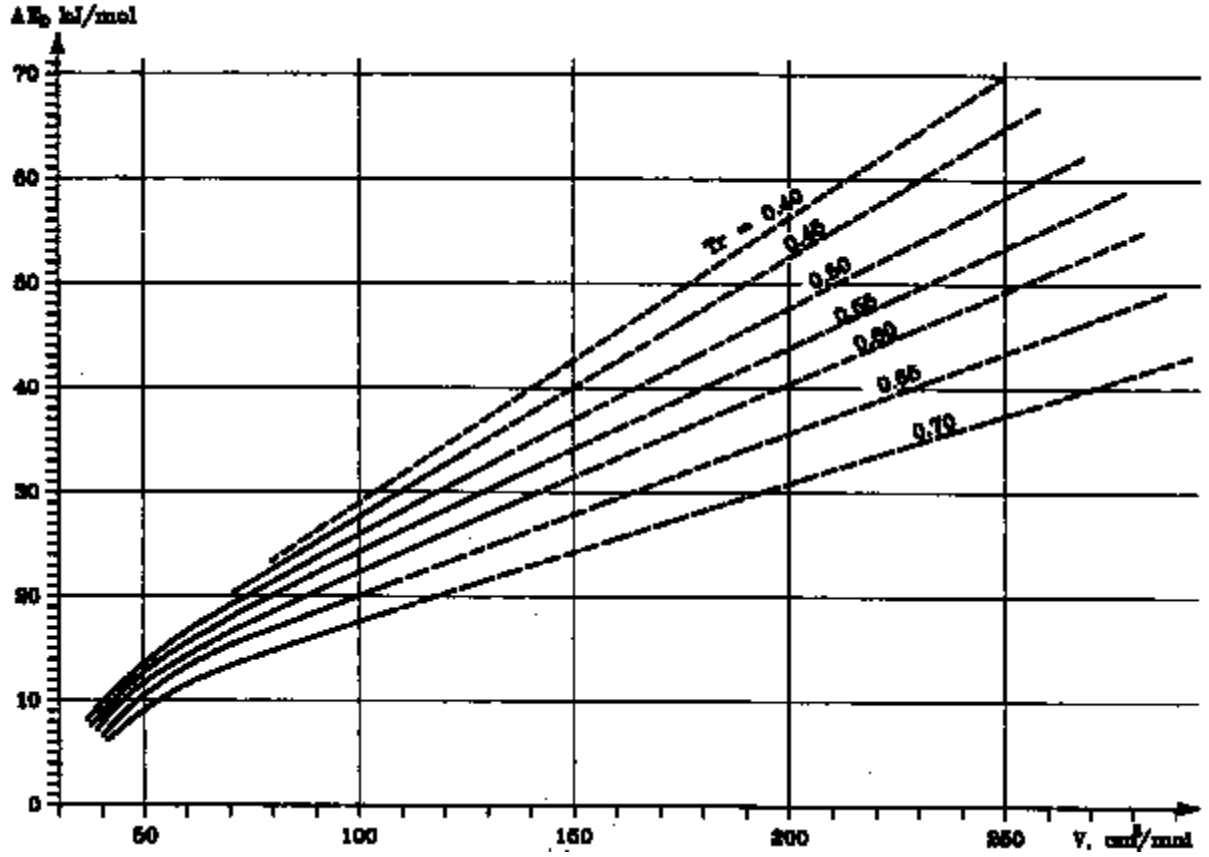
δ = Square Root of Cohesion Energy Density

δ_D

- HOMOMORPH CONCEPT ($\mathbf{E_D}$ = **E** FOR SIMILAR HYDROCARBON)
- CORRESPONDING STATE THEORY (CST)
- CST FIGURE FOR $\mathbf{E_D}$ FOR EACH OF ALIPHATIC, CYCLOALIPHATIC, OR AROMATIC STRUCTURE

  $\mathbf{E_D}$ versus V for $T_r = T_{298.15.}/T_{CRITICAL}$

FIGURE FOR E_D FOR ALIPHATIC HYDROCARBONS



δ_P

Böttcher Equation cal/cm^3

$$\delta_P^2 = \frac{12108}{V^2}\frac{\varepsilon - 1}{2\varepsilon + n_D^2}\left(n_D^2 + 2\right)\mu^2$$

Beerbower Equation MPa^{½}

$$\delta_P = 37.4(\mu)/V^{½}$$

δ_H

1. $E_H = E - E_D - E_P$
2. Panayiotou – statistical thermodynamics directly
3. Group Contributions

$$\delta_H = (E_H/V)^{1/2}$$

4. CHECK where possible that:

$$\delta^2 = \delta^2_D + \delta^2_P + \delta^2_H$$

THERMODYNAMIC BASIS OF HSP

Exchange Energy (Density)

$A_{12} = \varepsilon_{11} + \varepsilon_{22} - 2\varepsilon_{12}$

Geometric Mean

$\varepsilon_{12} = (\varepsilon_{11}\varepsilon_{22})^{1/2}$

Scatchard

$A_{12} = (\varepsilon^{1/2}_{11} - \varepsilon^{1/2}_{22})^2$

Hildebrand (Cohesive Energy Density)

$\varepsilon_{11} = \Delta E_1/V_1; \quad \varepsilon_{22} = \Delta E_1/V_1$

Hildebrand/Scott

$\Delta E_M = \varphi_1\varphi_2(x_1V_1 + x_2V_2)(\delta_1 - \delta_2)^2$

Patterson/Delmas

$\Delta G_{noncomb} = \varphi_1\varphi_2V_M(\delta_1 - \delta_2)^2$

THERMODYNAMIC BASIS (CONT.)

Hansen HSP

$$Ra^2 = 4(\delta_{D1} - \delta_{D2})^2 + (\delta_{P1} - \delta_{P2})^2 + (\delta_{H1} - \delta_{H2})^2$$

Hansen Relative Energy Difference (RED)

$$RED = Ra/Ro$$

Flory/Hansen

$$X/Xc = (RED)^2$$

Prigogine (With Geometric Mean)

$$v^2 = (\delta^2_{Prig}/\mathbf{4} + 9\rho^2) \text{ where } \delta_{Prig} = (\varepsilon_2 - \varepsilon_1)/\varepsilon_1$$

Prigogine/Hansen

$$\delta^2_{Prig} = [(\delta_{i1} - \delta_{i2})/\delta_o]^2 \qquad \text{For “i” = P,H}$$

Panayiotou - Direct Calculation of Hydrogen Bonding

STATISTICAL THERMODYNAMICS - PANAYIOTOU

Equation of state:

$$\tilde{P}+\tilde{T}\left[\ln(1-\tilde{\rho})-\tilde{\rho}\left(\frac{l}{r}-\nu_H\right)-\frac{z}{2}\ln\left(1-\tilde{\rho}+\frac{q}{r}\tilde{\rho}\right)+\frac{z}{2}\ln\Gamma_{00}\right]=0$$

Chemical potential:

$$\frac{\mu}{RT}=\frac{\mu_{dp}}{RT}+\frac{\mu_H}{RT}$$

$$\frac{\mu_{dp}}{RT}=\ln\frac{1}{\omega r}-\tilde{\rho}l+\ln\tilde{\rho}-\frac{z}{2}q\ln\left[1-\tilde{\rho}+\frac{q}{r}\tilde{\rho}\right]+\frac{zq}{2}\left[\ln\Gamma_{rr}\right]-\frac{q}{\tilde{T}}+r\frac{\tilde{P}}{\tilde{T}}$$

$$\frac{\mu_H}{RT}=r\nu_H-d\ln\frac{d}{d-\nu_H}-a\ln\frac{a}{a-\nu_H}$$

PANAYIOTOU δ^2_D, δ^2_P, and δ^2_H

$$\delta_d = \sqrt{\frac{\Gamma_{rr} q N \theta_r \varepsilon^*}{V}}$$

$$\delta_p = \sqrt{\frac{\Gamma_{rr} q N \theta_r \varepsilon^* \left[\pi \left(\frac{m}{r} \right)^2 s^2 \right]}{V}}$$

$$\delta_{hb} = \sqrt{\frac{-N_H E_H}{V}}$$

δ^2_H - COMPARISON

	HANSEN	PANAYIOTOU
Toluene	2.00	2.00
Tetralin	2.90	2.90
Acetone	6.95	7.00
Methyl Methacrylate	5.40	5.40
Ethanol	19.43	19.98
1-Butanol	15.80	15.80
Dimethyl sulfoxide	10.20	10.28
Water	42.32	42.17

δ^2_H – POLYMER COMPARISON

	HANSEN	PANAYIOTOU
Lin. Polyethylene	2.80	2.80
Polystyrene	2.90	2.90
PVC	3.40	3.42
PMMA	5.10	5.10
PC	6.90	6.90
Nylon 66	24.00	23.90

FREE ENERGY CHANGE, G, DETERMINES SOLUBILITY OR NOT

- **Free energy G must be negative for solution**

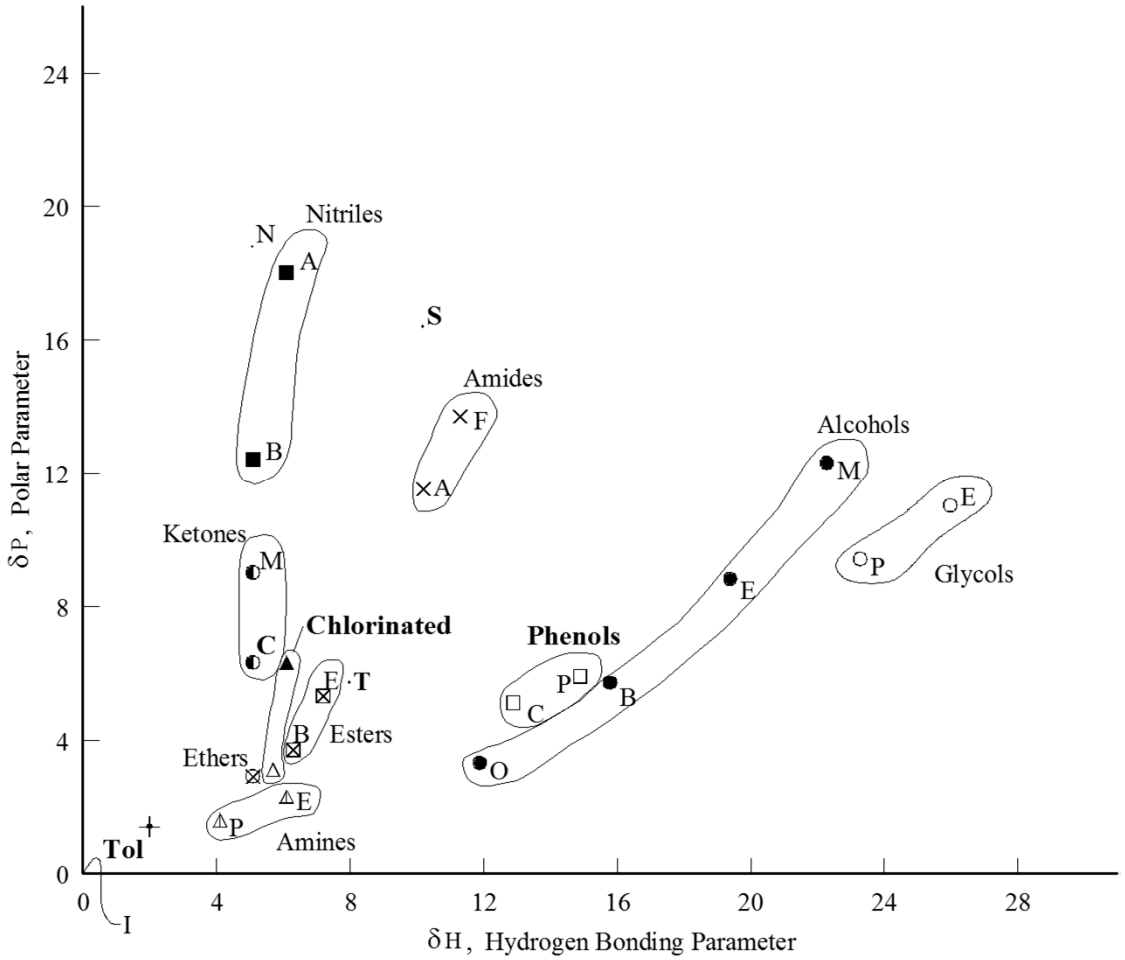
- $G = (1/N)\phi\ln(\phi) + (1 - \phi)\ln(1 - \phi) + X\phi(1 - \phi)$

- **ø is the solvent volume fraction**
- **N is the number of monomers in chain**

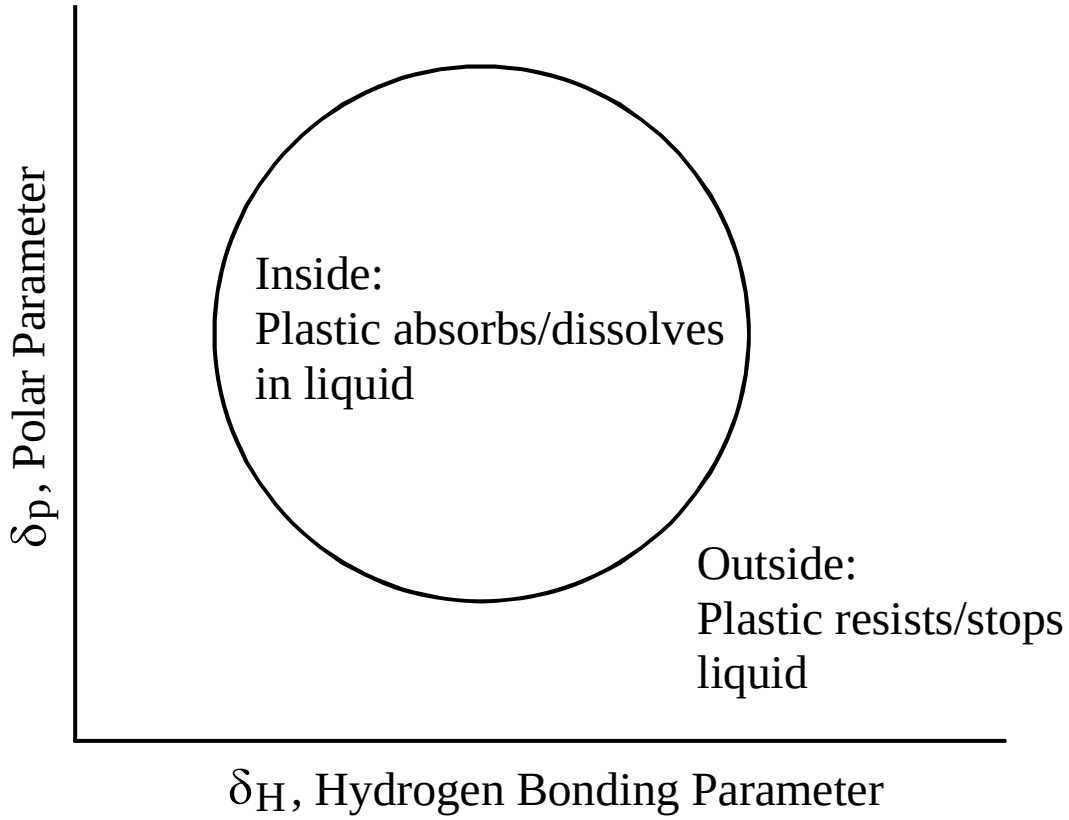
- $X = V_m/RT[(\delta_{D1} - \delta_{D2})^2 + 0.25(\delta_{P1} - \delta_{P2})^2 + 0.25(\delta_{H1} - \delta_{H2})^2]$

- **X is the chi parameter, V_m is the molar volume**

δ_P VERSUS δ_H PLOT



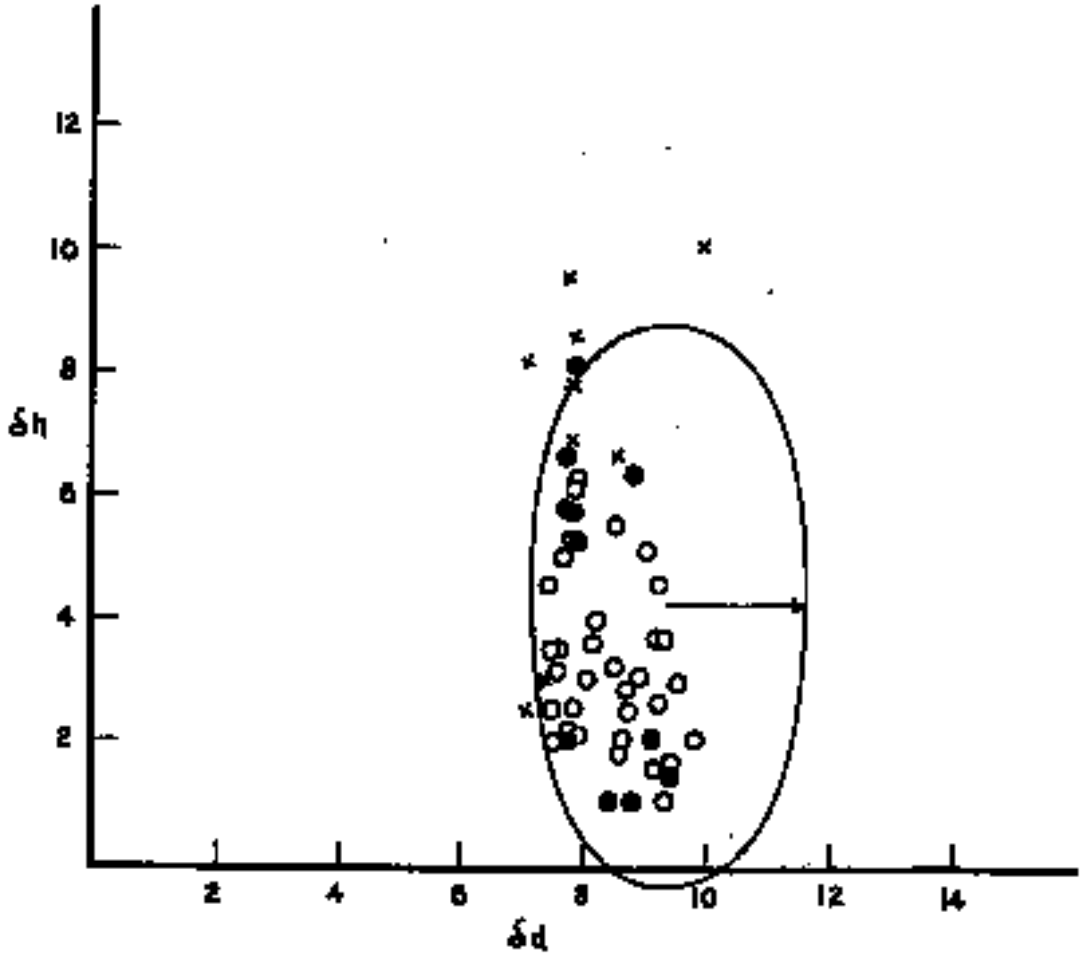
HANSEN SOLUBILITY PARAMETER DIAGRAM



KEY EQUATIONS

- $Ra^2 = 4(\delta_{D1} - \delta_{D2})^2 + (\delta_{P1} - \delta_{P2})^2 + (\delta_{H1} - \delta_{H2})^2$
- The experimentally verified ”4” is also found in Prigogine’s CST theory
- RED = Ra/Ro (Distance to sphere center divided by its radius)
- $(RED)^2 = (Ra/Ro)^2$ corresponds to χ_{12} / χ_c in Huggins/Flory Theory

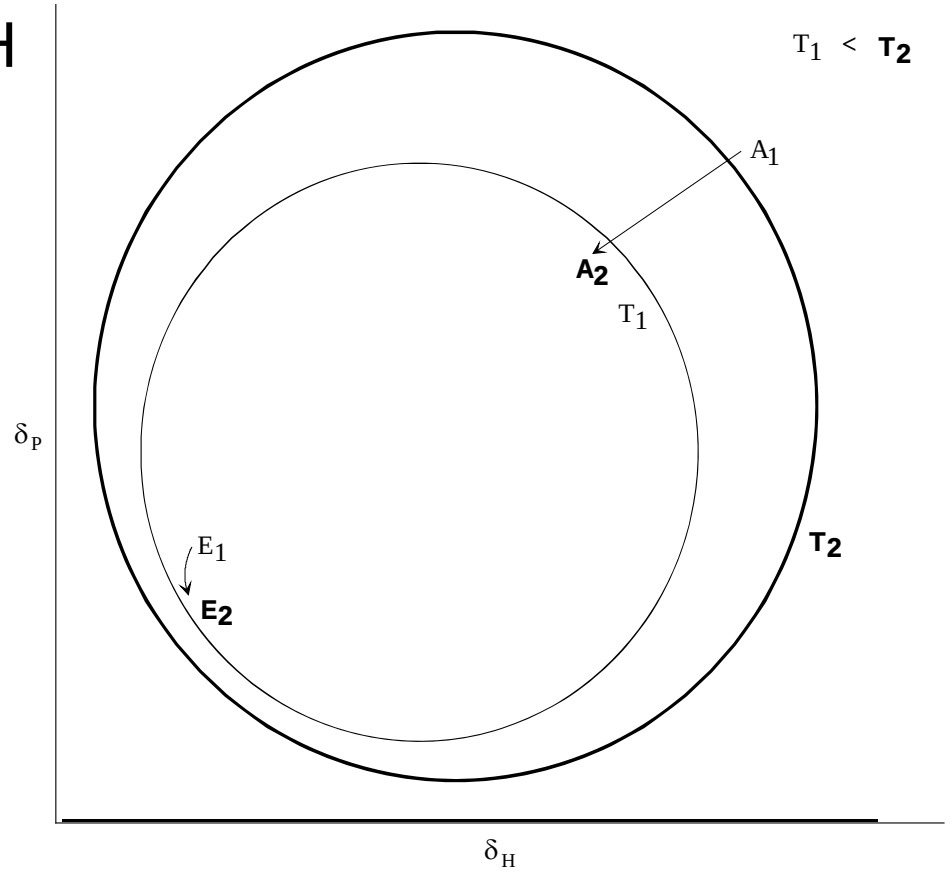
SPHEROIDS OF SOLUBILITY UNLESS ”4” IS USED



EFFECT OF TEMPERATURE

Higher temperature – Lower values

Larger effect for δ_H



CHANGE OF δ_H WITH TEMPERATURE (Williams)

$$\left(\frac{\partial \delta_h}{\partial T}\right)_P = -\delta_h\left(\frac{2.64\times10^{-3}}{2}+\frac{\alpha}{2}\right)$$

$$= -\delta_h\left(1.32\times10^{-3}+\frac{\alpha}{2}\right)$$

Functional Group	E_H Cal/mol	dE_H/dT Cal/mol/°K
-OH (aliphatic)	4650 ± 400	-10
$-NH_2$ (aliphatic)	1350 ± 200	-4.5
-CN (aliphatic)	500 ± 200	-7.0
-COOH (aliphatic)	2750 ± 250	-2.9

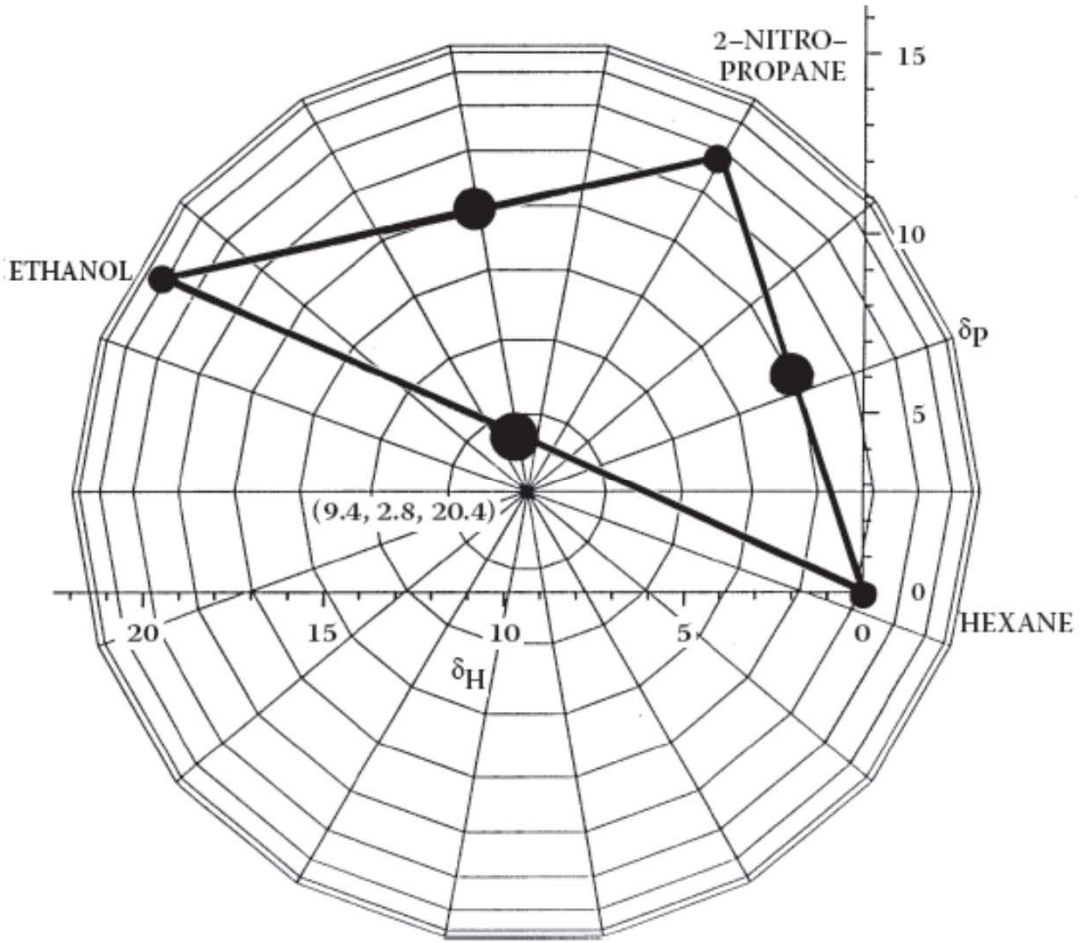
TYPES OF MATERIALS

- SOLVENTS
- POLYMERS
- PIGMENT SURFACES
- FIBER SURFACES
- DRUGS
- CHEMICAL PROTECTIVE CLOTHING
- BIOLOGICAL MATERIALS
- SALTS - BOTH ORGANIC AND INORGANIC

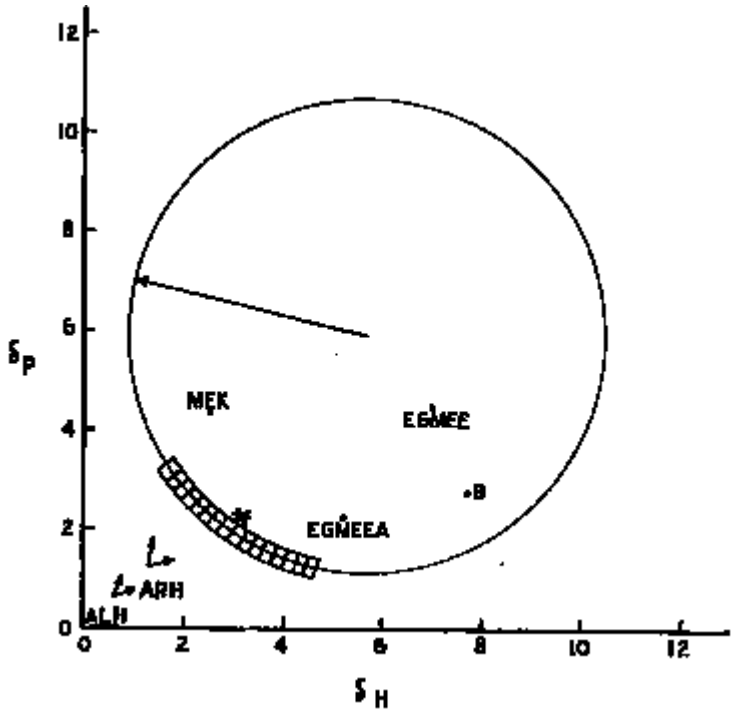
EXAMPLES OF USES OF HSP

- Solvent Selection and Substitution (REACH, Ozone Depletion, VOC, etc.)
- Solubility, Swelling, Related Phenomena
- Surface Characterization and Adhesion
- Permeation, Breakthrough Times
- Physical Properties
- Polymer and Biological Compatibility
- Controlled Drug Release

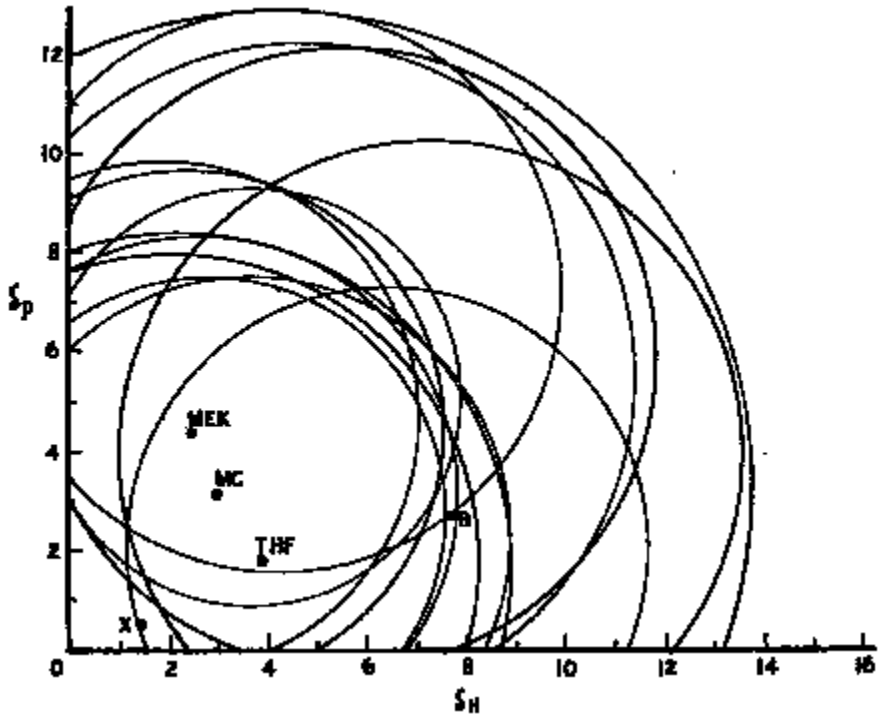
CHOLESTEROL NONSOLVENT SYNERGISM



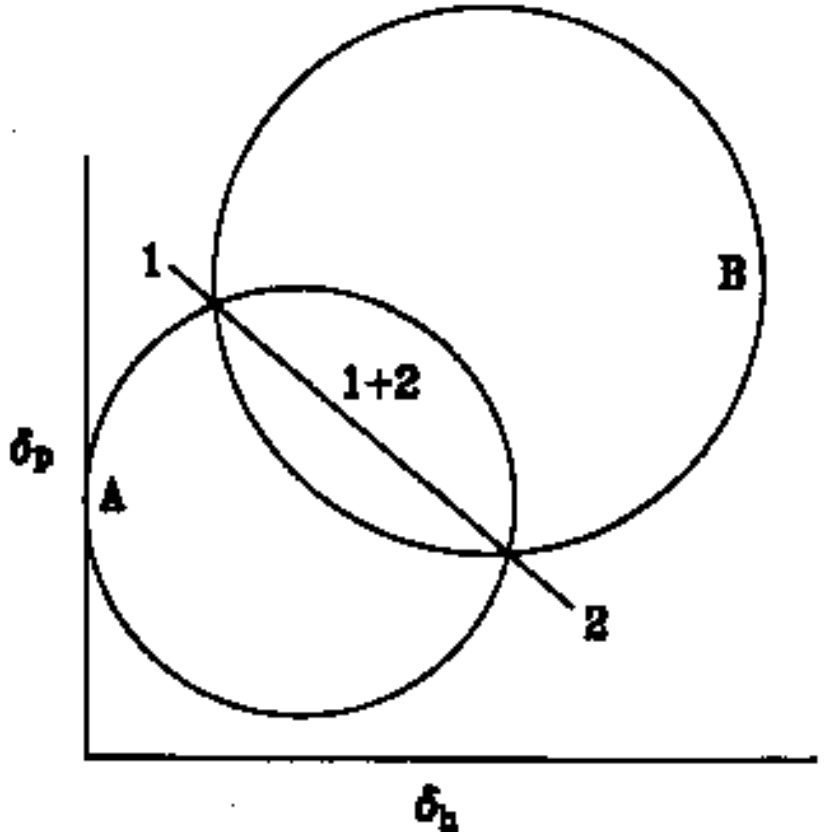
BOUNDARY SOLVENTS (MIXTURES) HAVE TRADITIONALLY BEEN THE LEAST EXPENSIVE



XYLENE PLUS n-BUTANOL CAN OFTEN APPROACH THE PERFORMANCE OF OTHER WIDELY USED SOLVENTS

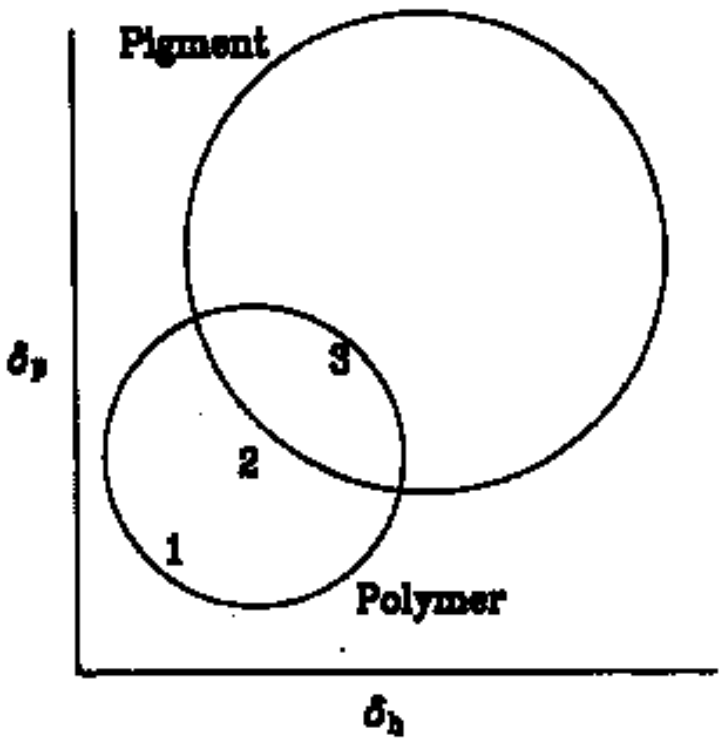


NON – COMPATIBLE POLYMERS DISSOLVED IN A MIXTURE OF NON-SOLVENTS

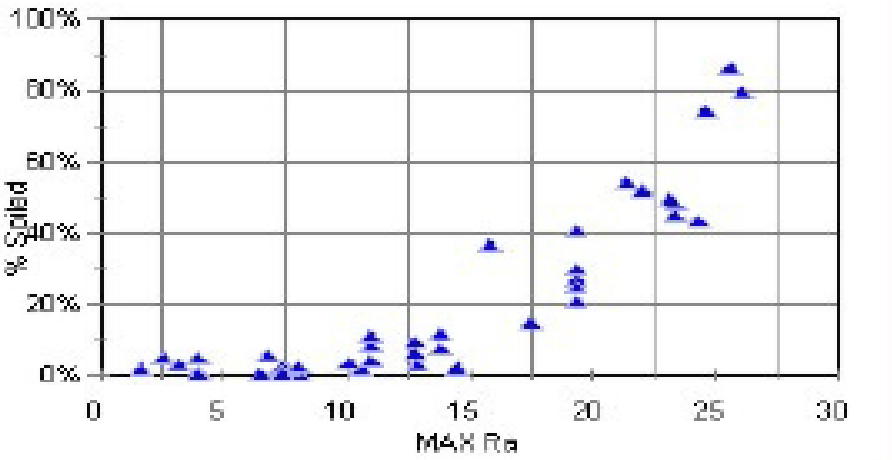


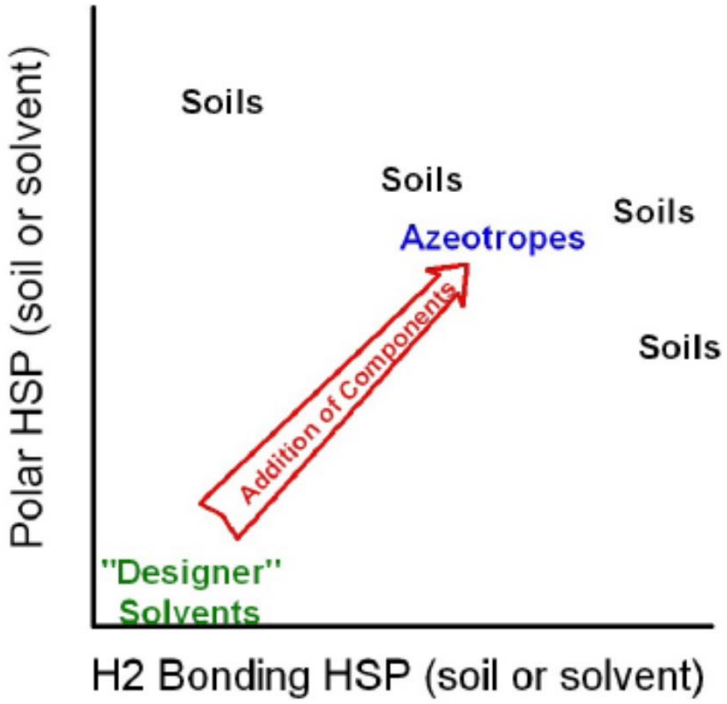
SOLVENT AFFECTS PIGMENT DISPERSION STABILITY

- Solvent 1 – Optimum in most cases – binder on pigment
- Solvent 2 – Too good for binder – removes binder
- Solvent 3 – Too good for pigment – replaces binder

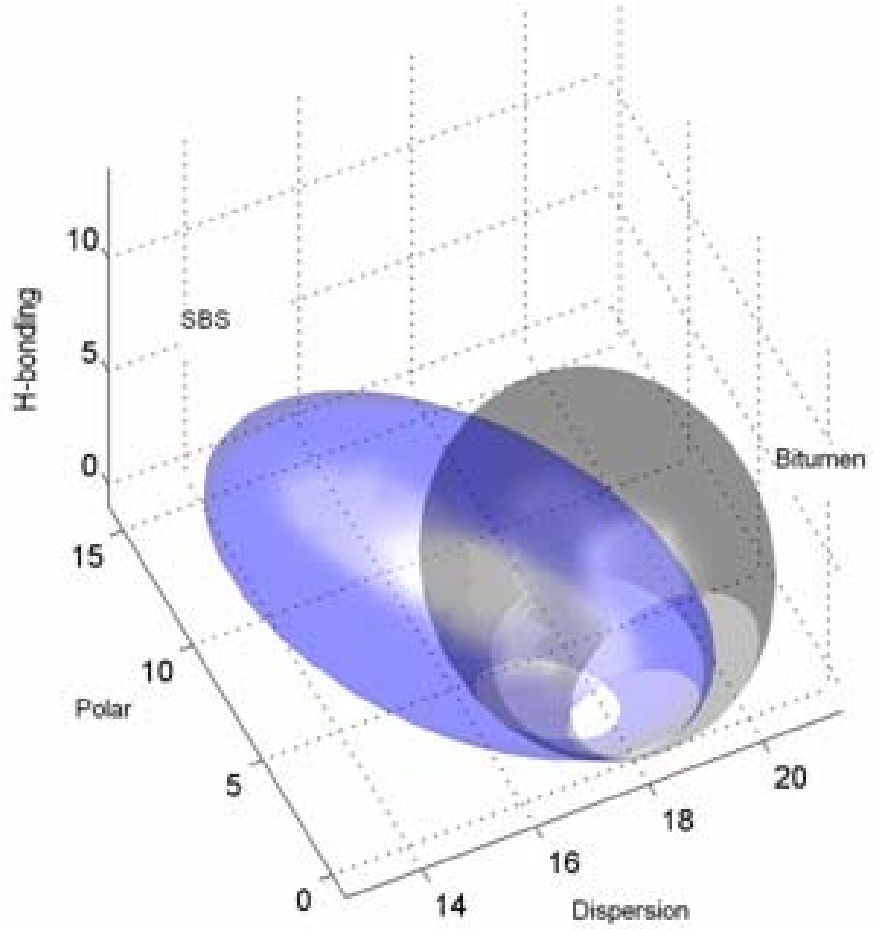


REPLACE OZONE DEPLETERS
Match Soil HSP
Use Azeotropes





SBS MUST BE PARTLY COMPATIBLE WITH BITUMEN



VARNISH REMOVAL FROM OLD PAINTINGS

Teas Triangular Plot for Solvent Selection

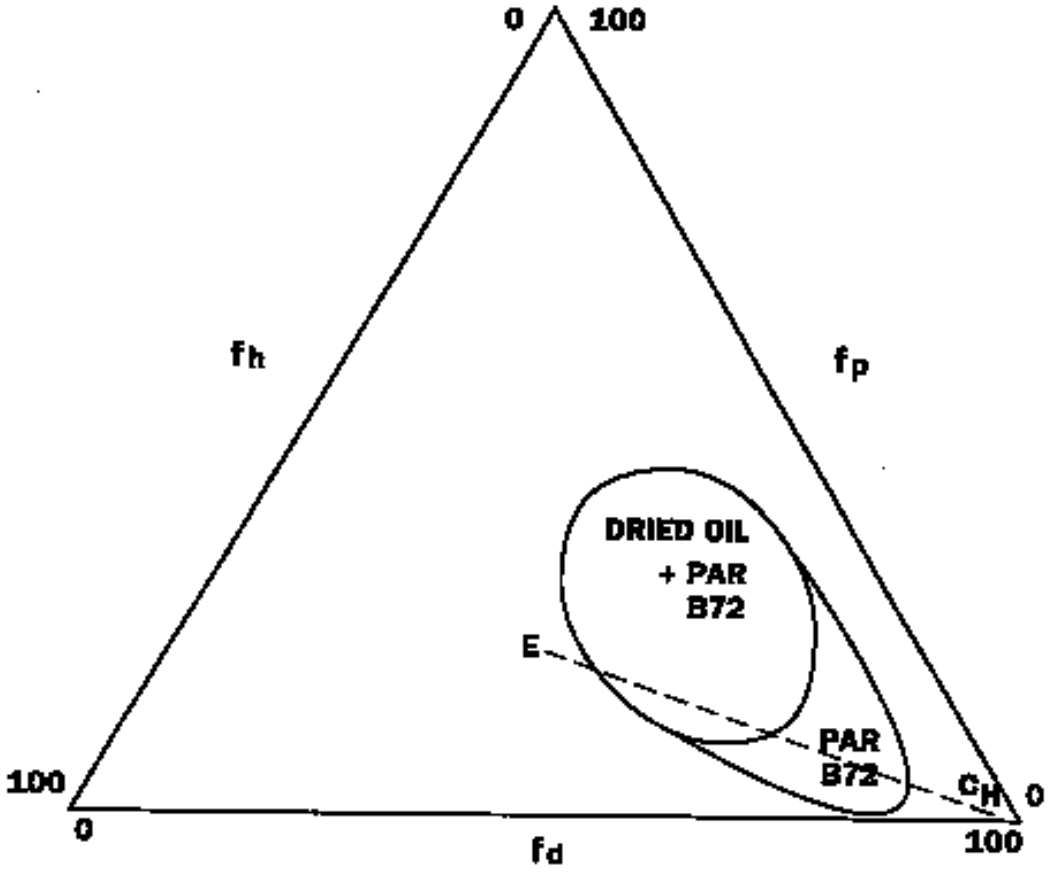
MODIFICATION OF HANSEN PARAMETERS

$$f_d = 100\delta_D/(\delta_D + \delta_P + \delta_H)$$

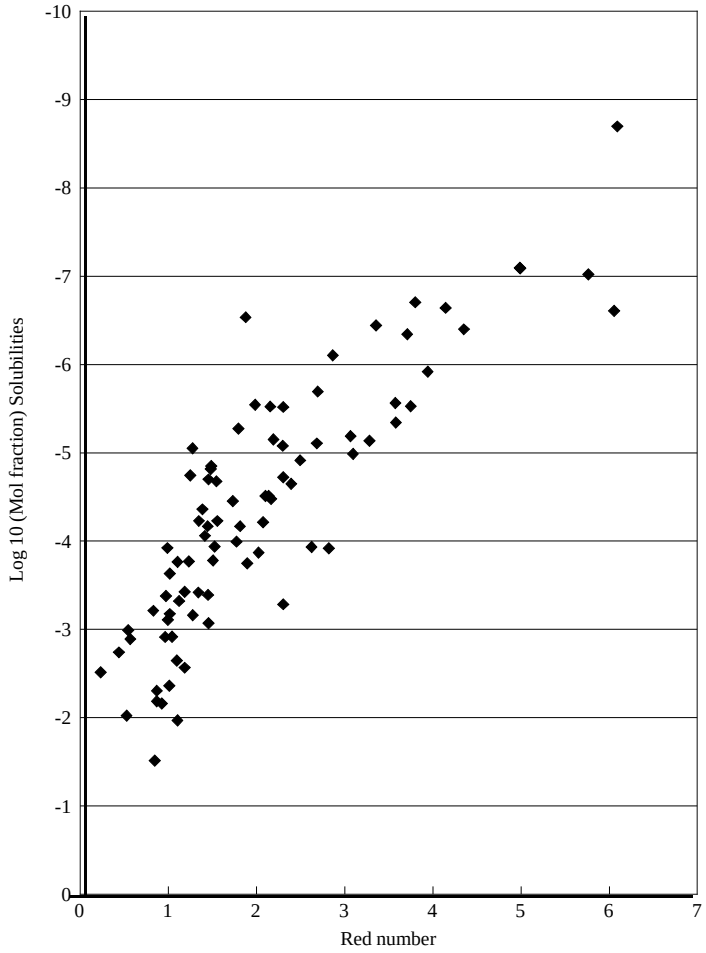
$$f_p = 100\delta_P/(\delta_D + \delta_P + \delta_H)$$

$$f_h = 100\delta_H/(\delta_D + \delta_P + \delta_H)$$

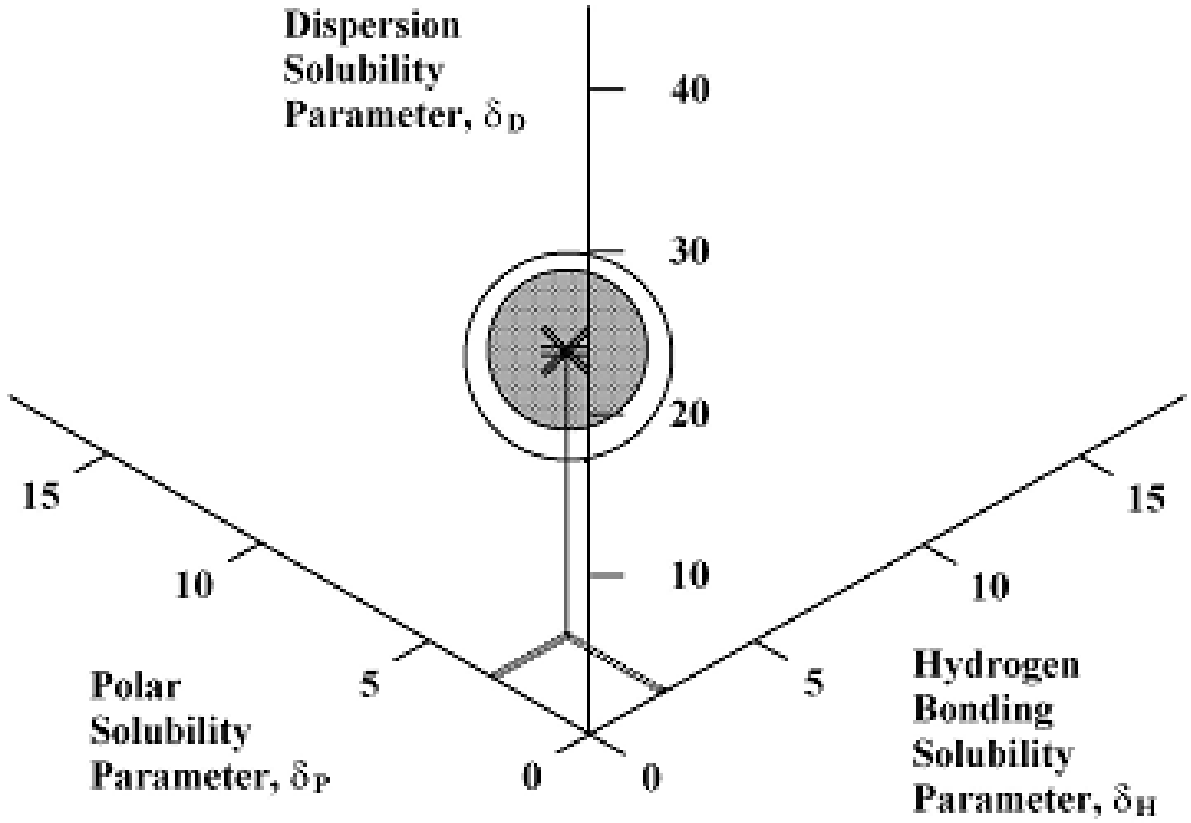
TEAS PLOT



SOLUBILITY OF CARBON-60

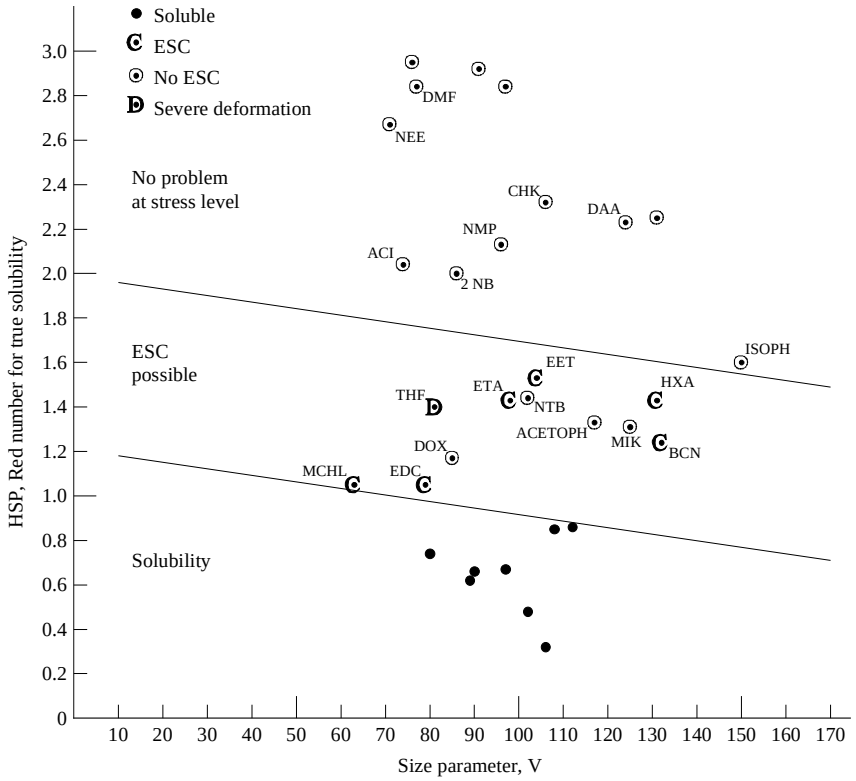


COC - SOLUBILITY SHADED ESC CLEAR

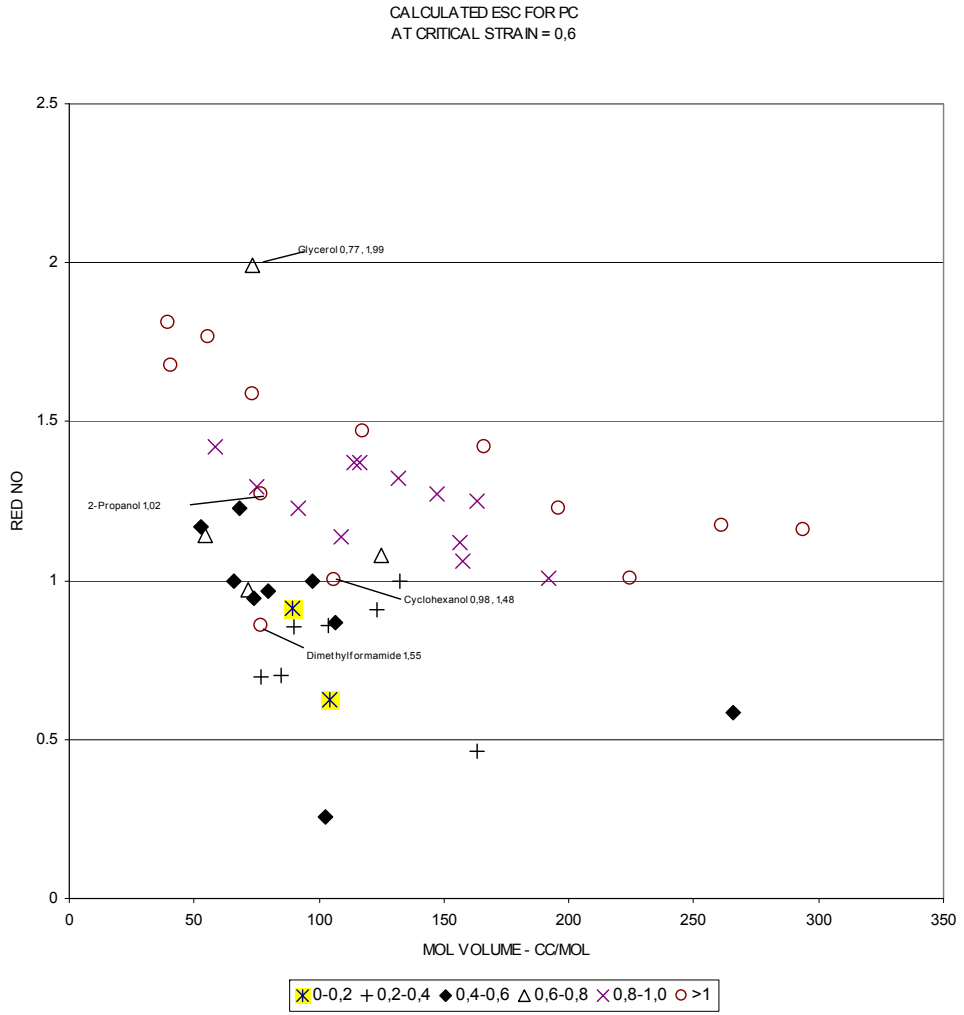


ENVIRONMENTAL STRESS CRACKING CORRELATES WITH RED NUMBER AND MOLAR VOLUME

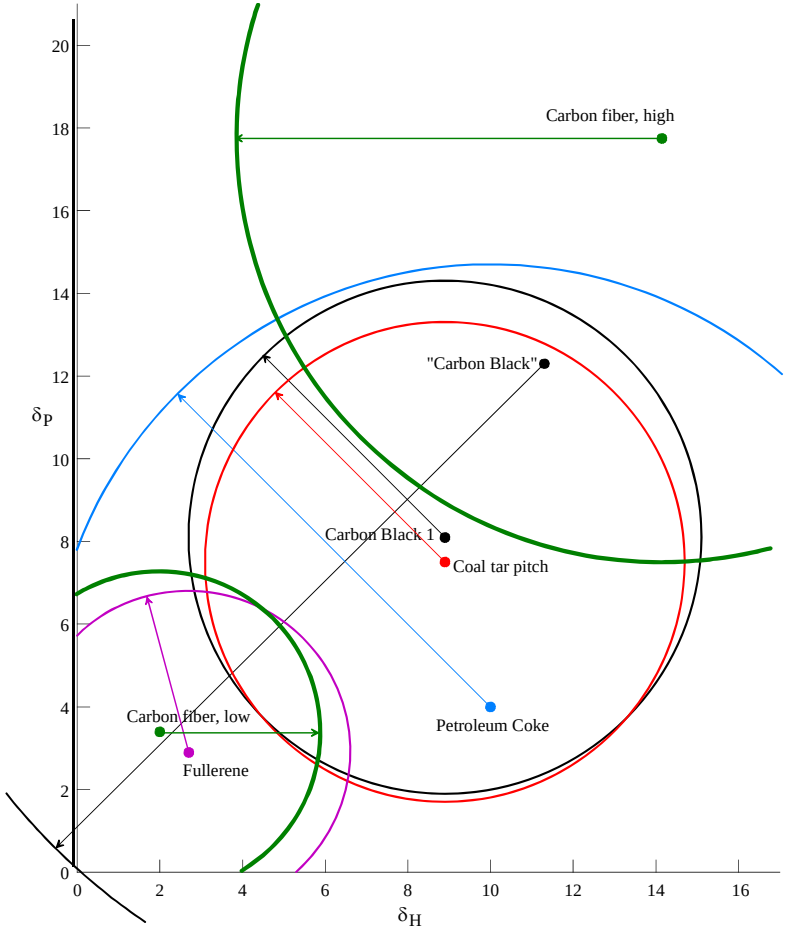
	δ_D	δ_P	δ_H	R_O
TOPAS 6013 solubility	18.0	3.0	2.0	5.0



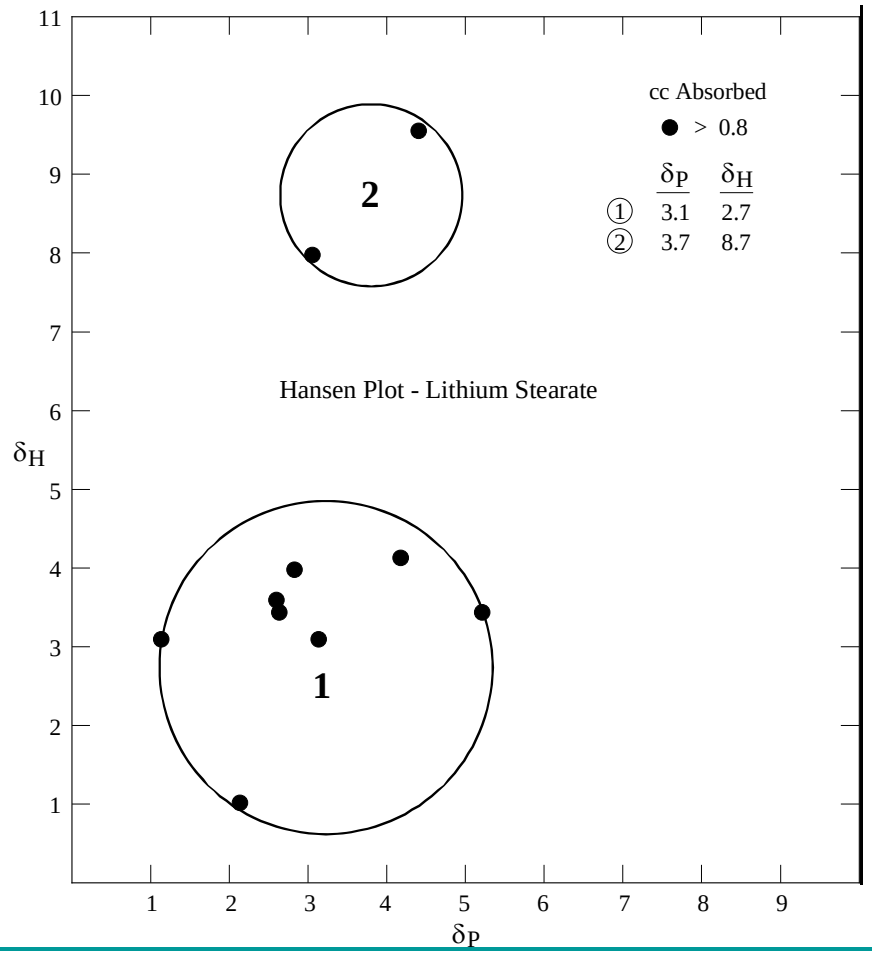
ESC in PC


CALCULATED ESC FOR PC
AT CRITICAL STRAIN = 0,6
RED NO
MOL VOLUME - CC/MOL
Glycerol 0,77 , 1,99
2-Propanol 1,02
Cyclohexanol 0,98 , 1,48
Dimethylformamide 1,55
0-0,2
0,2-0,4
0,4-0,6
0,6-0,8
0,8-1,0
>1

HSP FOR ”CARBON” MATERIALS

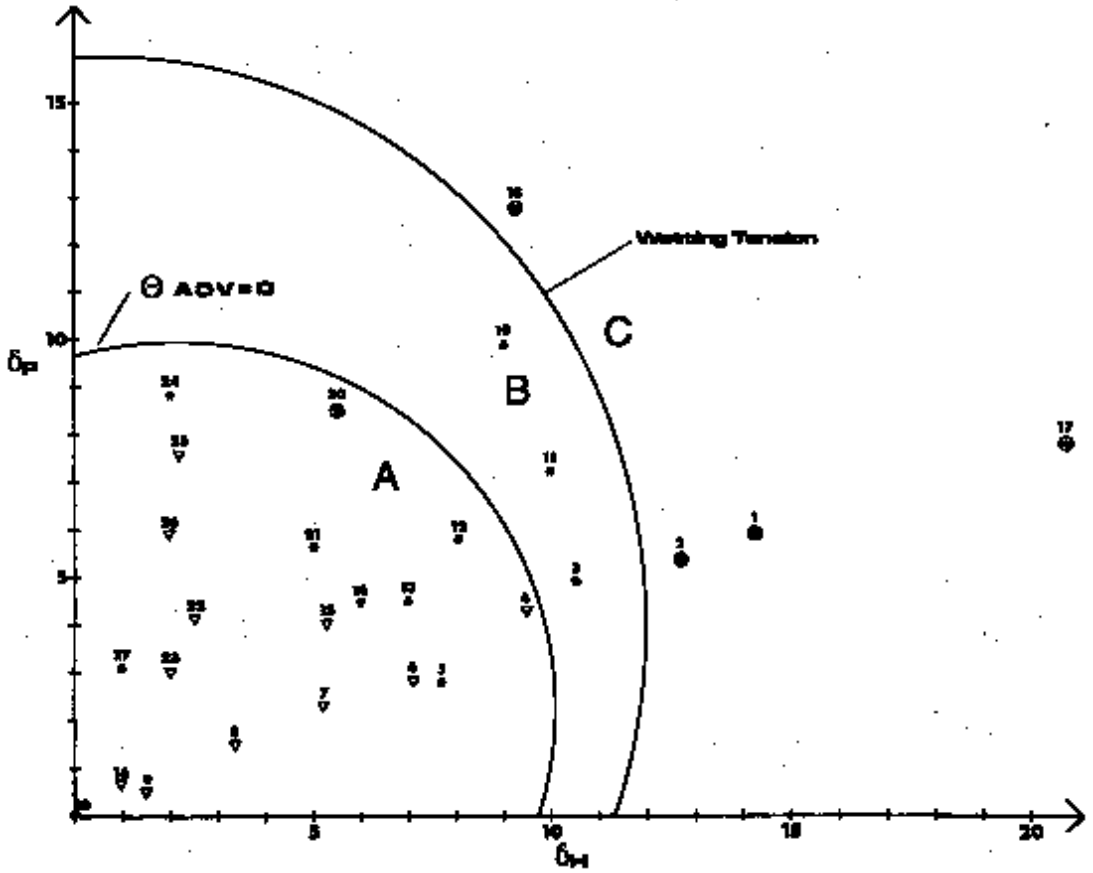


SURFACTANTS
Two HSP regions required



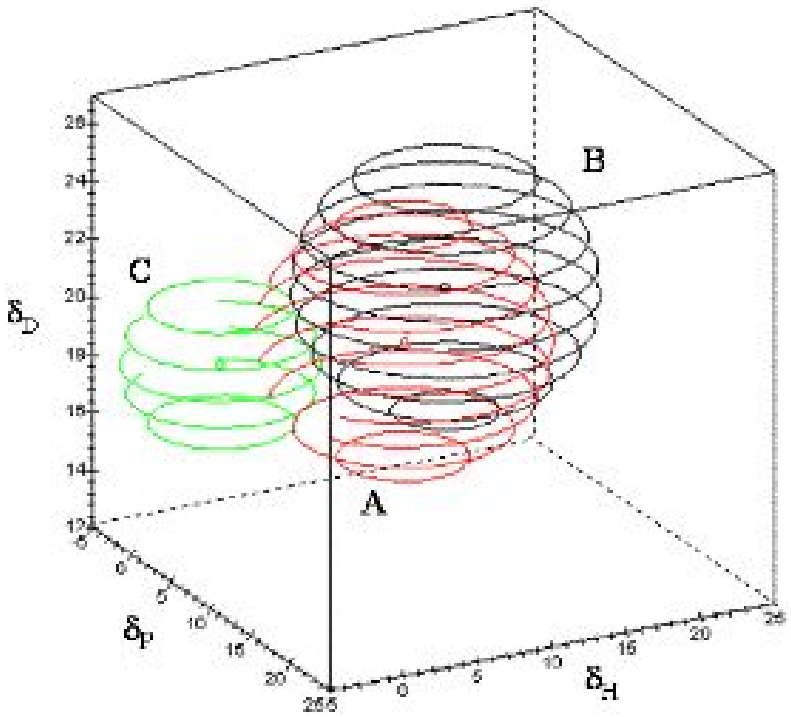
SURFACE PHENOMENA – EPOXY FILM

- A - Spontaneous spreading
- B - No dewetting
- C - Spontaneous dewetting



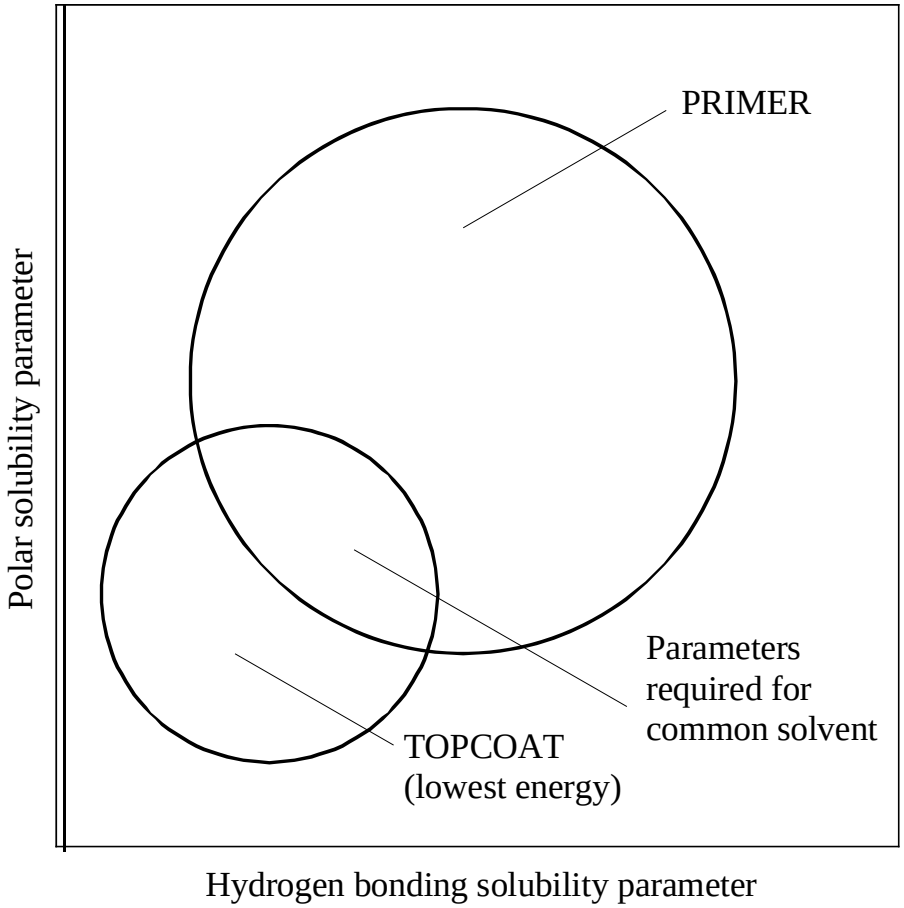
FIBER SURFACE CHARACTERIZATION

- **A – Glassy Carbon**
- **B – Carbon Fibers**
- **C – PP Fibers**



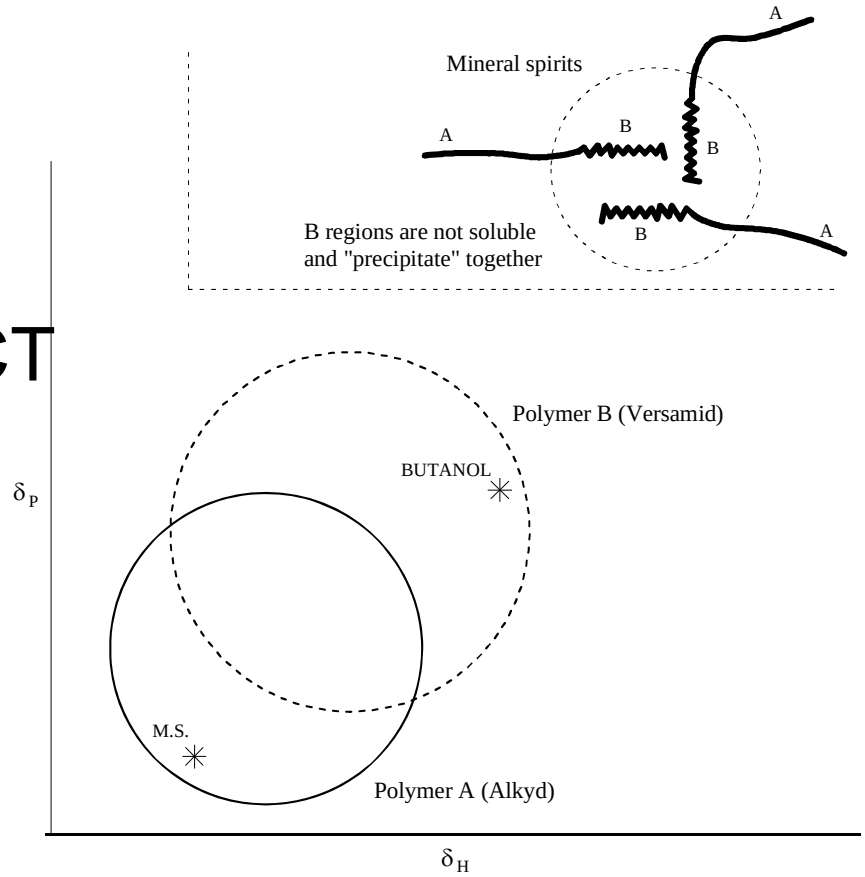
SELF-ASSEMBLY

Lower energy polymer is surface layer in two layer film deposited from true solution



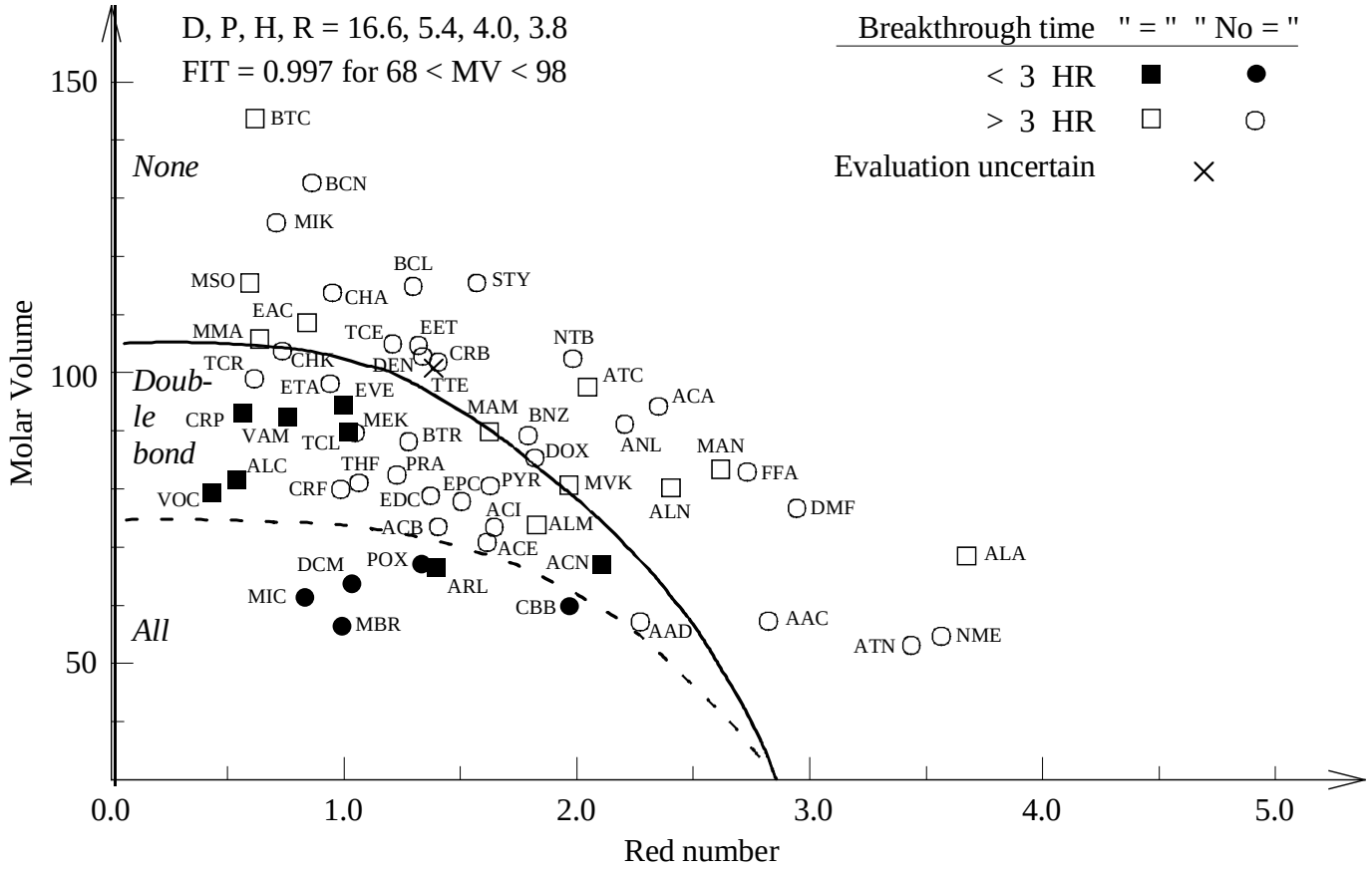
SELF-ASSEMBLY THIXOTROPIC PAINT

- VERSAMID SEGMENTS ASSOCIATE
- ALCOHOLS WILL DESTROY EFFECT
- SHEAR BREAKS STRUCTURE TEMPORARILY



BREAKTHROUGH TIME

Smaller molecules with linear structure and low RED diffuse faster - PTFE



HSP FOR CYTOTOXIC DRUGS FOR GLOVE SELECTION

CHEMICAL	D	P	H	V
Fluorouracil	18.0	11.7	11.6	118.3
Gemcitabine	19.0	12.6	15.5	260.6
Cyclophosphamide	17.5	11.9	12.6	279.1
Ifosfamide	17.5	11.9	9.8	261.1
Methotrexate	18.0	10.2	14.2	378.7
Etoposide	20.0	7.5	12.5	588.5
Paclitaxel (Taxol)	18.0	6.6	9.8	853.9
Average Group 1	18.3	10.3	12.3	-
Cytarabine (Pyrimidine/arabinose)	19.0	15.2	20.1	187.1
Carboplatin (Organic Pt)	27.3	9.0	10.4	185.1

CYCLOPHOSPHAMIDE BREAKTHROUGH TIMES NITRILE 45 MINUTES, BUTYL >>4 HOURS

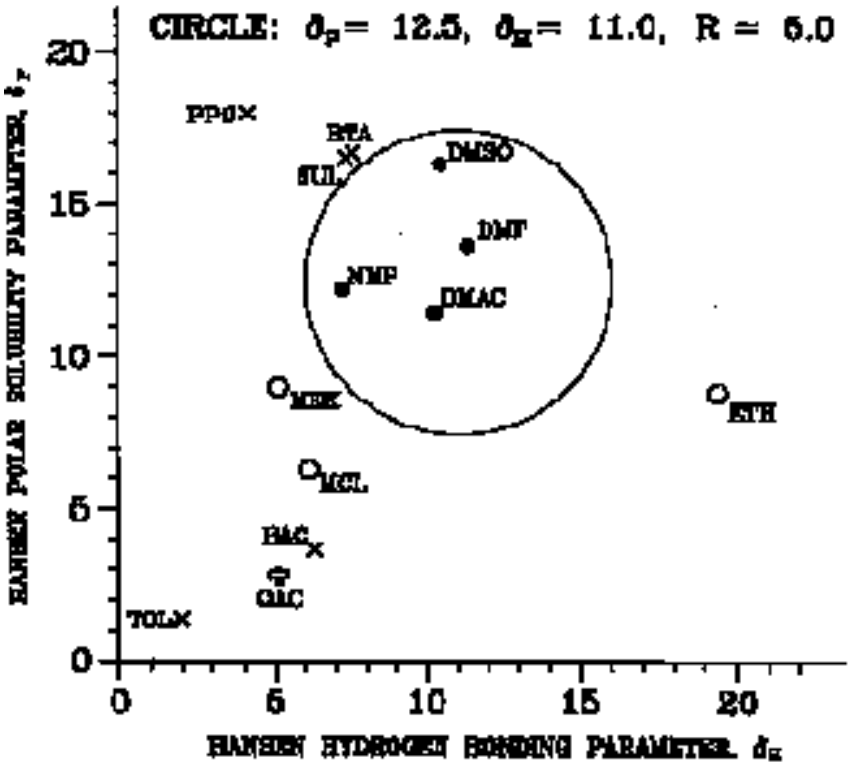
		D	P	H			
	Cyclophosphamide	**17.5**	**11.9**	**12.6**			
	MATERIAL	D	P	H	Ro	Ra	RED
117	**NR 20 MIN**	17.50	7.30	6.50	5.10	7.64	**1.50**
118	**NR 1 HR**	16.60	9.10	4.40	10.00	8.85	**0.88**
119	**NR 4 HR**	19.00	12.60	3.80	13.30	9.32	**0.70**
120	**BR 20 MIN**	16.50	1.00	5.10	5.00	13.38	**2.68**
121	**BR 1 HR**	15.80	-2.10	4.00	8.20	16.78	**2.05**
122	**BR 4 HR (2)**	17.60	2.10	2.10	7.00	14.36	**2.05**

PERMEATION - VIABLE HUMAN SKIN

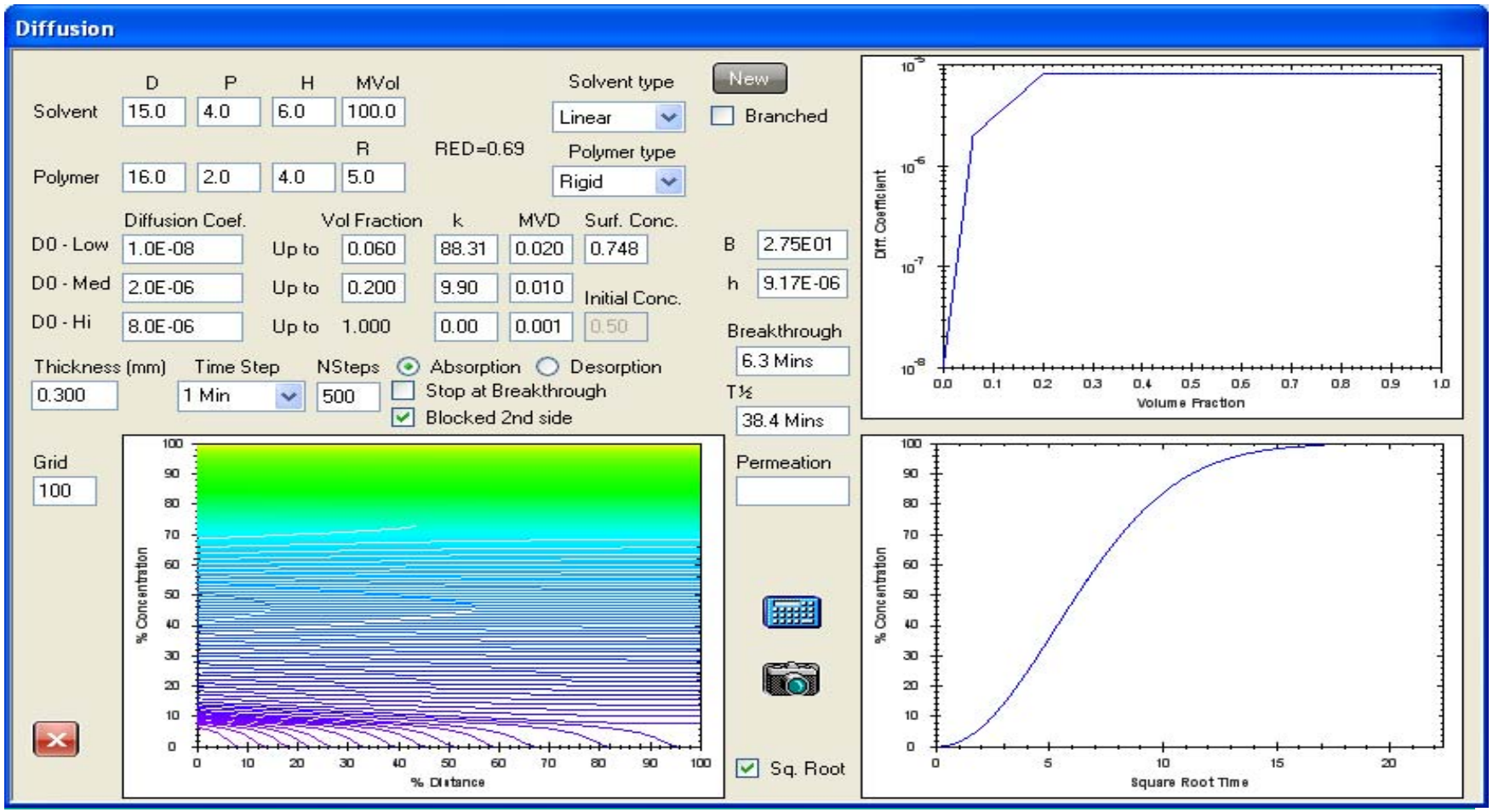
Ursin,et.al.,J.Am.Ind.Hyg.Assoc., 56, 651 (1995).

SOLUBILITY PARAMETER PLOT FOR SKIN PERMEATION RATE

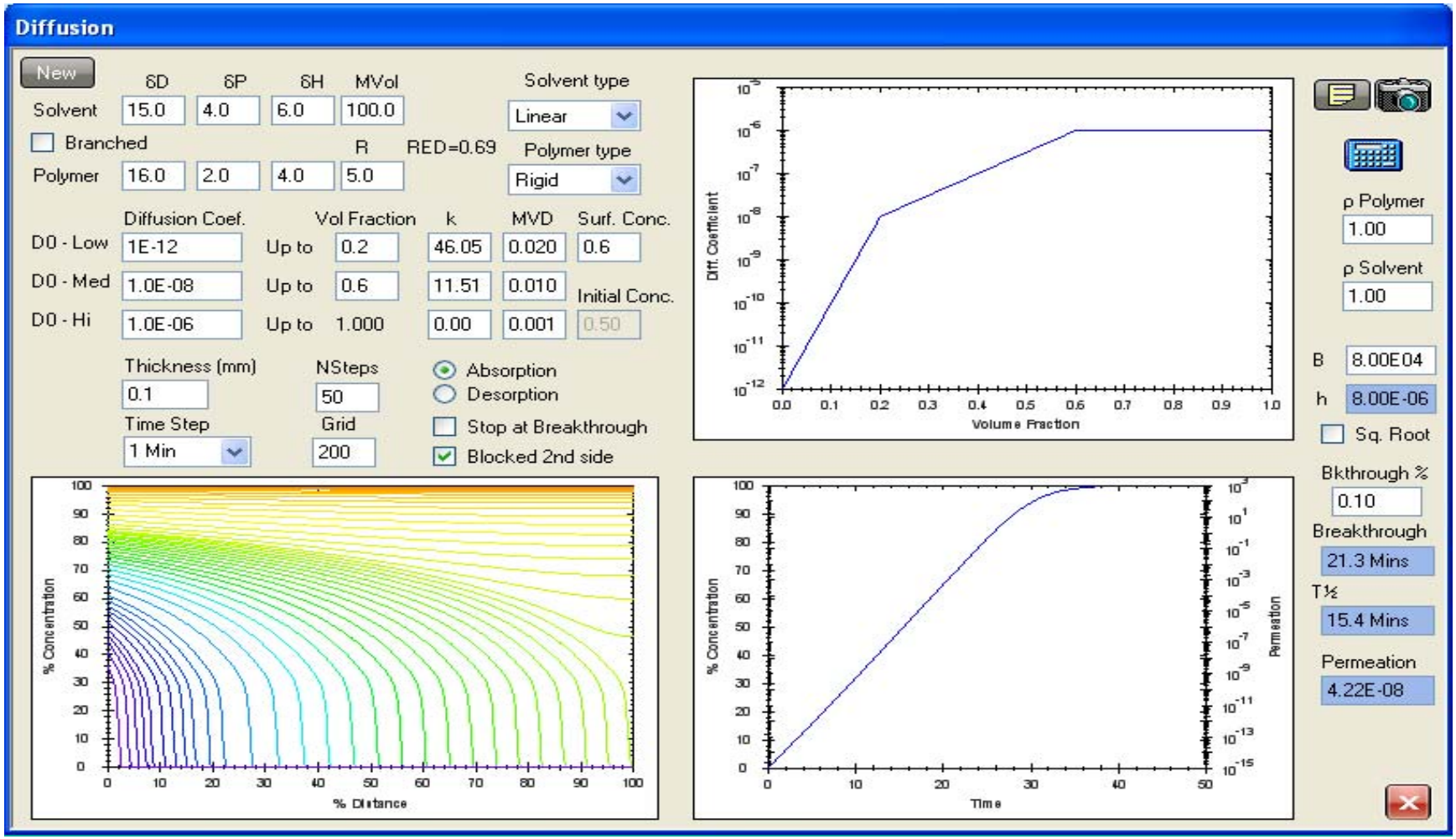
	δ_D	δ_P	δ_H	M_V	PERMEATION RATE
DMSO	18.4	16.4	102	71.3	
DMF	17.4	13.7	113	77.0	● HIGH
DMAC	16.8	11.5	102	92.5	
NMP	18.0	12.3	72	96.5	
MCL	18.2	6.3	6.1	63.9	
MEK	16.0	9.0	5.1	90.1	○ MODERATE
ETH	15.6	8.8	19.4	58.5	
BAC	15.8	3.7	6.3	132.5	
PPC	20.0	18.0	4.1	85.0	×
TOL	18.0	1.4	2.0	106.8	LOW
BTA	19.0	16.6	7.4	76.8	
SUL	18.4	18.6	7.4	95.3	
OAC	15.8	2.9	6.1	196.0	✣ "0"



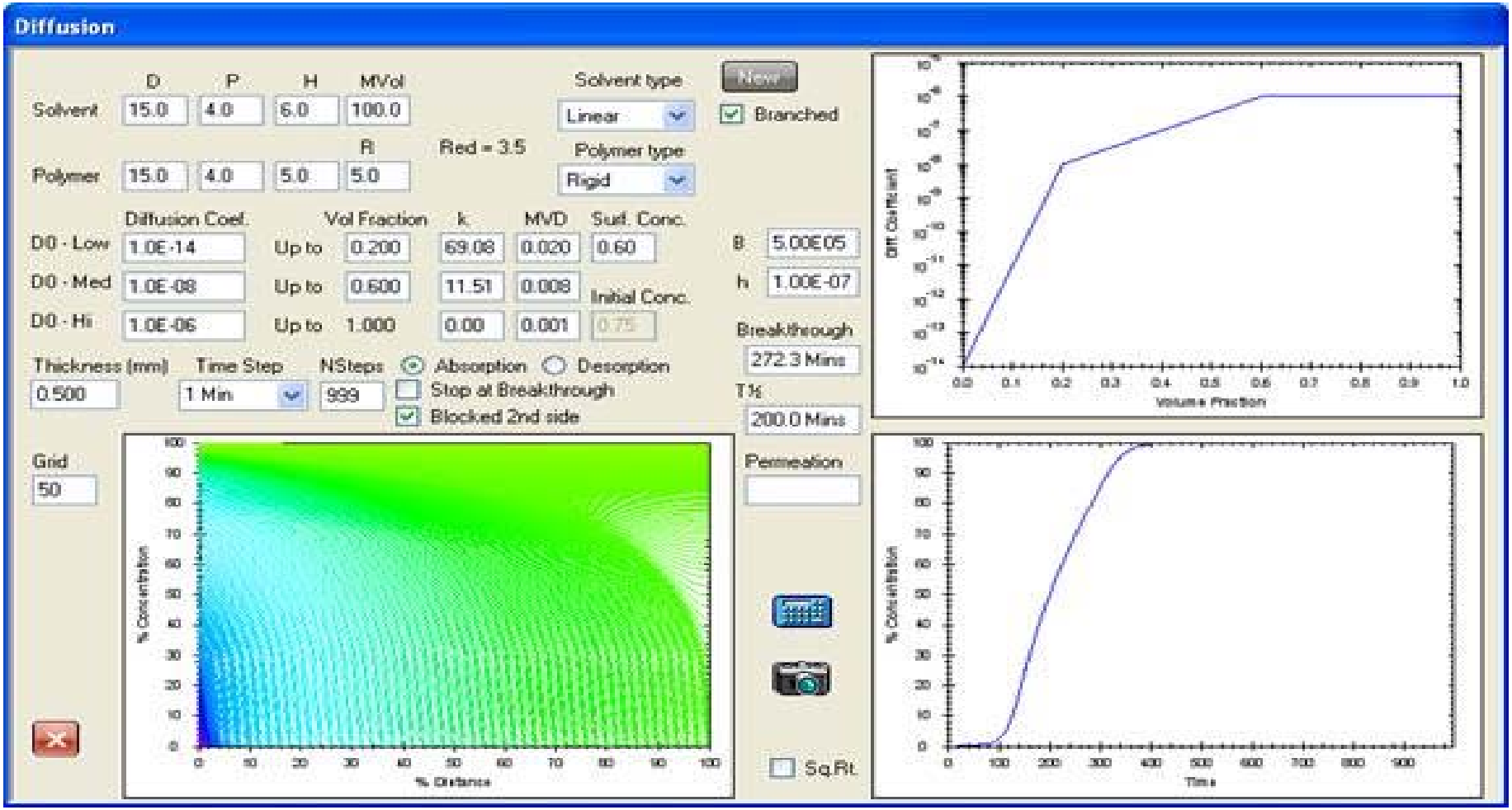
SIGMOIDAL ABSORPTION – TIME DELAY WITH SQRT TIME



ABSORPTION LINEAR WITH TIME CASE II



ABSORPTION FASTER THAN LINEAR WITH TIME – SUPER CASE II



HSP FOR ORGANIC SALTS

Material	D	P	H
DMEA - Dimethyl Ethanolamine	16.1	9.2	15.3
Formic Acid	14.3	11.9	16.6
Acetic Acid	14.5	8.0	13.5
DMEA/Formic Acid	17.2	21.5	22.5
DMEA/Acetic Acid	16.8	19.8	19.8

ALL VALUES HIGHER

HSP FOR IONIC LIQUIDS

Ionic liquid	δ_D	δ_P	δ_H	δ_t	V, cc/mole
[bmim]Cl	19.1	20.7	20.7	35.0	175.0
[bmim]PF_6	21.0	17.2	10.9	29.3	207.6
[omim]PF_6	20.0	16.5	10.0	27.8	276.0
[bmim]BF_4	23.0	19.0	10.0	31.5	201.4

[bmim] is butyl methyl imidazole (o is octyl)

Solvents having CO_2 solubility greater than Ideal x = 0.0229 at 25°C and P_{CO2} = 1 (Williams)

Solvent		δ_d **(MPa)$^{1/2}$**	δ_p **(MPa)$^{1/2}$**	δ_h **(MPa)$^{1/2}$**
Tributyl phosphate, ($C_{12}H_{27}O_4P$)	0.03550	16.3	6.3	4.3
Amyl acetate, ($C_7H_{14}O_{2)}$	0.02800	15.8	3.3	6.1
Butyl oleate, ($C_{22}H_{42}O_{2)}$	0.02790	14.7	3.4	3.4
Tetrahydrofuran (C_4H_8O)	0.02700	16.8	5.7	8.0
Methyl oleate ($C_{19}H_{36}O_2$)	0.02690	14.5	3.9	3.7
Isobutyl acetate ($C_6H_{12}O_2$)	0.02500	15.1	3.7	6.3
Methyl ethyl ketone (C_4H_8O)	0.02444	16.0	9.0	5.1
Propyl acetate ($C_5H_{10}O_2$)	0.02429	15.3	4.3	7.6
Ethyl acetate ($C_4H_8O_2$)	0.02300	15.8	5.3	7.2
Methyl acetate ($C_3H_6O_2$)	0.02253	15.5	7.2	7.6

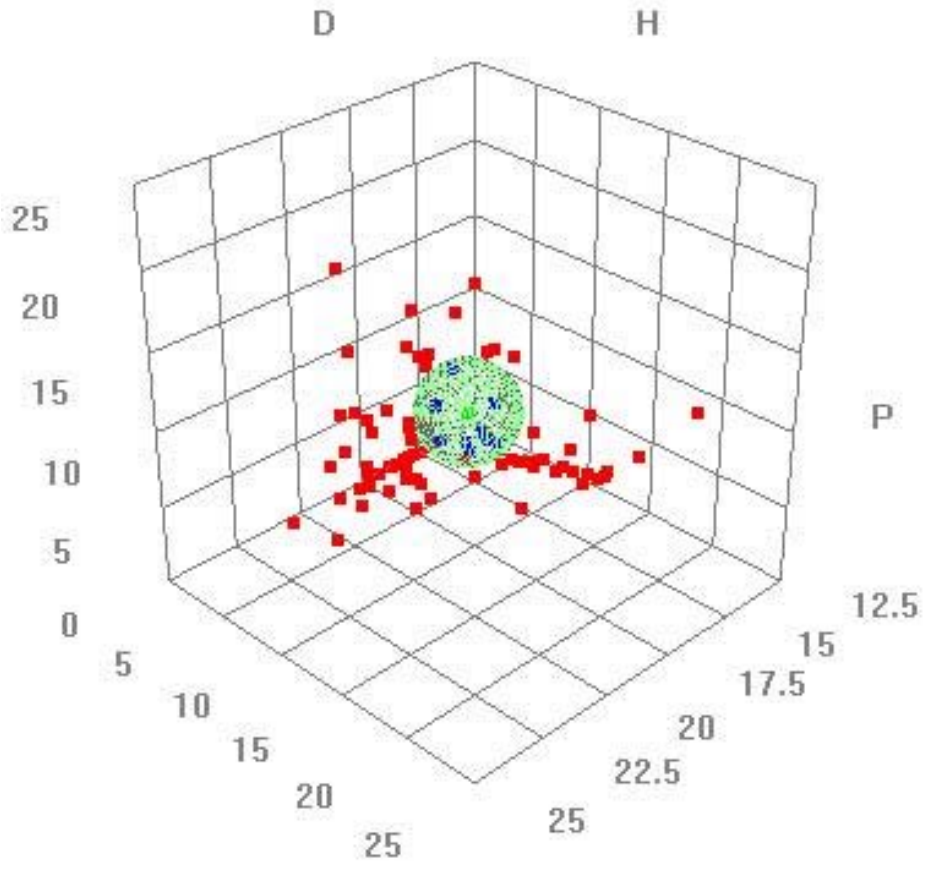
BEST SOLVENTS
CARBON DIOXIDE

No.	Solvent	Dispersion	Polar	Hydrogen	Soluble	RED	MolVol
328	Ethyl Acetate	15.8	5.3	7.2	1	0.331	98.5
464	Methyl Acetate	15.5	7.2	7.6	1	0.523	79.7
641	Tri-n-Butyl Phosphate*	16.3	6.3	4.3	1	0.714	274
617	Tetrahydrofuran	16.8	5.7	8	1	0.725	81.7
579	n-Propyl Acetate	15.3	4.3	7.6	1	0.737	115.3
45	Amyl Acetate	15.8	3.3	6.1	1	0.865	148
430	Isobutyl Acetate	15.1	3.7	6.3	1	0.879	133.5
502	Methyl Oleate	16.2	3.8	4.5	1	0.948	337.3
481	Methyl Ethyl Ketone	16	9	5.1	1	0.973	90.1
545	Oleic Acid*	16	2.8	6.2	0	1.013	317
1075	Dodecanol*	16	4	9.3	0	1.066	224.5
197	1-Decanol *	16	4.7	10	0	1.146	191.8
479	2-Methyl Cyclohexanone	17.6	6.3	4.7	0	1.173	121.3
183	Cyclohexanone	17.8	6.3	5.1	0	1.234	104
932	1-Nonanol	16	4.8	10.6	0	1.306	174.4
7	Acetone	15.5	10.4	7	0	1.327	74

HSP FOR CARBON DIOXIDE

- Data Fit = 1.000 for experimental data
- δ^2_D = 15.7 $MPa^{½}$
- δ^2_P = 6.3 $MPa^{½}$
- δ^2_H = 5.7 $MPa^{½}$
- Ro = 3.3 $MPa^{½}$

CARBON DIOXIDE SOLUBILITY



HSP FOR SPECIAL CHEMICALS

Chemical	δ_D	δ_P	δ_H
Amphetamine	17.5	4.3	6.3
Bisphenol A	19.2	5.9	13.8
d-Camphor	17.8	9.4	4.7
2-Ethyl hexyl phthalate (MEHP)	17.3	6.2	6.8
Hexanal	15.8	8.5	5.4
Nicotine	18.5	7.8	6.5
L-Menthol	16.6	4.7	10.6
Paracetemol	17.8	10.5	13.9
Paraquat	19.5	8.8	5.9
Skatole	20.0	7.1	6.2
2-Tert-butyl-4-methyl phenol	17.3	3.7	10.5
Triacetin	16.5	4.5	9.1
Triclosan	20.0	7.7	10.0
Vanillin	18.6	10.6	13.8

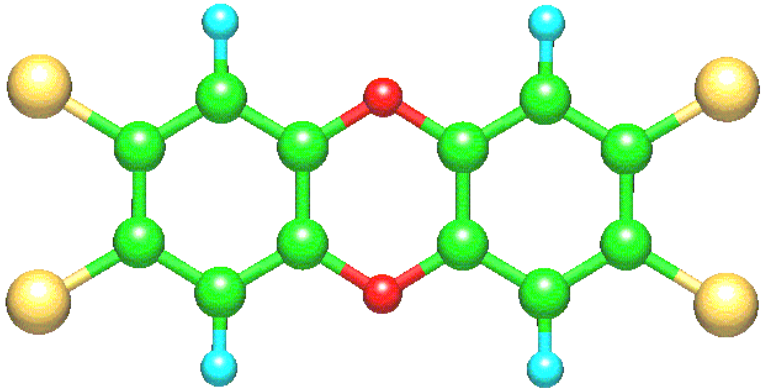
HSP AVAILABLE FOR 1200 CHEMICALS INCLUDING:

Adrenaline, Ascorbic Acid, Bethoxazin, Caffeine, Carbon Dioxide, Cholesterol, DNA, Dopamine, Ecstasy, Lignin, Meclofenoxate, Norephedrin, Palm Oil, Quinine, Saccarine, Serotonin, Spermidin, Sucrose, Urea, Zein, Etc., Etc.

SIMILARITY TO TETRABROMOBISPHENOL A

MATERIAL	δ_D	δ_P	δ_H	Ra	RED $_{TBBPA}$
TBBPA	20.2	9.1	13.8	-	0.0
PENTACHLORO-PHENOL	21.5	6.9	12.8	3.5	(close)
LIGNIN	21.9	14.1	16.9	6.8	0.5
RAPID SKIN PERMEABILITY	17.6	12.5	11.0	6.5	0.36
PSORIASIS SCALE SWELLING	24.6	11.9	12.9	9.3	0.49

DIOXIN PHYSICAL INTERACTIONS



D	P	H
20.0	9.2	7.6

PREDICTIONS:
Moderate Skin Permeation Rate (Large Size)
Ready Absorption into Lignin (Plants)

ULTRASTRUCTURE OF WOOD

HEMICELLULOSE SIDE CHAINS ORIENT

BOUNDARY HSP MATCH

(LIGNIN) (LIGNIN)

Ac Ac Ac Ac

2 3 2 3

M1β4M1β4M1β4G1β4M1β4G1β4M1β4M1β4G–

3 6

β α

1 1

M Ga

(CELLULOSE) (CELLULOSE)

GOOD HSP MATCH

HSP FOR WATER

	D	P	H	Ro
Single molecule	**15.5**	**16.0**	**42.3**	**—**
>1% soluble in	**15.1**	**20.4**	**16.5**	**18.1**
Data Fit 0.856				
Good/Total 88/167				
Total miscibility	**18.1**	**17.1**	**16.9**	**13.0**
Data Fit 0.880				
Good/Total 47/166				

CHEMICALS AFFECTING DNA -

Ts'o P.O.P., Et.Al. *Natl Acad Sci., U S A*, 48, 686-698, (1962)

Increasing activity was found to be: Adonitol, Methyl Riboside (both negligible) < Cyclohexanol < Phenol, Pyrimidine, Uridine < Cytidine, Thymidine < Purine, Adenosine, Inosine, Deoxyguanosine < Caffeine, Coumarin, 2,6-Dichloro-7-Methylpurine PLUS Formamide and Dimethyl Sulfoxide

HSP CORRELATION FOR DNA

Solvent	δ_D	δ_P	δ_H	RED	V
Dimethyl sulfoxide	18.4	16.4	10.2	0.353	71.3
2,6-Dichloro-7-methyl purine	20.5	11.7	14.2	0.651	162.4
Coumarin	20.0	12.5	6.7	0.807	156.3
Purine	20.5	11.7	14.2	0.853	100.0
Caffeine	19.5	10.1	13.0	0.923	157.9
Formamide	17.2	26.2	19.0	0.977	39.8
Pyrimidine	20.5	9.4	11.3	1.002	78.8
Phenol	18.0	5.9	14.9	1.342	87.5
Urea	20.9	18.7	26.4	1.447	45.8
Cyclohexanol	17.4	4.1	13.5	1.492	106.0
Methyl riboside	17.0	12.0	32.8	2.142	117.2
Adonitol	18.0	12.0	36.0	2.393	95.1
DNA	D = 19.0 P = 20.0 H = 11.0 RAD. = 11.0 FIT = 1.000 NO = 12				

HSP FOR DNA

- Chemicals ordered correctly
- Those not calculated have molecules that are too complicated and too large to be directly compared with the other smaller molecules.

RESULT ($MPa^{1/2}$)		
δ_D^2	δ_P^2	δ_H^2
19.0	20.0	11.0

E_H is 14% of E

HSP FOR DNA BASES

Segment	D	P	H	"V"	In H_2O Parts/100
Guanine	20.0	12.7	12.5	126.1	Insol.
Cytosine	19.5	12.1	9.9	107.8	0.77
Adenine	20.0	10.2	13.7	131.5	0.05
Thymine	19.5	14.2	12.6	121.7	0.4
Average	19.75	12.3	12.2	-	-

ESSENTIALLY INDENTICAL HSP: DNA BASES, CYTOTOXIC DRUGS AND RAPID SKIN PERMEATION

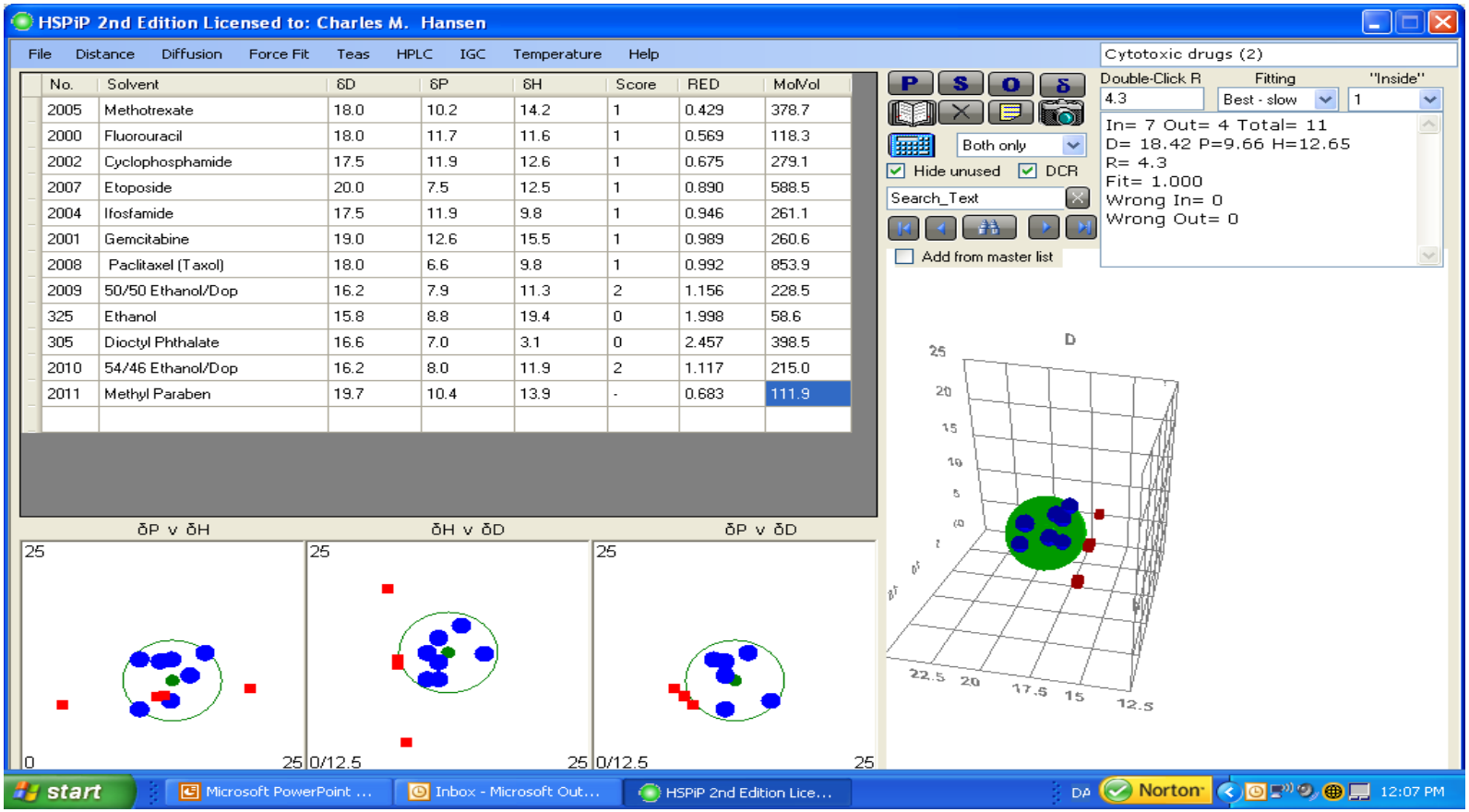
	D	P	H	Ra (bases)	Ra (Gp 1)
Rapid Skin Perm.	17.6	12.5	11.0	4.47	2.91
DNA bases	19.75	12.3	12.2	-	3.52
Ave. Group 1 Drugs	18.3	10.3	12.3	3.52	-

Synergism will be found for any of:
Phthalate plasticicizers, tricresyl phosphate, N-methyl-2-pyrrolidone, …
Mixed with any of:
Ethanol, 2-propanol, ethylene glycol, propylene glycol, or glycerol

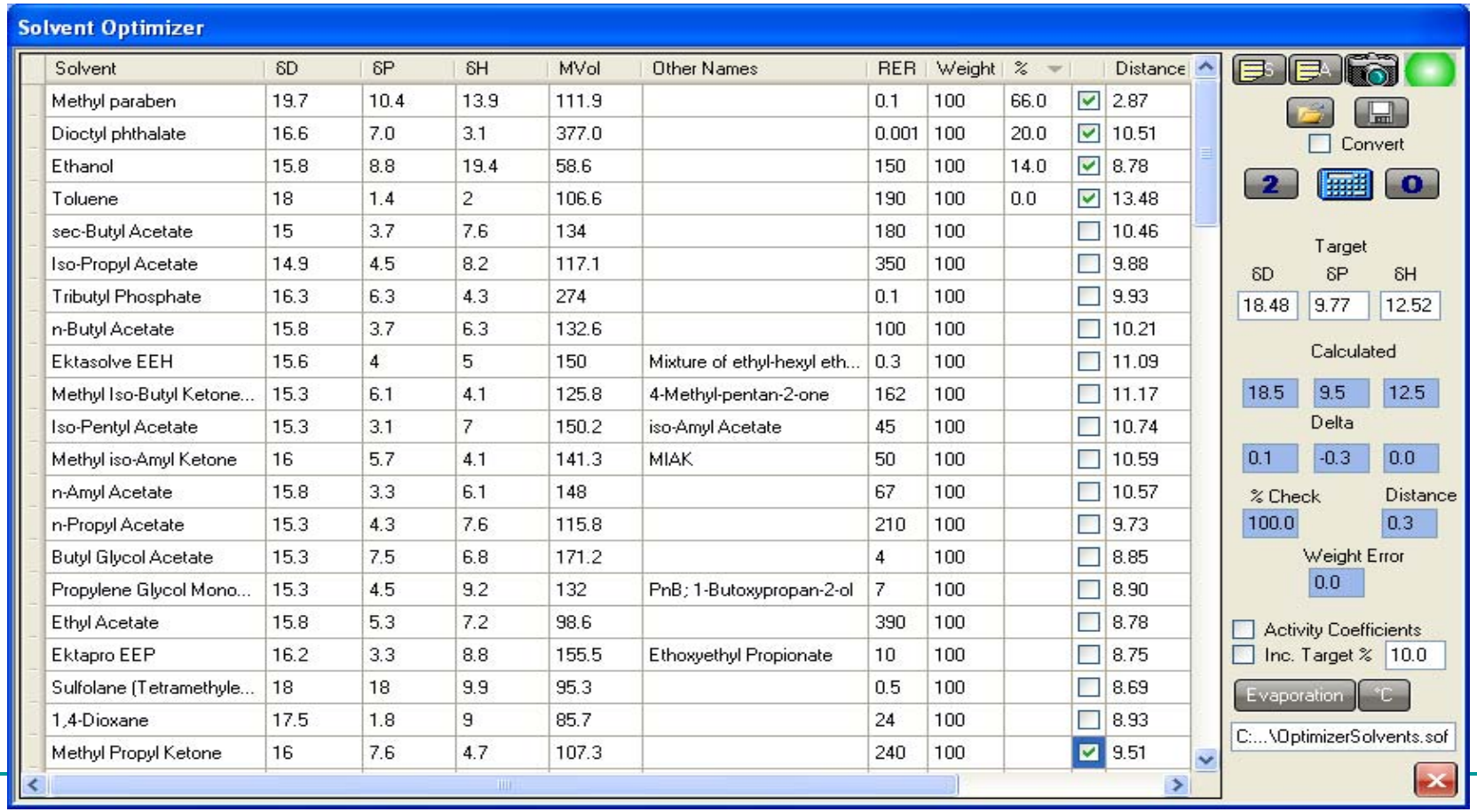
HSP DIFFERENT FOR DNA BASES, DNA, PROTEINS, AND DEPOT FAT

	D	P	H	Ro	Fit	Ra (Bases)
DNA (Molecule)	19.0	20.0	11.0	11.0	1.000	7.93
Zein (Protein)	22.4	9.8	19.4	11.9	0.964	9.28
Lard (Depot Fat)	15.9	1.2	5.4	12.0	1.000	15.87

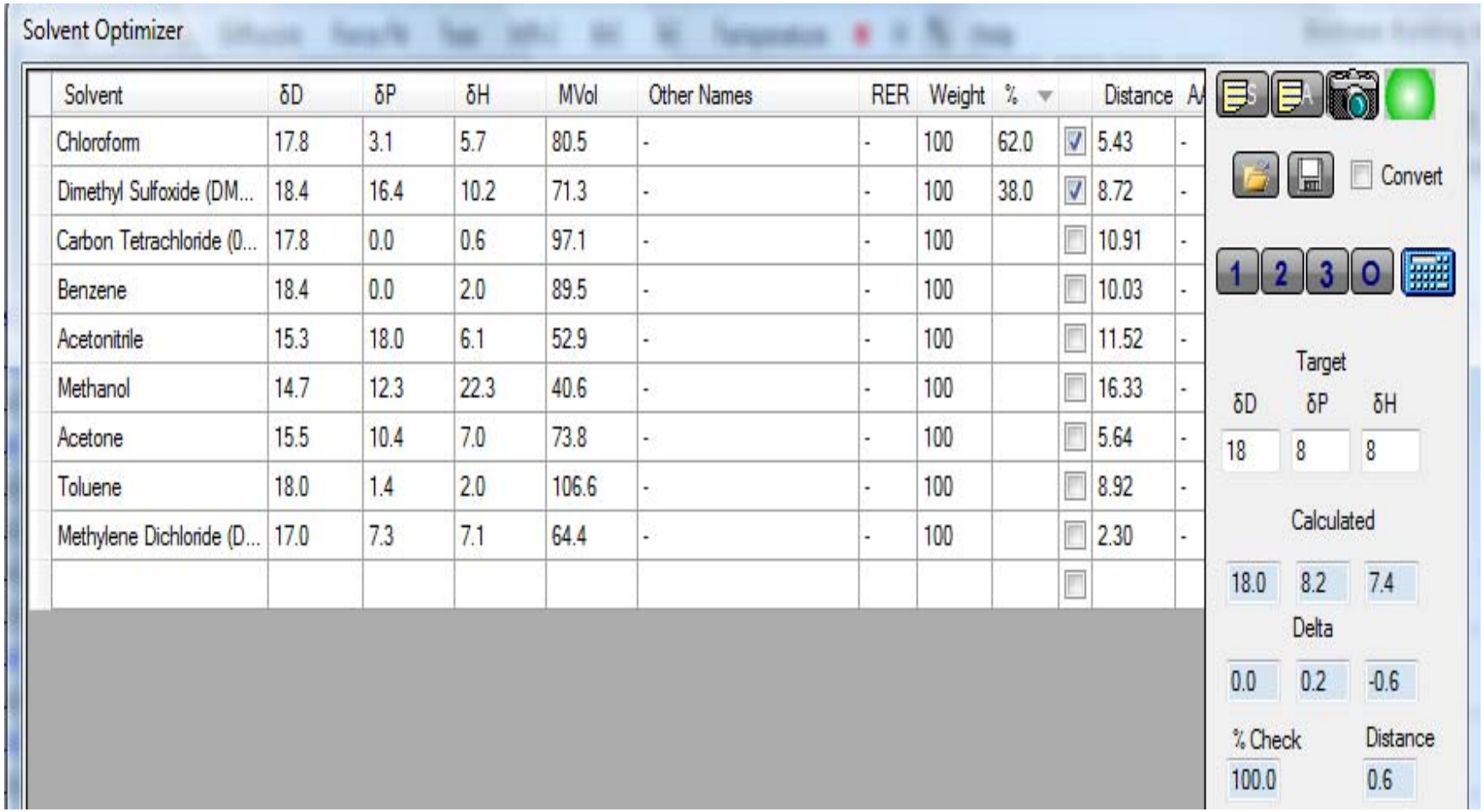
CHEMOTHERAPY DRUGS WITH ETHANOL/DOP MIXTURES



COCKTAIL FOR CONSIDERATION METHYL PARABEN+DOP+ETHANOL TARGET: CHEMODRUG HSP SPHERE

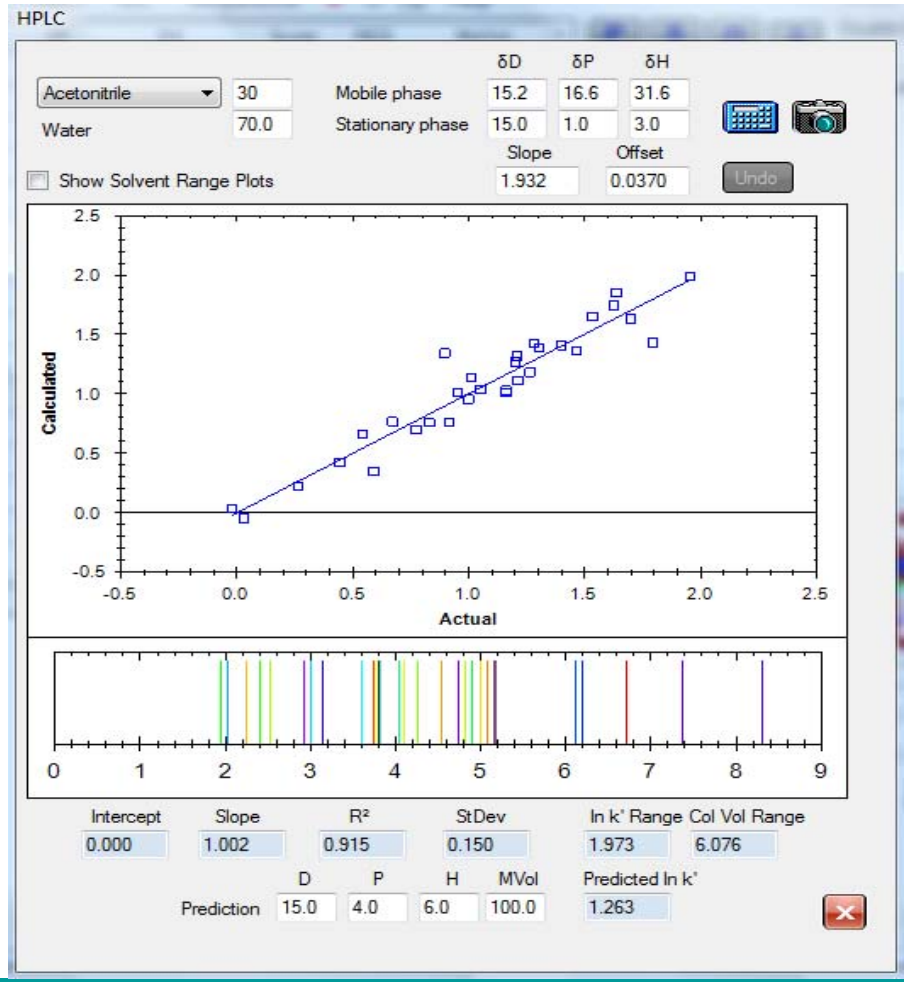


OPTIMUM NMR SOLVENT MIXTURES ARE POSSIBLE



HPLC RETENTION TIME

Retention time based on HSP of solute, mobile and stationary phases



WHOLE EQUALS SUM OF PARTS

E = COHESION ENERGY = ΔE_{vap}

- $E = E_D + E_P + E_H$
- D - Dispersion (Hydrocarbon)
- P - Polar (Dipolar)
- H - Hydrogen Bonds (Electron Interchange)
- V - Molar Volume
- $E/V = E_D/V + E_P/V + E_H/V$

$$\delta^2 = \delta^2_D + \delta^2_P + \delta^2_H$$

HANSEN SOLUBILITY PARAMETERS (HSP)

δ = Square Root of Cohesion Energy Density

SUMMARY

HSP have now existed since 1967

The first edition of HSPiP came in November, 2008.

Uses: Solubility (Gases, Liquids, Polymers, Solids), Compatibility, Swelling, Selection of Chemical Protective Clothing, Permeation Rates, Controlled Drug Release, Environmental Stress Cracking, Self-Assembly, Physical Properties, Conservation of Paintings, Surface Characterization, Improvement of Physical Adhesion, Bitumen, Asphalt, Organic Salts, Inorganic Salts, Explosives, Biologicals, Aromas, Surfactants, Subcritical Extraction, Supercritical gases

What Else?

Hansen Solubility Parameters in Practice eBook, Software, and Examples

The HSPiP software:

Finds HSP for solute (drug) with solubility data

Optimizes solvent blends for given target HSP

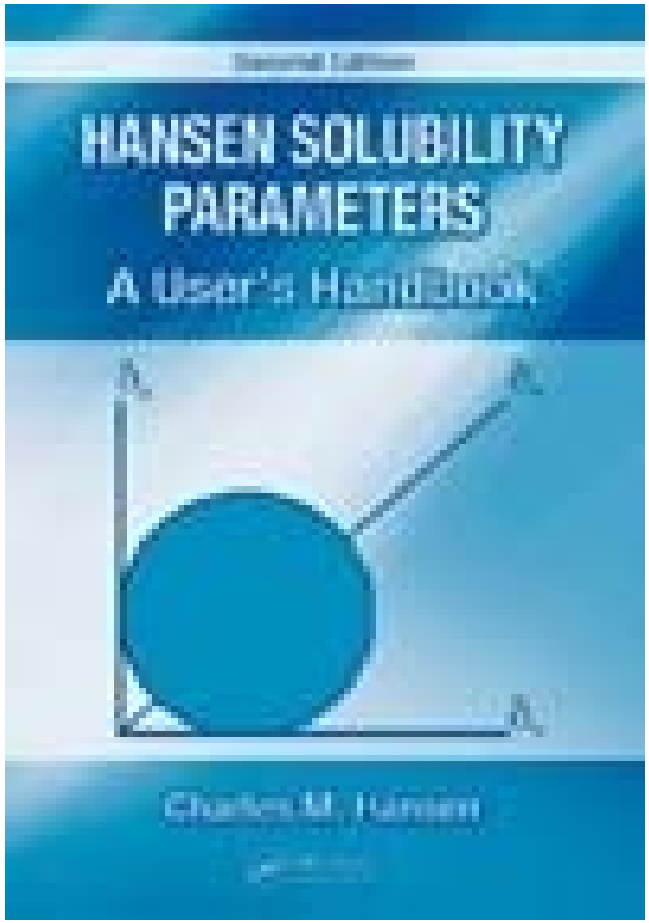
Shows which solvents can dissolve a solute

Shows polymers that are likely to be compatible

Models absorption, desorption, and permeation

HSP for chemicals/polymers with structure

Calculates HPLC solvents and IGC results



Thank you for your attention!

For further contact please visit:

www.hansen-solubility.com