



Hansen Solubility Parameters

Efficient and faster time-to-market



**Open Innovation Platform for
Materials & Coating Research**

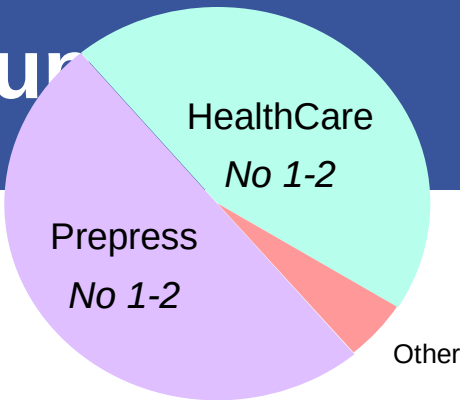


Extend your Reach

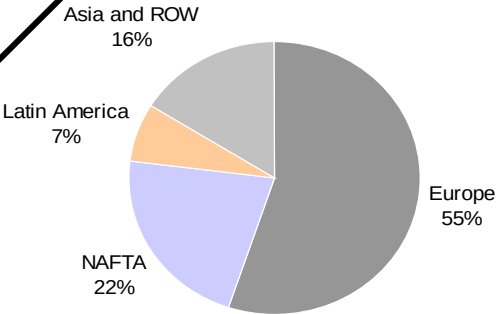
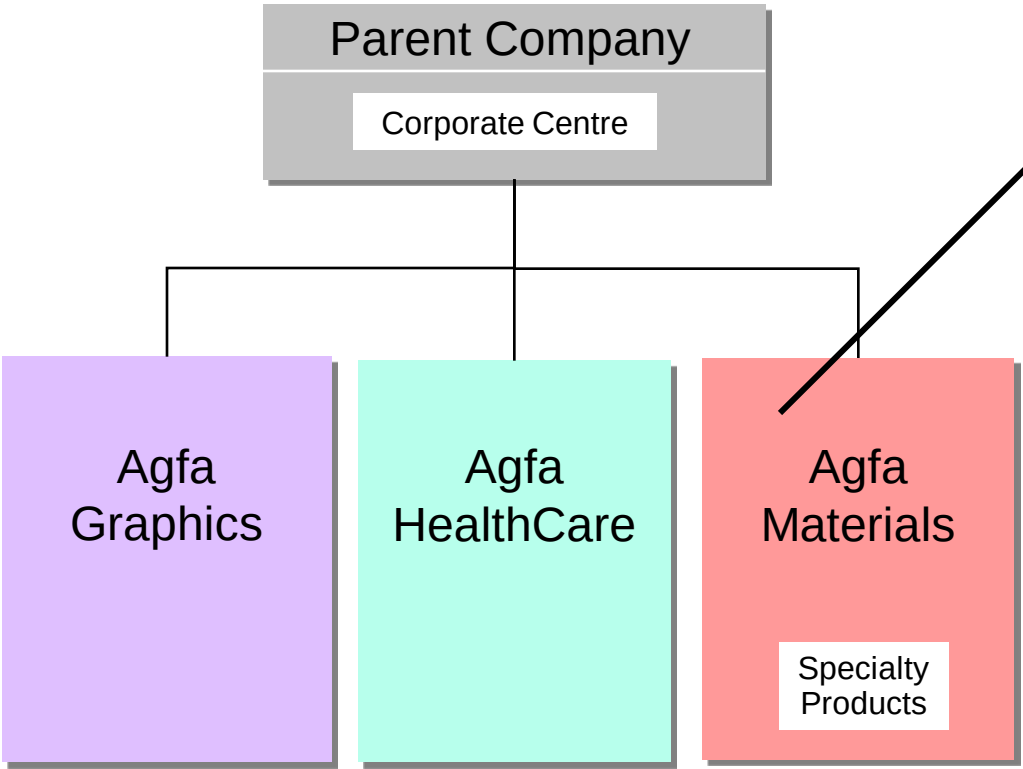
**Advanced Chemical and Physical Analytics
Joint Development Projects**



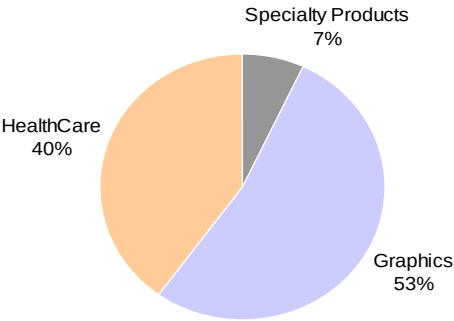
Agfa-Gevaert Group



Agfa-Gevaert Group

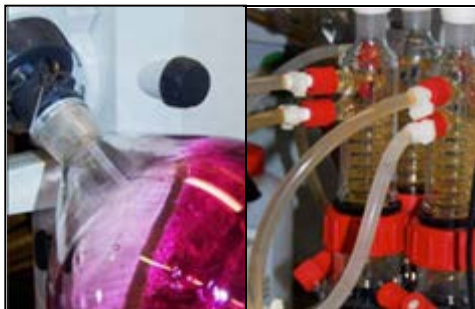


Sales by region



Sales per business group

Agfa's Materials Technology Centre



■ Molecular Ingredients

■ Sourcing, design and synthesis

- Functional polymers
- Dispersants
- Dyes
- Pigments
- Functional ingredients

■ Structure – activity relation

■ Formulations and dispersions

- Formulation discovery
- Structure – activity relation
- Dispersion technology
- Process scale-up
- Pilot Lab

Reaction calorimetry

Security

REACH

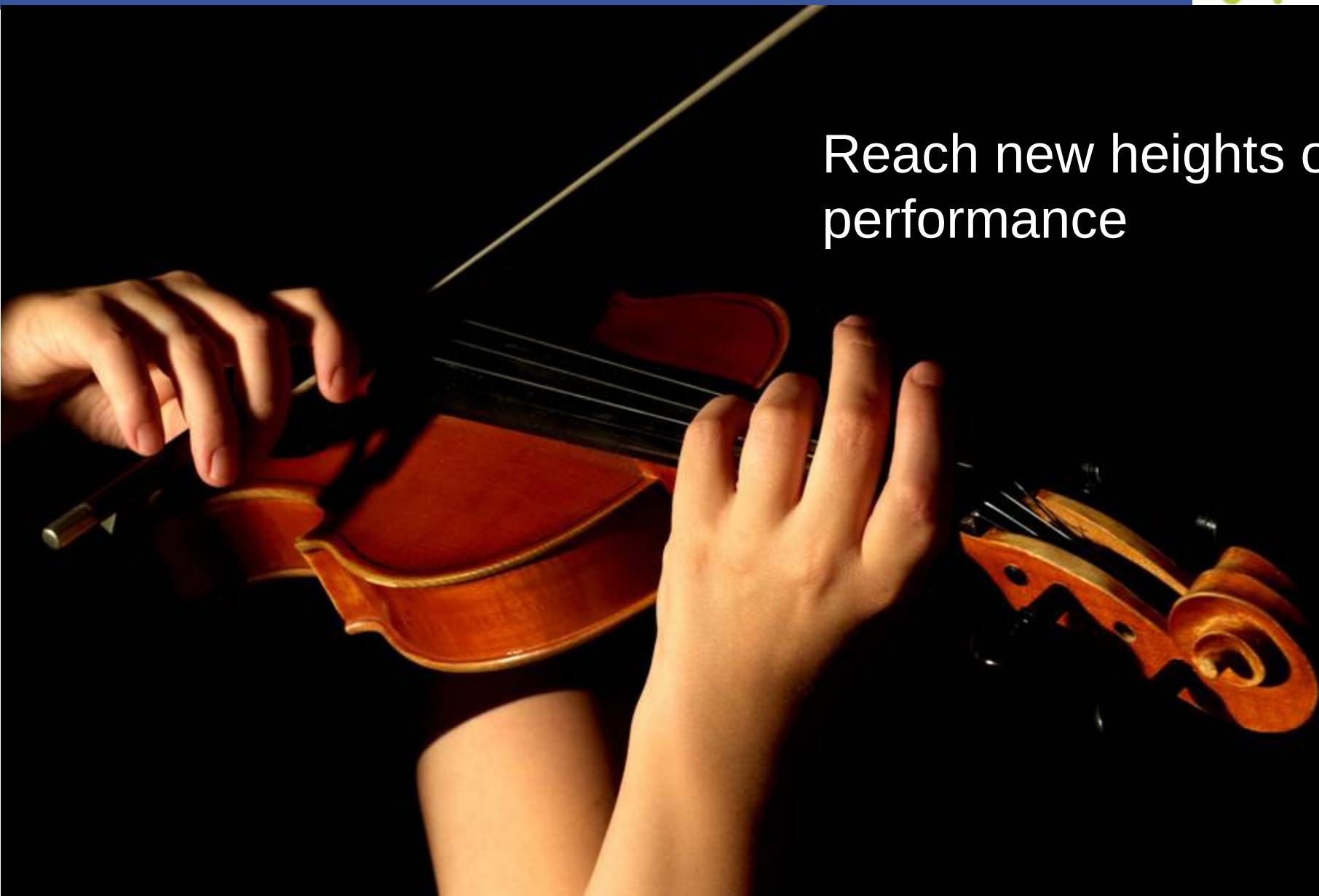
■ Analytical competences

- Organic and Inorganic Analysis
- Colloids, Surfaces and Particles
- Thermal Analysis
- Microscopy and Material Optics
- High Throughput Techniques and Mechanical Testing
- Climate Testing and Weathering

Agfa's Advanced Analytical Services



Reach new heights of
performance



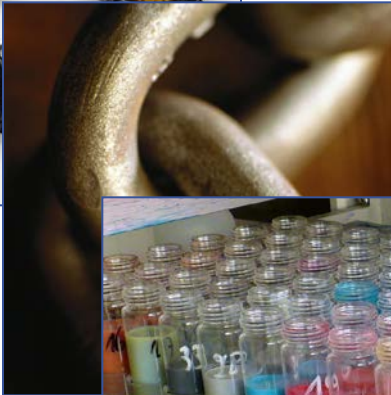
Agfa's Advanced Analytical Services



Trouble shooting and Failure Analysis



Contaminant Identification



Materials Analysis and Testing



High Throughput Analytics



Deformulation

Agfa-Labs' toolbox



High
Throughput
Formulation

n

High
Throughput
Analysis



Hansen
Solubility
Parameters

Miscellanea



Hansen Solubility Theory



Hildebrand solubility parameter δ



- Based on the principle :
 - Like seeks like
 - Like dissolves like
 - Similia similibus solvuntur

Cohesive energy density

Energy of evaporation

$$\delta^2 = \left(\frac{E}{V_m} \right) = \left(\frac{\Delta H_{evap} - R.T}{V_m} \right)$$

Molar volume

Hansen Solubility Parameters



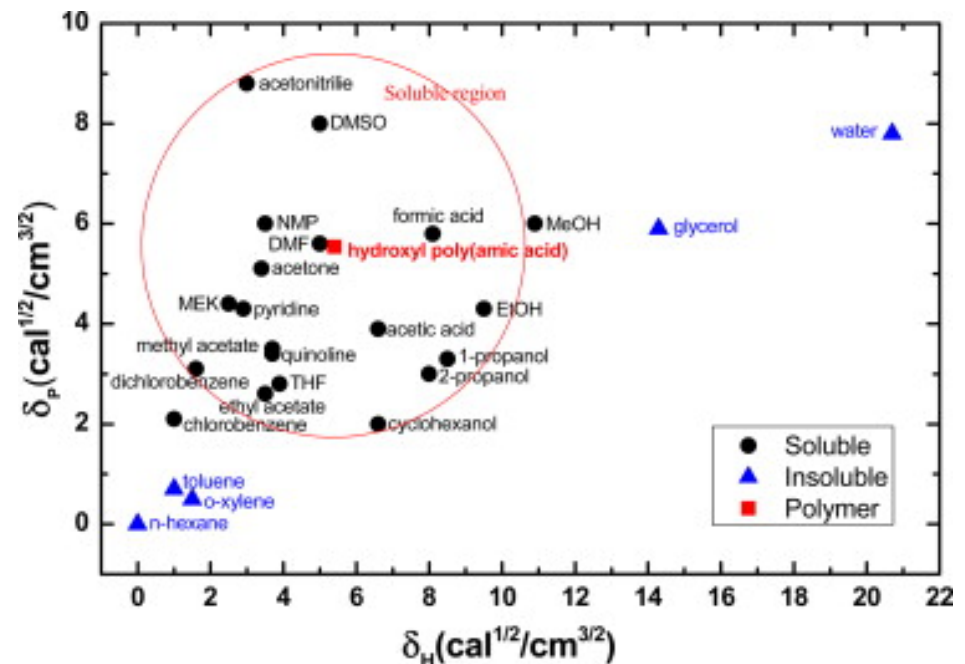
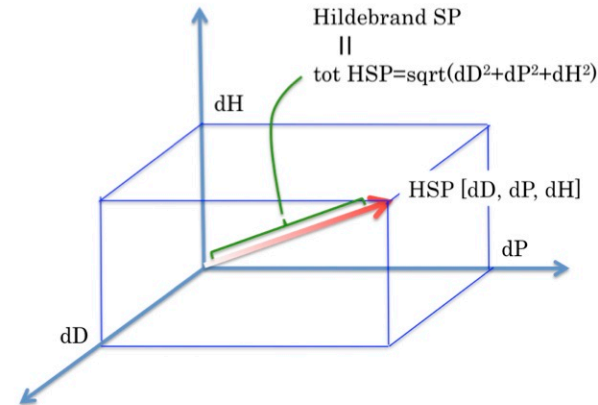
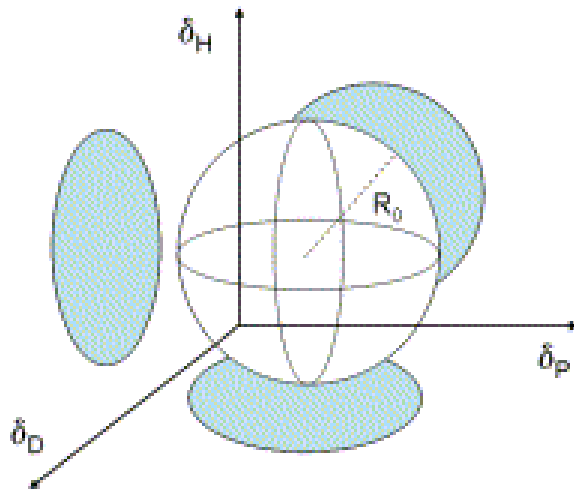
- The total cohesive energy can be divided in 3 components
 - (atomic) dispersion forces (VanderWaals...)
 - (molecular) permanent dipole-permanent dipole forces
 - (molecular) hydrogen bonding (electron exchange)

$$\delta^2 = \delta_D^2 + \delta_P^2 + \delta_H^2$$

Each solvent, polymer,
pigment... can be described by
a set of ($\delta_D, \delta_P, \delta_H$) coordinates

Hansen solubility parameters

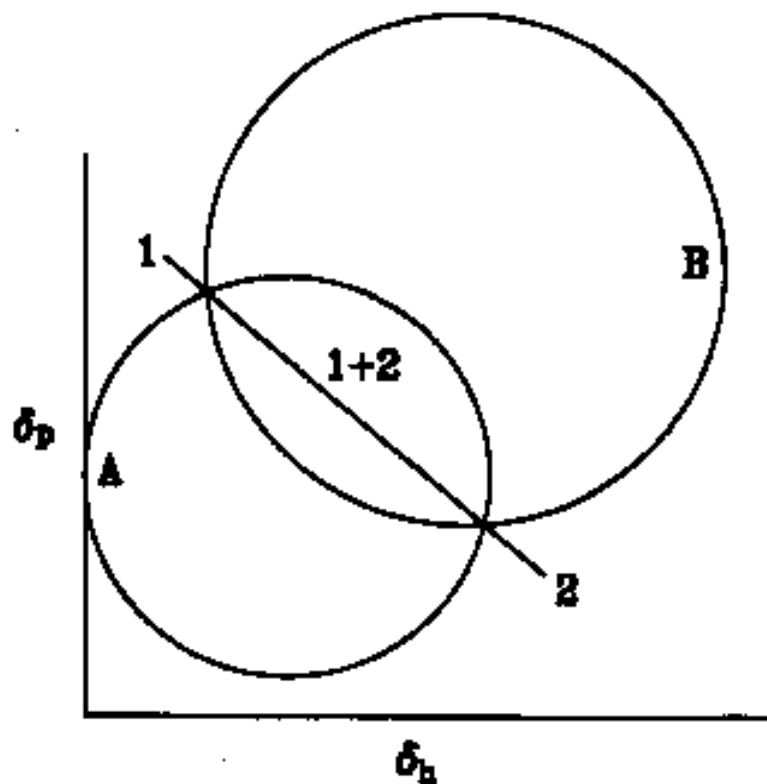
- 3D representation
 - cartesian space coordinates ($\delta_D, \delta_P, \delta_H$)
 - Sphere of solubility



Hansen solubility parameters



- Solvent mixtures
 - Two non-solvents can be mixed to a good solvent
 - Two immiscible polymers can be brought to an homogeneous solution

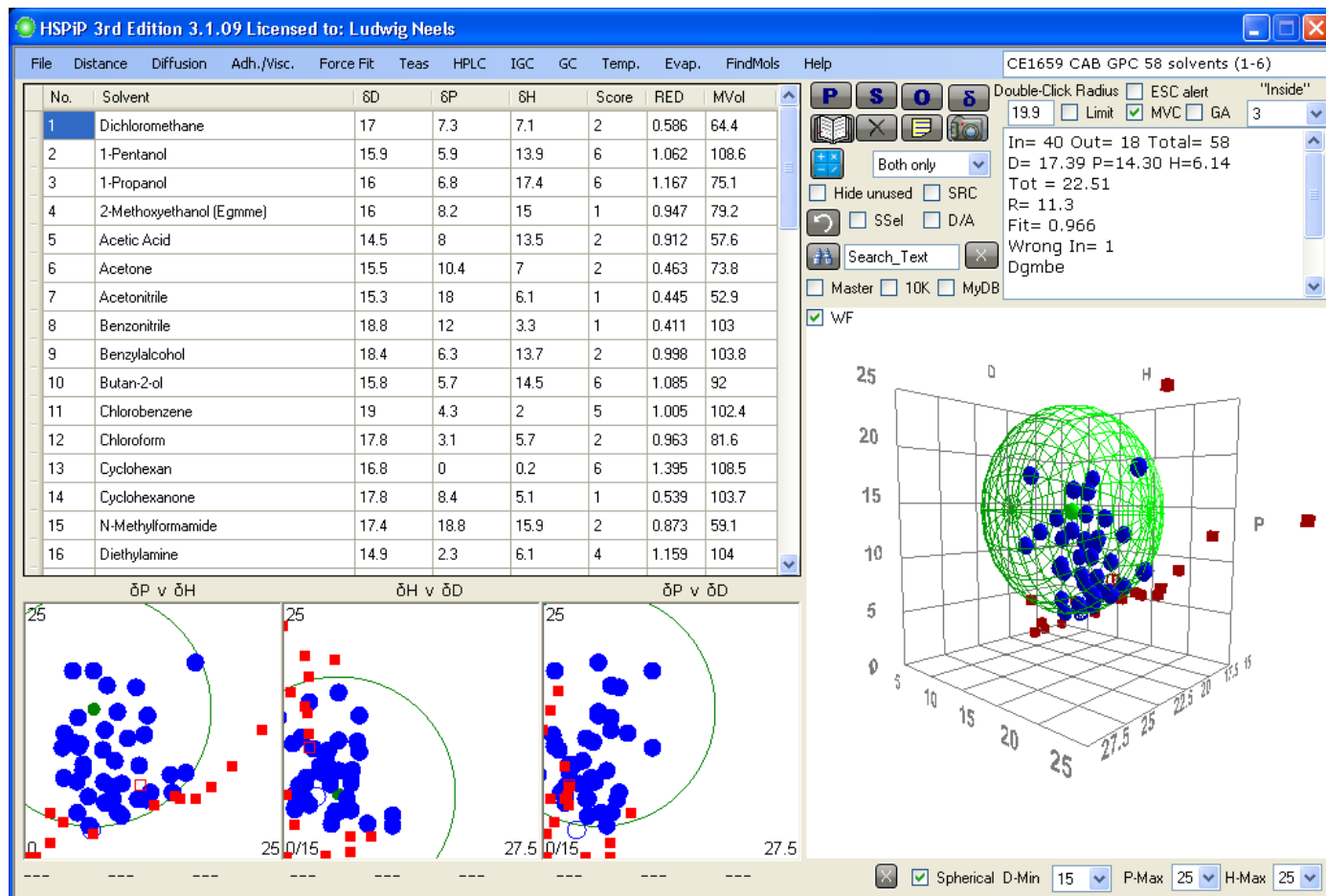


A,B : Polymers
1,2 : solvents

Hansen solubility parameters

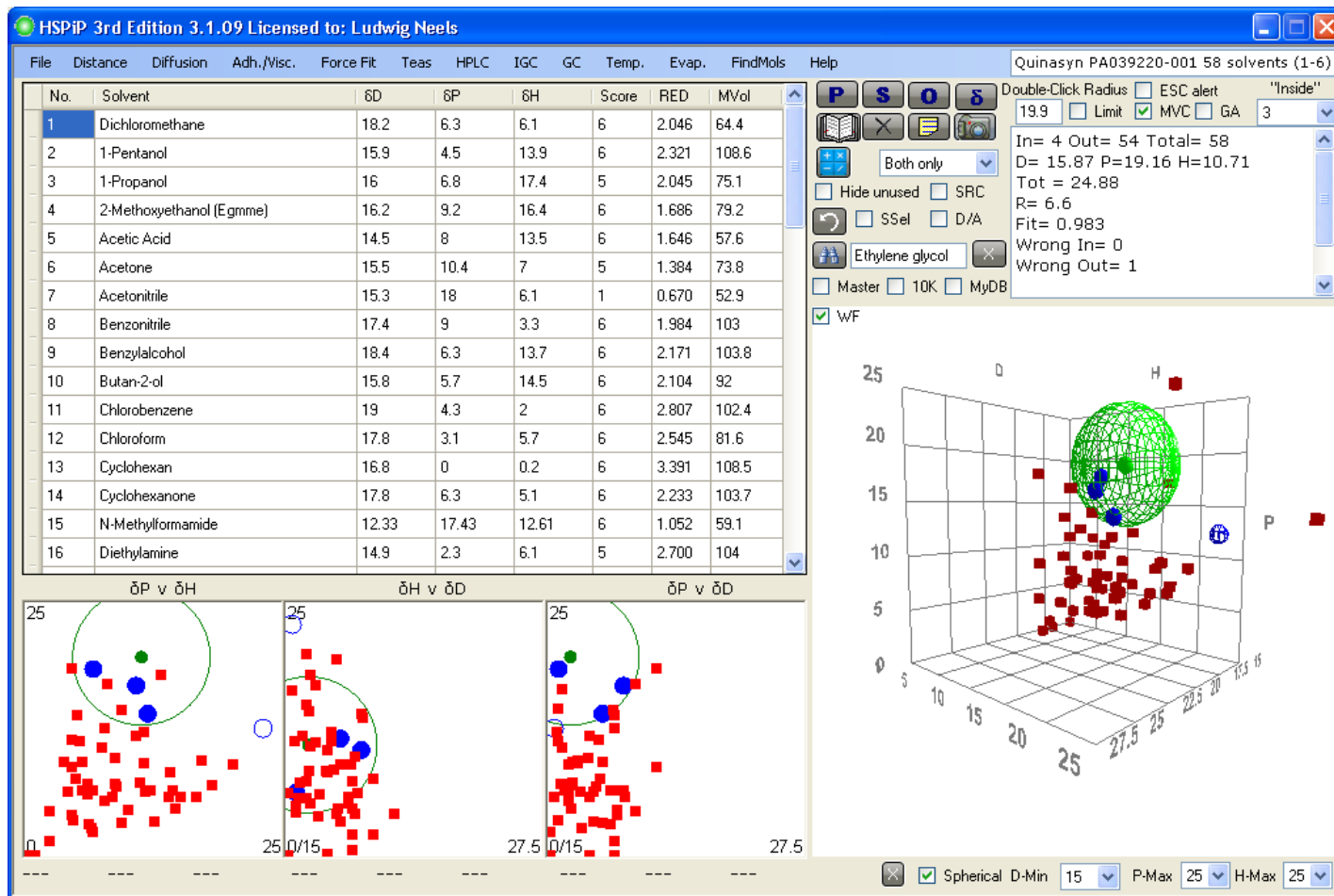


- Solubility sphere of a polymer : CAB



Hansen solubility parameters

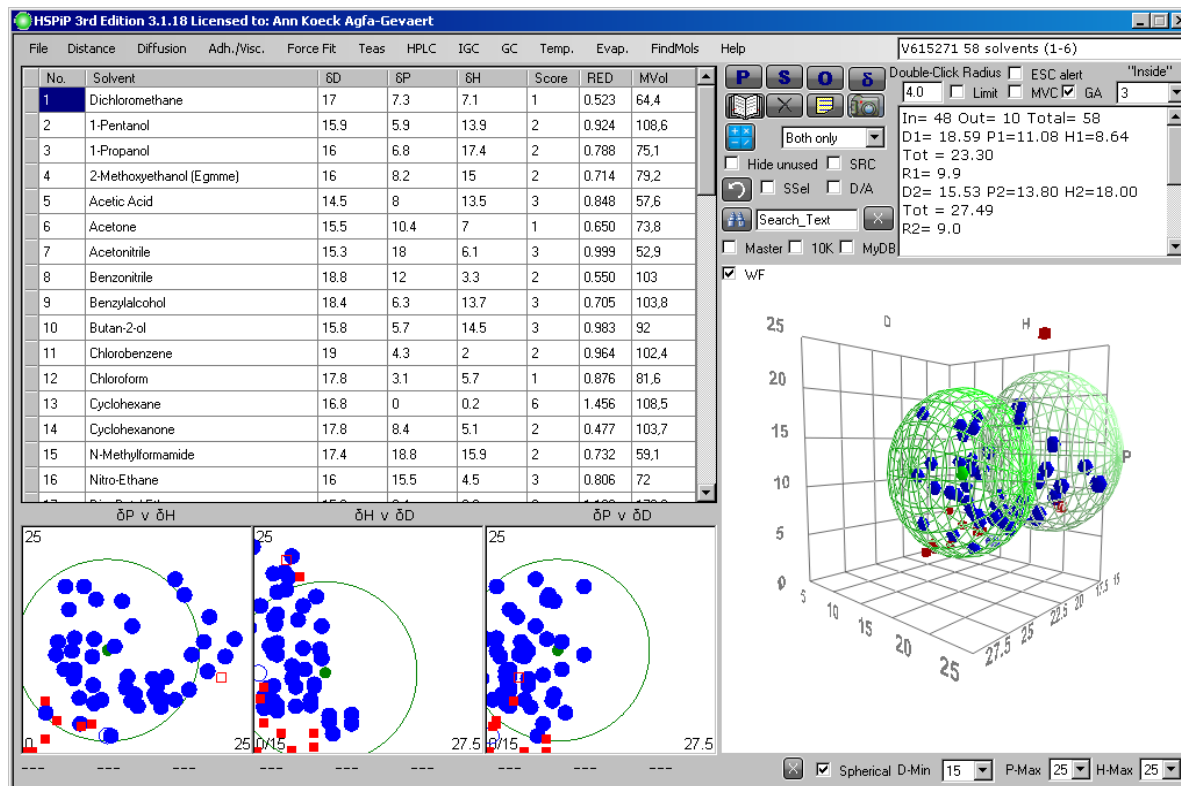
■ “Solubility” sphere of a pigment



Hansen solubility parameters



- Solubility sphere S for a dispersant
 - sphere 1 : $dD = 18.59$ / $dP = 11.08$ / $dH = 8.64$ ($R = 9.9$)
 - sphere 2 : $dD = 15.53$ / $dP = 13.80$ / $dH = 18.00$ ($R = 9.0$)





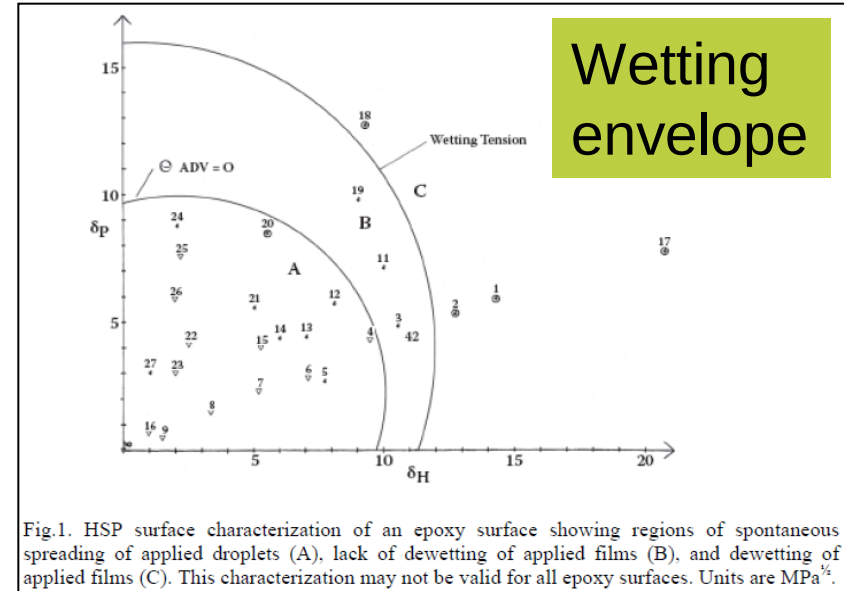
524 references in CAS



HSP aid in coating technology

■ when wet :

- Dispersion stability (23 cit)
- Thinners
- Wetting of substrate
- Solvent evaporation
- Cross-linking
- Skin formation
- Stratification
- Diffusion

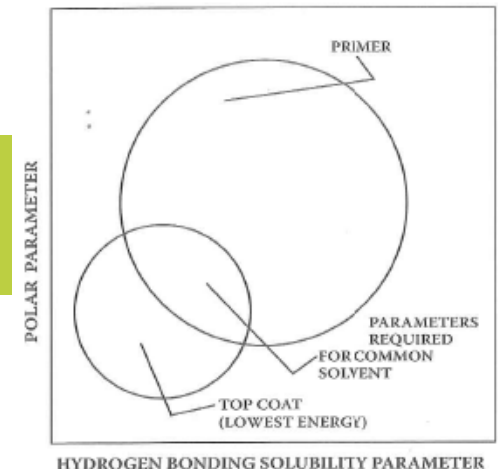


■ When dry

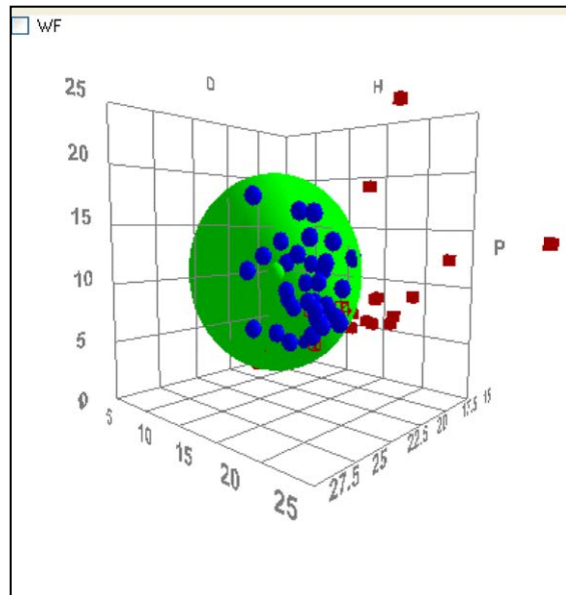
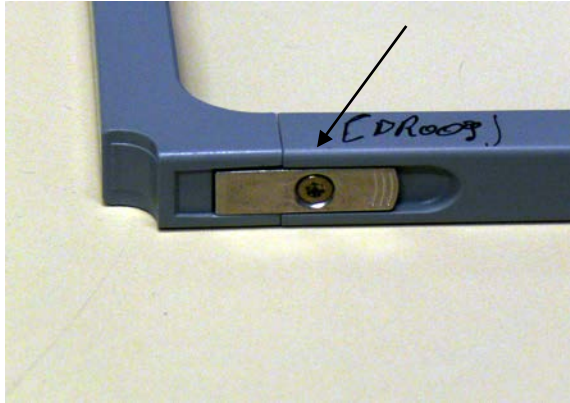
- Mechanical strength
- Chemical resistance (15 cit)
- Adhesion to substrate
- Crazing
- swelling
- Gas permeability
- Paint stripping

Self-stratifying
coating system

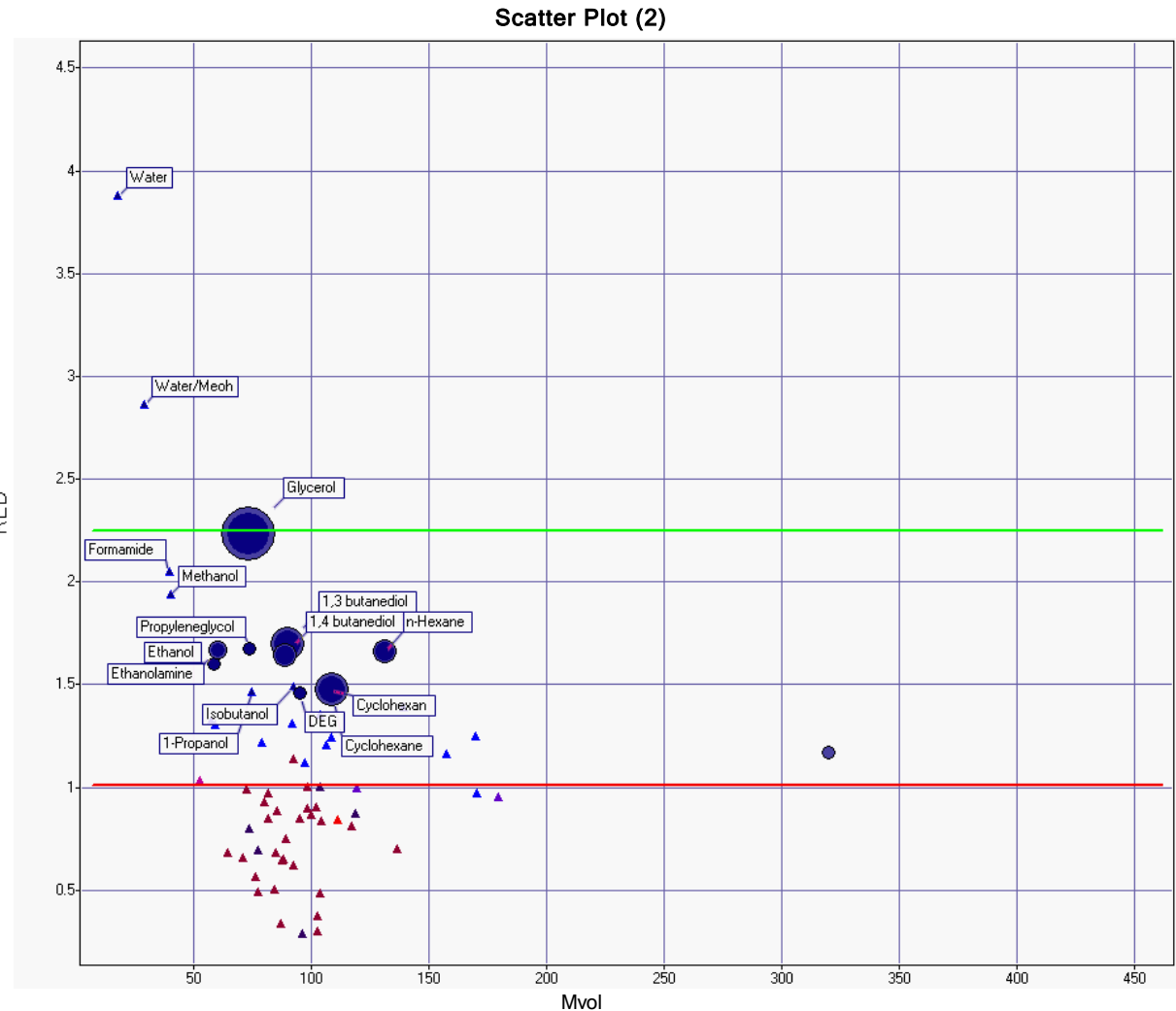
:



HSP aid in Environmental stress cracking and chemical resistance



Hansen sphere for
ABS



HSP aid in “green” Designer Solvents



- Cleaning of soils
- Safety and toxicity
- Biodegradable
- Ionic liquids
- Supercritical CO₂
- Subcritical fluid extraction (food)
- Skin protection
- Toner print removal
- Fatty acid Me-esters (FAME's)

Reference soil materials

Soil	#	δ Dispersion MPa ^{1/2}	δ Polar MPa ^{1/2}	δ Hydrogen Bonding MPa ^{1/2}	Molecular Model Image
ASTM Fuel "A"	1	14.3	0	0	
Butyl Stearate	2	12.6	6.3	6.1	
Castor Oil ²⁷	3	13.6	6.0	10.5	
Ethyl Cinnamate	4	16.0	10.8	7.5	
Linseed Oil	5	13.5	3.5	3.7	
Tricresyl Phosphate	6	15.9	13.9	13.5	

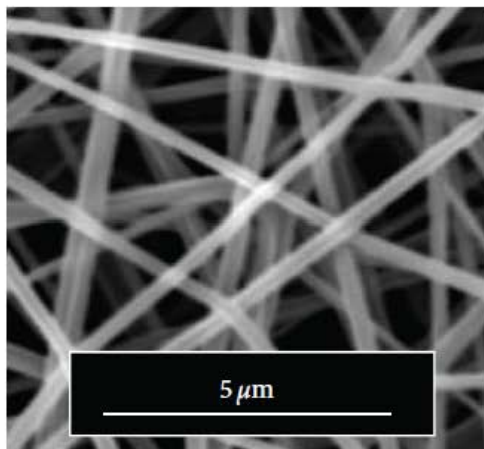
Controlled Morphology of Porous Polyvinyl Butyral Nanofibers

Daniela Lubasova and Lenka Martinova

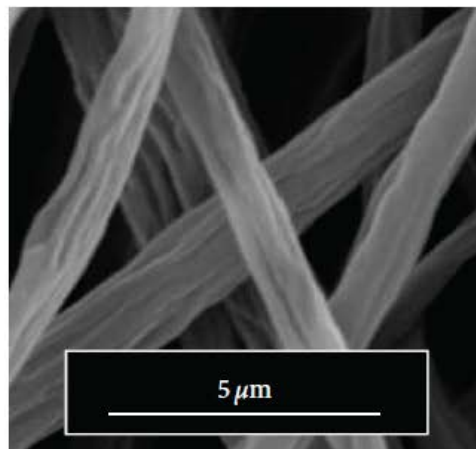
Department of Nonwovens, Technical University of Liberec, 46117 Liberec, Czech Republic

Correspondence should be addressed to Daniela Lubasova, daniela.lubasova@tul.cz

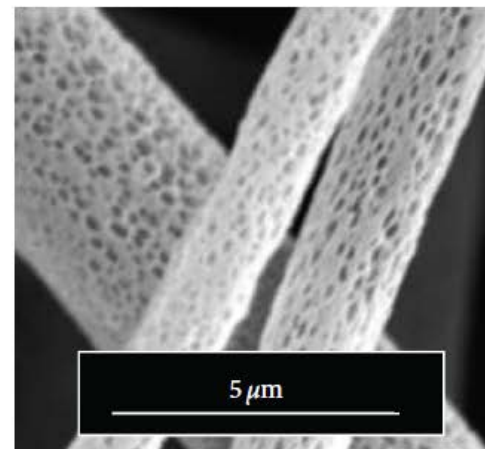
Received 12 August 2010; Revised 3 December 2010; Accepted 17 January 2011



(a)



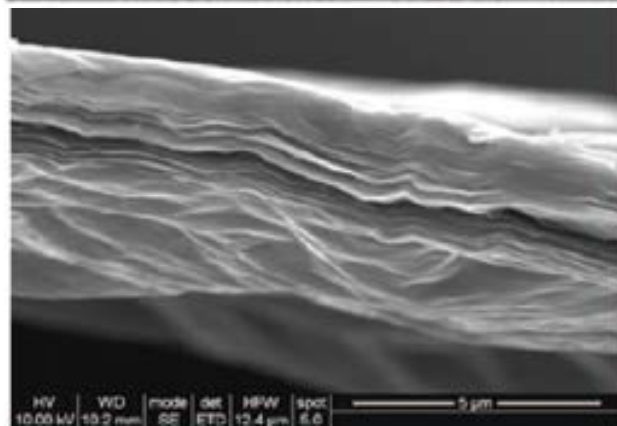
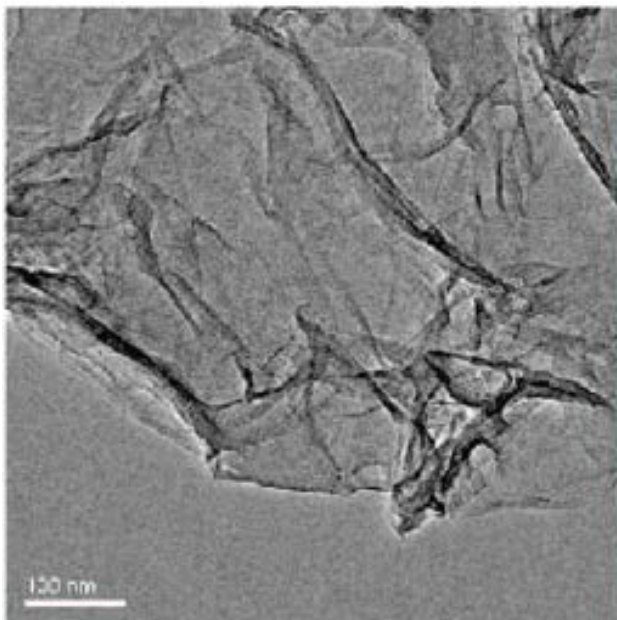
(b)



(c)

FIGURE 4: SEM images of PVB nanofibers prepared from 10 wt.% polymer solution from the mixtures: (a) ethanol/methanol (9/1 v/v), (b) ethanol/DMSO (9/1 v/v), (c) THF/DMSO (9/1 v/v).

HSP aid in nanotechnology

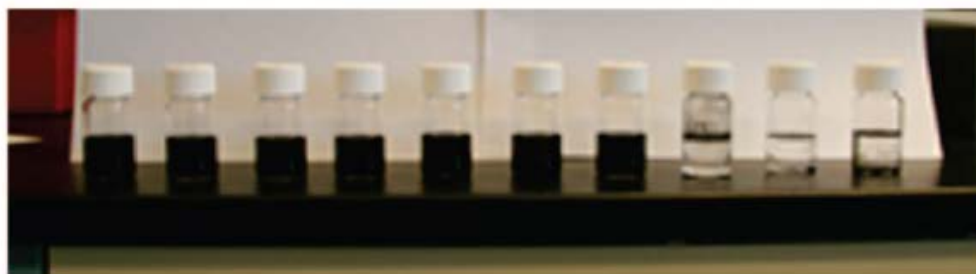


Colloidal Suspensions of Highly Reduced Graphene Oxide in a Wide Variety of Organic Solvents

Sungjin Park, Jinho An, Inhwa Jung, Richard D. Piner, Sung Jin An, Xuesong Li, Aruna Velamakanni, and Rodney S. Ruoff*

Department of Mechanical Engineering and the Texas Materials Institute, The University of Texas at Austin, One University Station C2200, Austin, Texas, 78712-0292

Received December 16, 2008; Revised Manuscript Received February 3, 2009

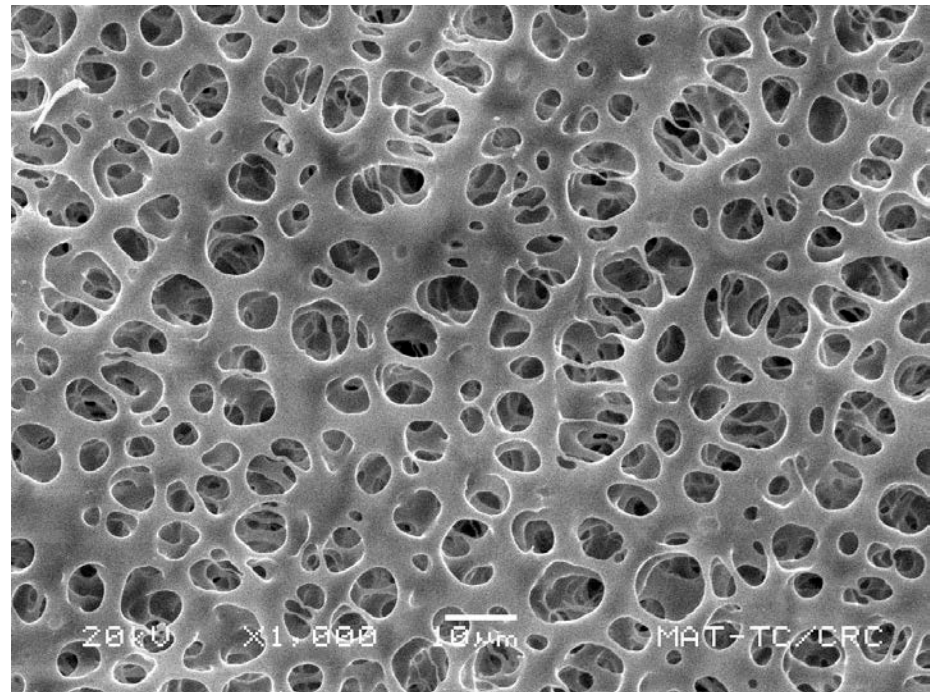


Colloidal suspensions of HRG sheets in various organic solvents, Volume ratio of added solvents:DMF:H₂O = 90:9:1, Added solvents from left: DMF, ethanol, acetone, THF, DMSO, NMP, acetonitrile, DCB, diethylether, and toluene

HSP aid in Barrier layers and Membranes



- Renewable barrier film design based on wood hydrolysate
- Gas separation
- Pervaporation membranes for separation of solvents (28 cit.)
- Permeability of membranes
- Phase diagrams
- Anti-biofouling
- Resist layers
- Pesticide
- Fire retardants
- Skin protection
- H-storage



HSP aid in Pharmaceutical

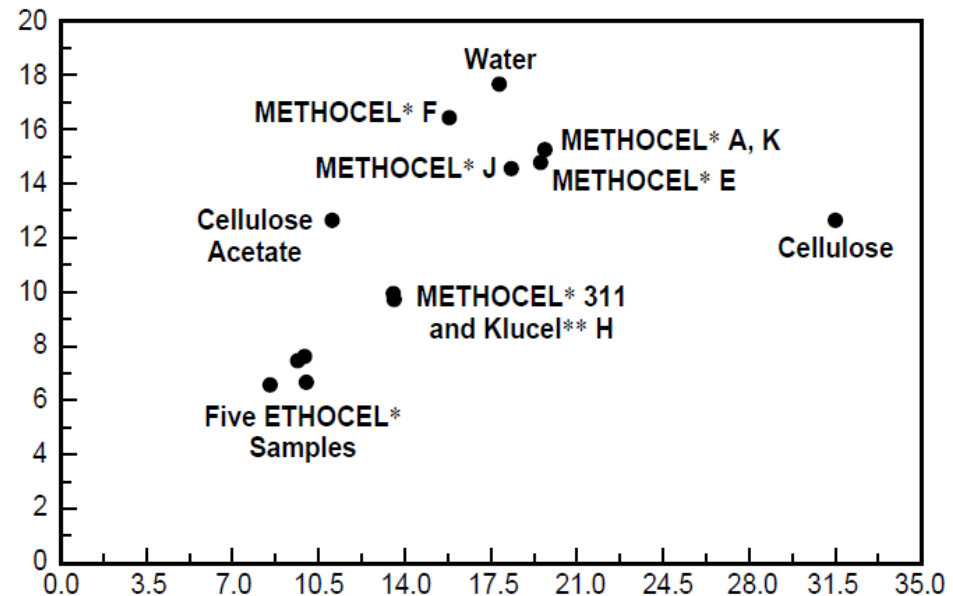


- Controlled drug release
- Drug solubility in rats
- Hot melt extruded drug delivery
- Drug distribution in microsphere
- Co-crystallization
- Adsorption of cytotoxic drugs to nucleic acids
- Nucleic acid hybridisation in polar aprotic solvents
- Adsorption of proteins to polymers
- Bootstrap statistics
- Enzymology
- Extraction of bioactive components



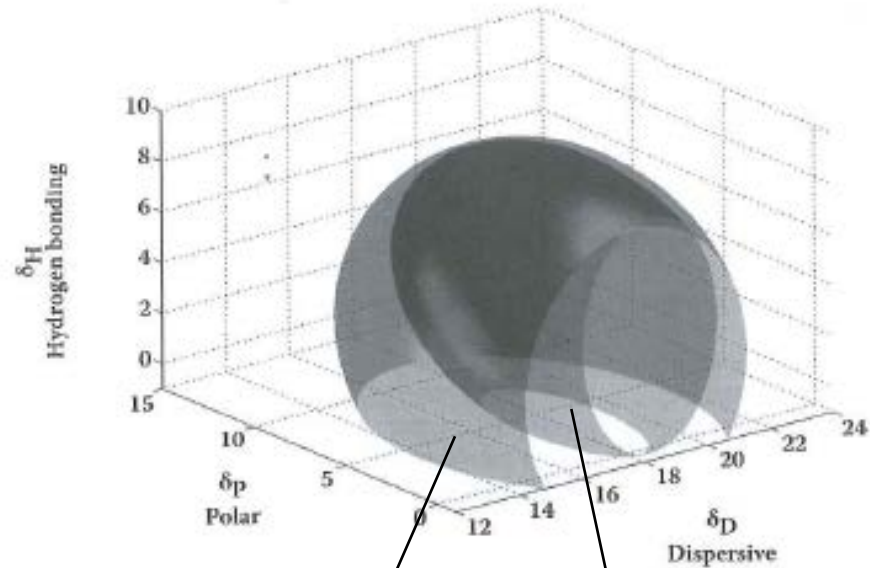
Hansen Solubility Parameters for Selected Cellulose Ether Derivatives and Their Use in the Pharmaceutical Industry

Figure 3 – Hansen Solubility Parameters for Cellulose Derivatives



HSP aid in Petrochemistry

- Asphaltene aggregation
- Bitumen
- Asphalt
- Crude oils
- Coal tar pit extraction
- Oil recovery
- Breaking heavy fuel
- Solute partition coefficients between polyolefins



Solubility sphere for
light crude North Sea
oil

Solubility sphere for
heavy Venezuelan crude
oil

HSP aid in Biological materials



- Cellulose
- Lignine
- Cholesterol
- Blood serum

Important source for
biobased aromatic
building blocks

- Fat
- DNA
- Skin

SOLUBILITY PARAMETER PLOT
FOR SKIN PERMEATION RATE

- Poly-L-lactine
- Hop
- Extraction bioactive components
- enzymology

	δ_D	δ_P	δ_H	M_V	PERMEATION RATE
DMSO	18.4	16.4	10.2	71.3	● HIGH
DMF	17.4	16.7	11.3	77.0	
DMAC	16.8	11.5	10.2	92.5	
NMP	18.0	12.3	7.2	96.5	
MCL	18.2	6.3	6.1	63.9	○ MODERATE
MEK	16.0	9.0	5.1	90.1	
ETH	15.8	8.8	19.4	58.5	
BAC	15.8	3.7	6.3	132.5	✕ LOW
PPC	20.0	18.0	4.1	85.0	
TOL	18.0	1.4	2.0	106.8	
BTA	19.0	16.6	7.4	76.8	
SUL	18.4	16.6	7.4	95.3	
OAC	15.8	2.9	5.1	196.0	⊕ "0"

HSP in plastic processing



- Vulcanised NBR-rubber
- Composites with plasticizers
- Composite polymer blends
- Composites with fillers
- CAB, SBS, ABS, BR, CA, polyimide (19 cit)
- Precipitation polymerization (7 cit)
- Biopolymers
- Recycling plastics

And so many other applications...



HSP in Textiles

- Treating stained fabrics
- SFE surfactants on nylon
- Adsorption of colorants to fibers
- Whitening agents for cellulose

■ HSP in cosmetics

- HSP of skin
- Coloring of keratin fibres (hair)
- Eye make-up removal

■ HSP in Graphics

- Ink Jet
- Flexography
- Paper industry
- Adhesives for low SFE surfaces

■ HSP in electronics

- Organic semiconductors
- Alternative etching liquids for semi-conductors
- Nano-lithography
- Laminating resist layers
- Conductive inks

■ HSP in energy

- Liquifaction of PS in fuel
- OPV (thiophene in acetophenone & mesitylene)
- H-storage materials
- Organic conductive coatings

HSP aid in Aromas and fragrances



- Hiroshi Yamamoto

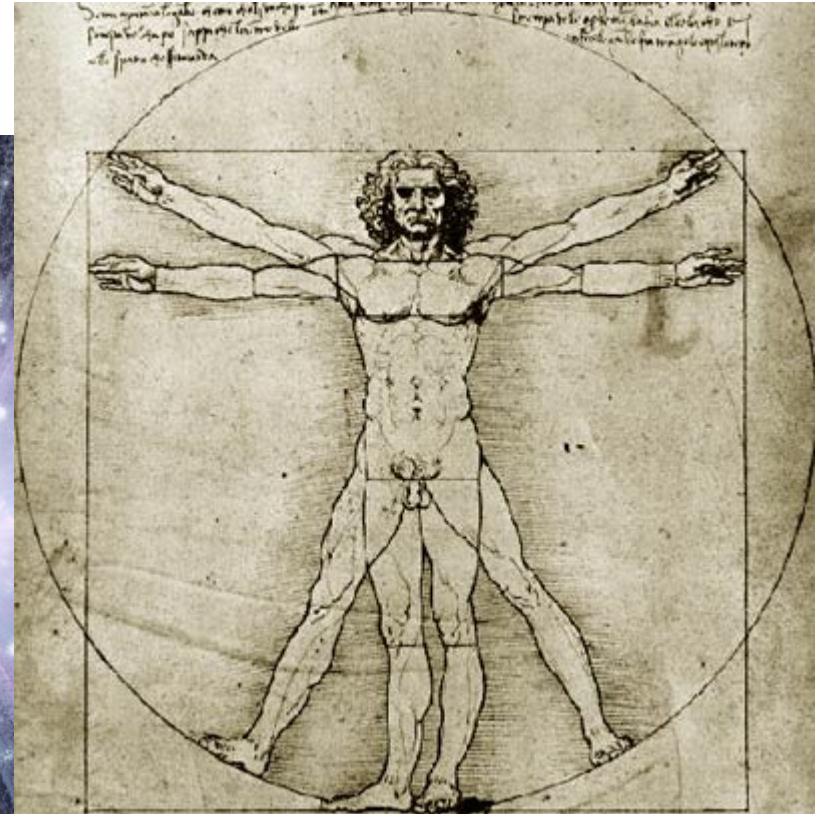


- HSP of natural herbs
- Offensive odor
- Hot and spicy
- Allergens for cosmetics

- 20 polymer sensored electronic nose
- Sensates in edible, oral, throat, skin, hair : menthanes = “fresh”
- Dispersion in air by aminoacids (aerosol)

Hansen solubility parameters

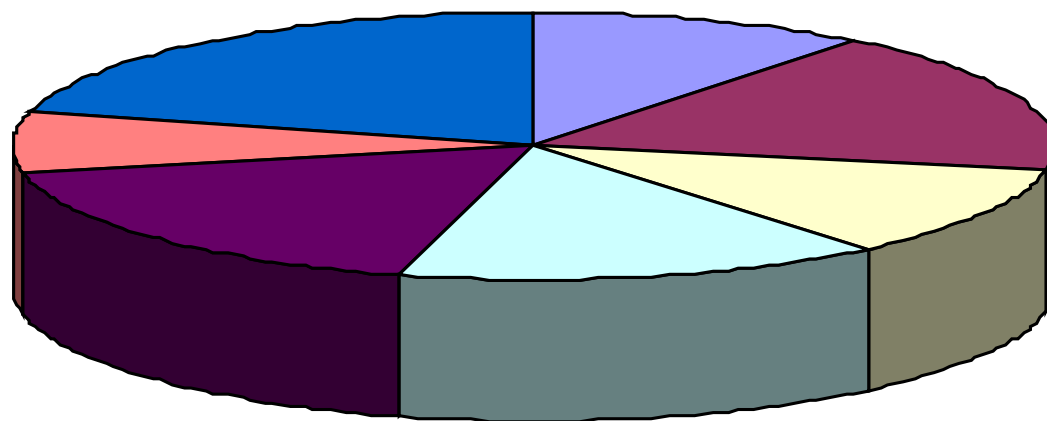
- The Grand Unification Theory?



Hansen solubility parameters



Number of references out of 524 CAS articles



- green solvents
- polymer processing
- membranes
- nanotechnology
- pharmaceutical
- petrochemistry
- coatings

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A close-up photograph of a hand holding a small, dark, irregular object. The hand is positioned on the right side of the frame, with the thumb and index finger gripping the object. The object is dark and has a rough, textured surface. The background is a solid, light blue color. The text "Keen to innovate" is overlaid on the bottom left of the image.

Keen to innovate

Agfa-Labs: Where we are...



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