Hansen Solubility Parameters

F. Ruttens

Efficient and faster time-to-market
Extend your Reach
Advanced Chemical and Physical Analytics
Joint Development Projects
Molecular Ingredients
- Sourcing, design and synthesis
  - Functional polymers
  - Dispersants
  - Dyes
  - Pigments
  - Functional ingredients
- Structure – activity relation

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

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

Reaction calorimetry
Security
REACH
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
- Hansen Solubility Parameters
- High Throughput Analysis
- Miscellanea
Hansen Solubility Theory
Hildebrand solubility parameter $\delta$

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

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

- Cohesive energy density
- Energy of evaporation
- Molar volume
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 (δD, δP, δH)
  - Sphere of solubility

![3D representation of Hansen solubility parameters](image)
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 spheres** for a dispersant
  - sphere 1: $d_D = 18.59 / d_P = 11.08 / d_H = 8.64$ (R = 9.9)
  - sphere 2: $d_D = 15.53 / d_P = 13.80 / d_H = 18.00$ (R = 9.0)
Literature screening

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

Fig. 1. HSP surface characterization of an epoxy surface showing regions of spontaneous spreading of applied droplets (A), lack of dewetting of applied films (B), and dewetting of applied films (C). This characterization may not be valid for all epoxy surfaces. Units are MPa.

Self-stratifying coating system:

Wetting envelope
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)
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

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).
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:H$_2$O = 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 microspheres
- 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
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
Important source for biobased aromatic building blocks
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 semiconductors
  - 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 sensor 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

www.hansen-solubility.com
www.agfa-labs.com
Agfa-Labs: contact us

Keen to innovate
Agfa-Labs: Where we are...

- **Mail:**
  Agfa-Labs
  Customer Service (3190)
  Agfa-Gevaert NV
  Septestraat 27
  2640 Mortsel /Belgium

- **Web:** [www.agfa-labs.com](http://www.agfa-labs.com)
- **E-mail:** info@agfa-labs.com
- **Phone:** +32 (0)3 444 3190
- **Fax:** +32 (0)3 444 3299