The use of Hansen Solubility Parameters (HSP) in the development of inkjet inks

Els Mannekens

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The Inkjet Conference
Inkjet Engineering & Inkjet Chemistry
24-25 Oct 2017, Neuss/Düsseldorf, Germany
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Chemstream: The Chemical R&D Company

Profile

- Founded in April 2010
- **Staff profile: 9 PhD's**
  - Chemistry
  - Material Science
  - Bio Engineer
- **Located near Antwerp – Belgium**
- **Lab-facilities (500 m2)**
  - Organic Synthesis
  - Chemical Formulation
  - Characterization



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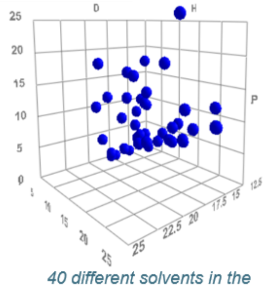
Hansen Solubility Parameters (HSP)

3 main numbers to capture **the solubility behaviour of a substance**:

- **δD – the Dispersion**, van der Waals properties of a molecule
- **δP – the Polar** contribution (related to dipole moment)
- **δH – the Hydrogen bonding** contribution

=> **3D Hansen solubility space**



40 different solvents in the 3D Hansen solubility space

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Hansen Solubility Parameters (HSP)

In relation to inkjet printing technology:

Sedimentation of pigments in ink carrier

Nano-dispersion stability

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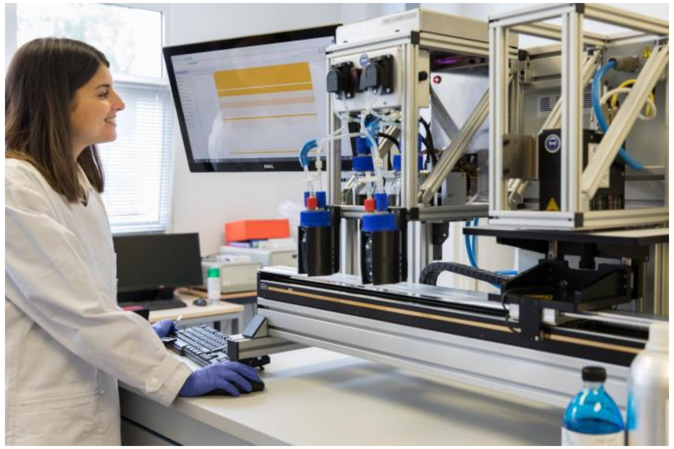

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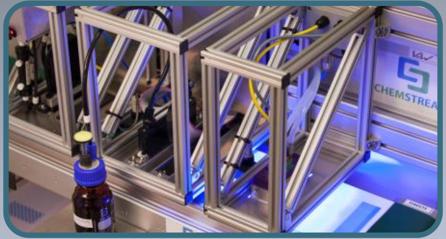
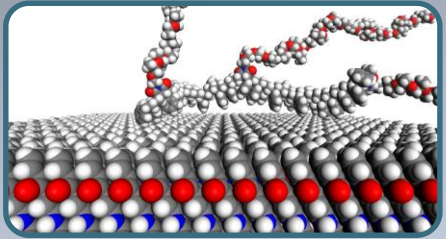
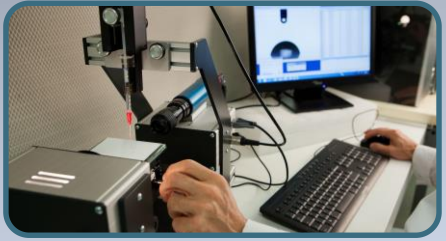
Chemstream: The Chemical R&D Company

Mission

To translate customer requirements into chemical formulations with dedicated functionalities, from **design to prototyping and implementation**







Organic Synthesis
* Crystal, colorant and dispersant design
* Photochemistry
* Interfacial chemistry, wetting and adhesion
* Superabsorbing polymers

Technology
* Dispersion technology
* Coating, printing, jetting (Modular printing unit MPU)
* Radiation curing (UV, UV-LED, e-Beam)
*Atmospheric plasma

Methodology
* Molecular Modeling
* Design of Experiment (D.O.E.)
* High throughput screeining
* Hansen solubility parameters (HSP)

Analytical and physical chemical tools
* UVVIS, FTIR, GCMS, LCMS, GPC
* Particle size distribution (PSD)
* Contact angle, surface tension, Viscosity

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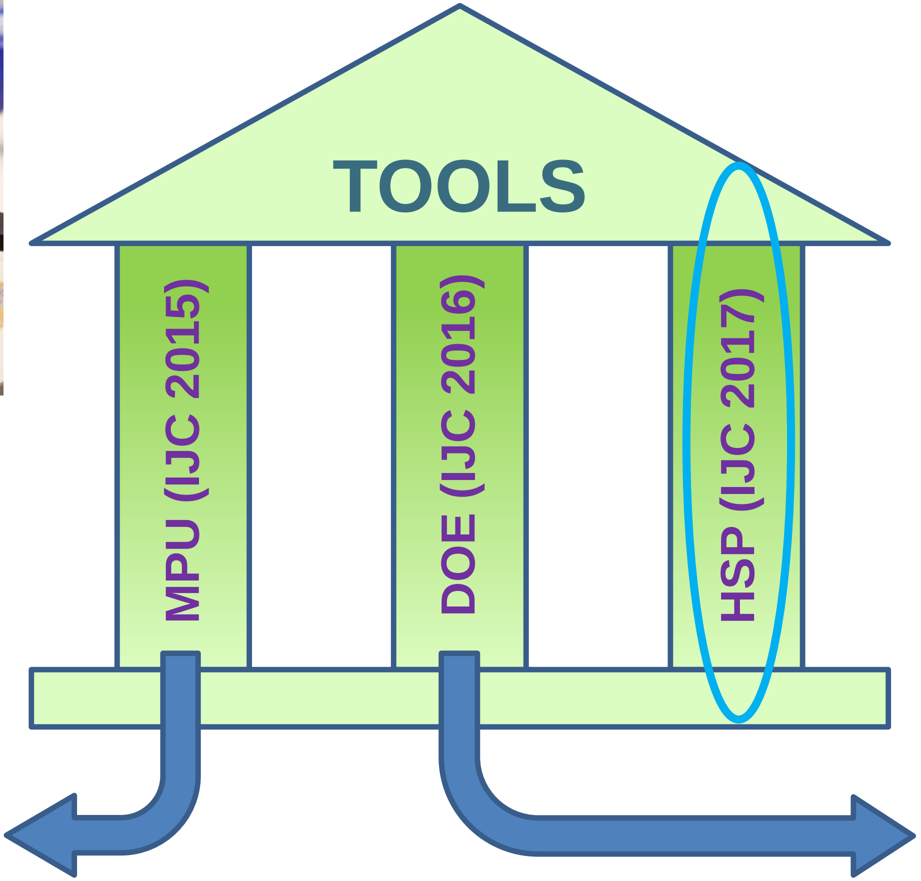
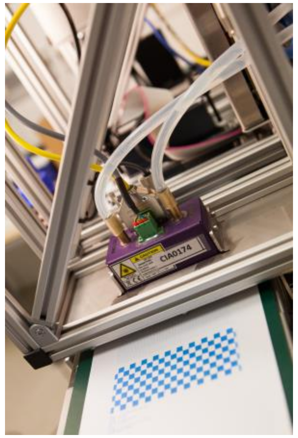
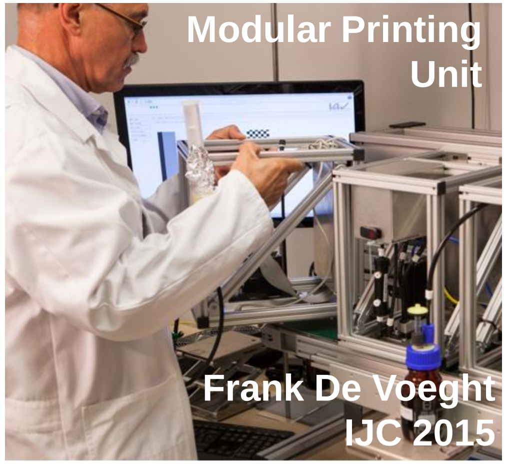
Ink development is a Dynamic Collaboration between R&D and Technology

Ink design (R&D)
Mechanical properties
Process characteristics
Colour (pigment / dye)
Hydrophobicity
Rheology
Legislation
...





Technology
Type of printhead
Resolution printhead
Printing speed
Belt speed
Curing method
…



Hansen Solubility Parameters (HSP)

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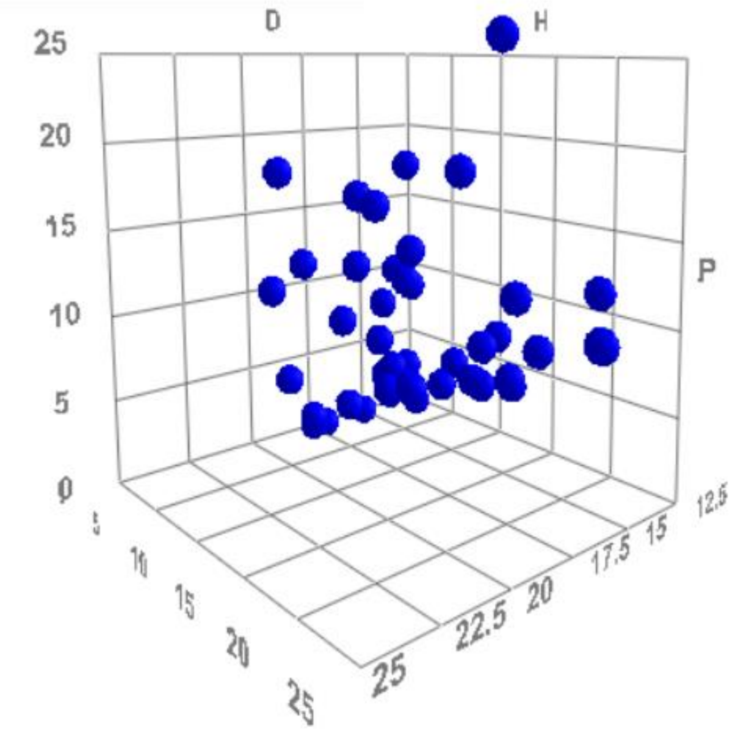
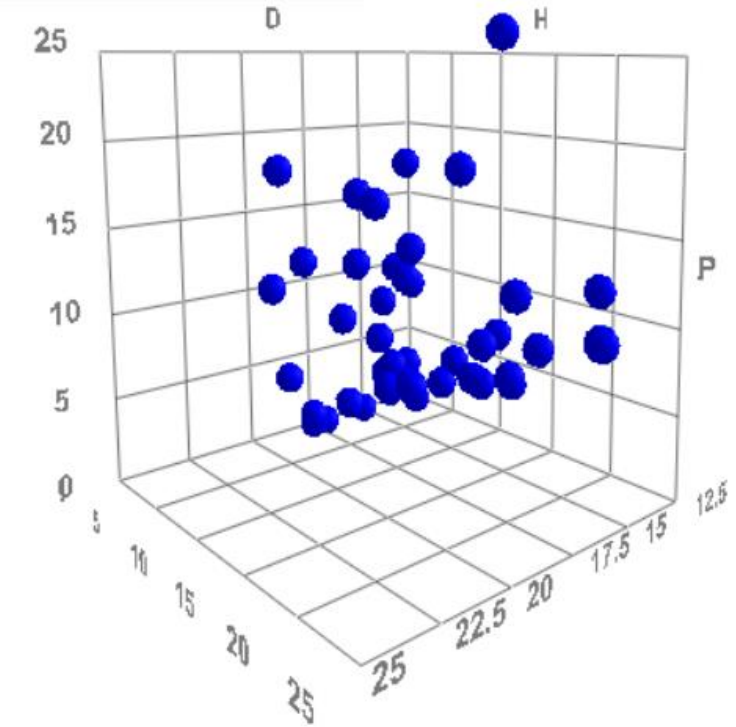
=> **3D Hansen solubility space**



40 different solvents in the 3D Hansen solubility space

Hansen Solubility Parameters (HSP)

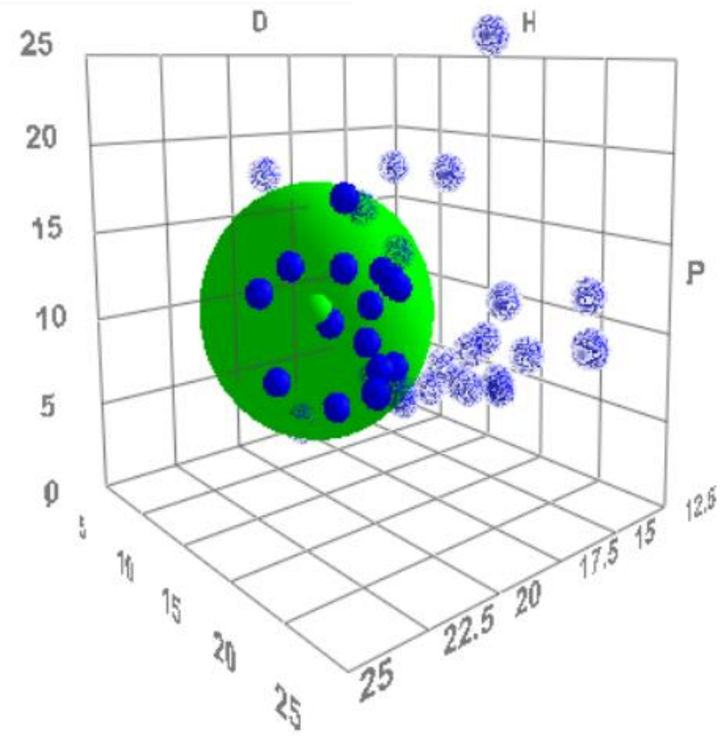
- **The closer the position** of compounds in the 3D solubility space, **the more 'alike'** they are.



40 different solvents in the 3D Hansen solubility space

Hansen Solubility Parameters (HSP)

- **The closer the position** of compounds in the 3D solubility space, **the more 'alike'** they are.
- Each molecule can be checked for its 'compatibility' using a selected set of solvents and obtains its own **solubility sphere**.
- **The radius** of the HSP sphere is **a measure of its 'solubility'** within the 3D solubility space.

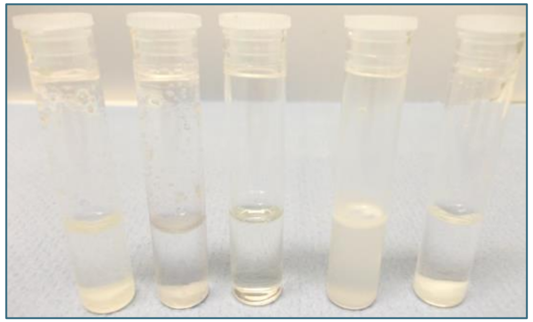


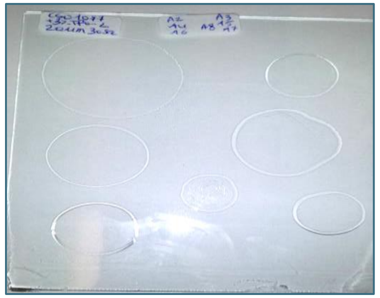
The Hansen solubility sphere of 1 molecule in the 3D Hansen solubility space

Hansen Solubility Parameters (HSP)

'Compatibility' or 'Solubility' are broad terms:

- **Dissolving** (of a powder/drug/compound in solvents)
- **Miscibility** (of solvents)
- **Sedimentation** (of a solid/pigment in solvents)
- **Diffusion/permeability** (of solvents through a polymer film, skin,…)
- **Swelling** (of polymers in solvents)
- **Attack** of a surface by solvents
- …





Hansen Solubility Parameters (HSP)

In relation to inkjet printing technology:

Sedimentation of pigments in ink carrier

- **Nano-dispersion stability**

Swelling/attack of polymers in ink carrier

- **Material compatibility**

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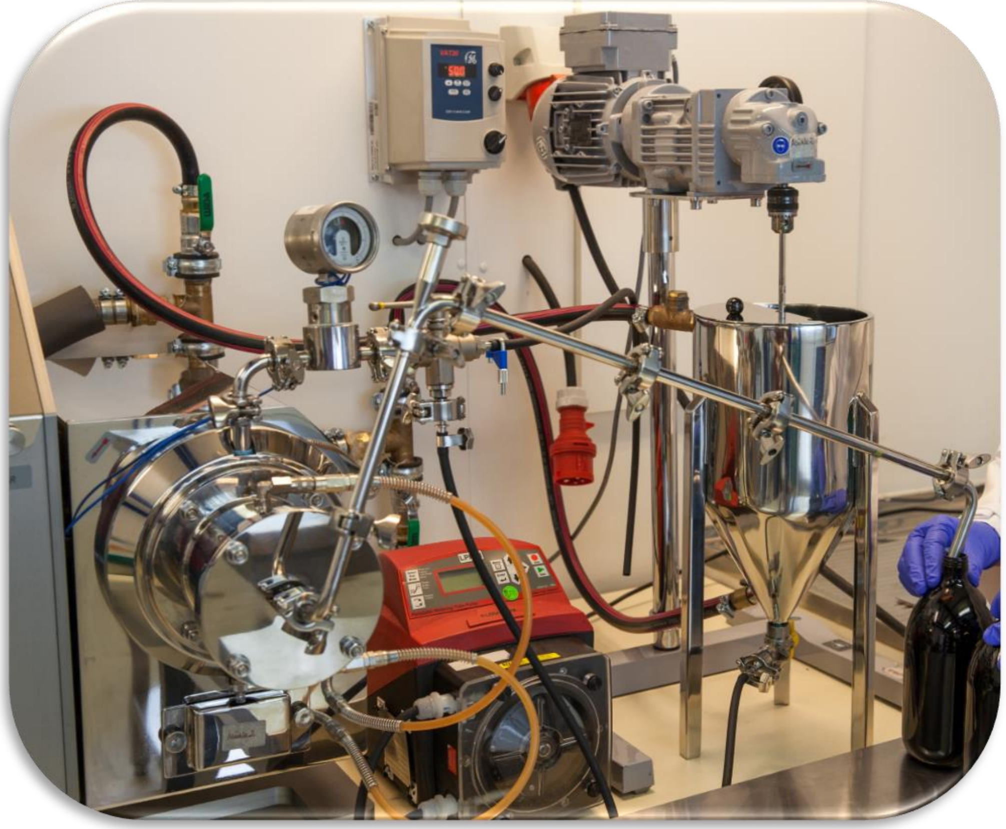
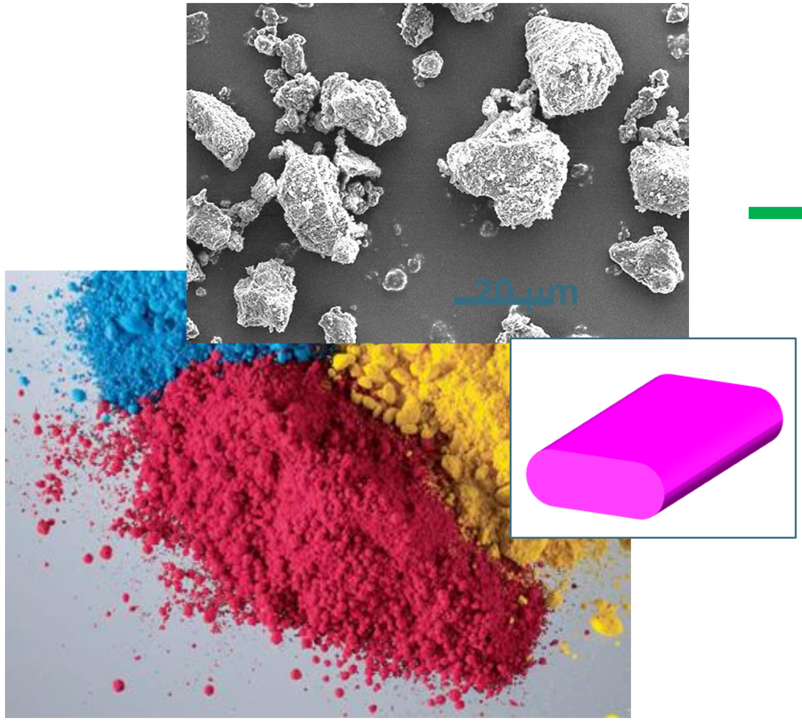
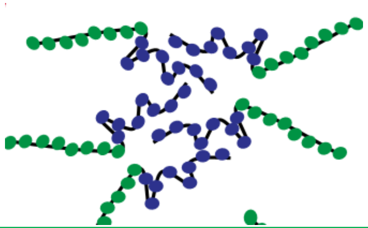


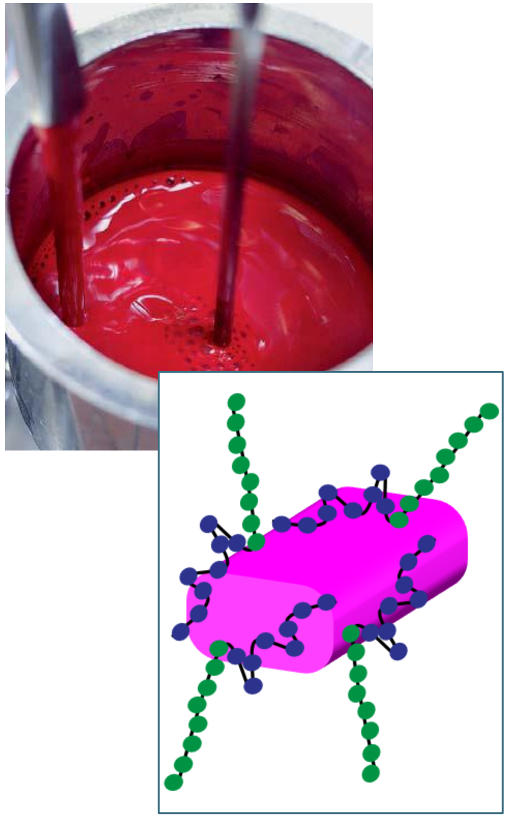
Nano-dispersion stability



Agglomerated pigment particles



Milling in ink carrier



Stabilized pigment nano-dispersion

Nano-dispersion stability

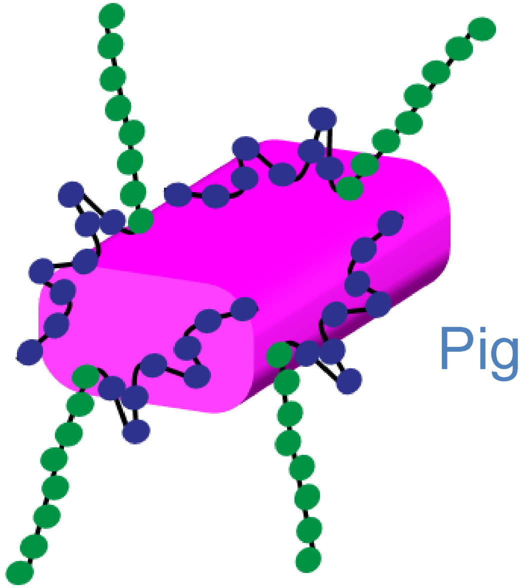
The surface of the pigment should be available for interaction with the pigment'ophilic part of the dispersing agent (anchoring).

FOR EXAMPLE:

UV-curable pigmented nano-dispersions

Matrix = UV-curable monomer

Pigment surface = more polar character



Steric stabilization

Nano-dispersion stability

Commercial pigments = very diverse!

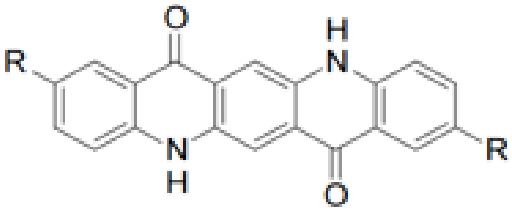
- different work-up processes after production
- different surface modifications of the pigments

=> Different surfaces for the same pigment types!

But: mostly, the details are not known.

FOR EXAMPLE:
Mixed crystal Magenta 'PV19/PR202'

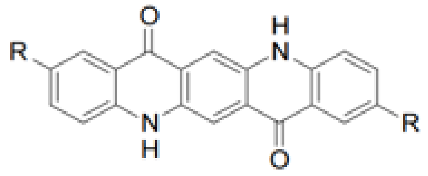
- **Quality A**
- **Quality B**
- **Quality C**



PV19 R = H
PR202 R = Cl

Studied with Hansen solubility parameters (HSP)

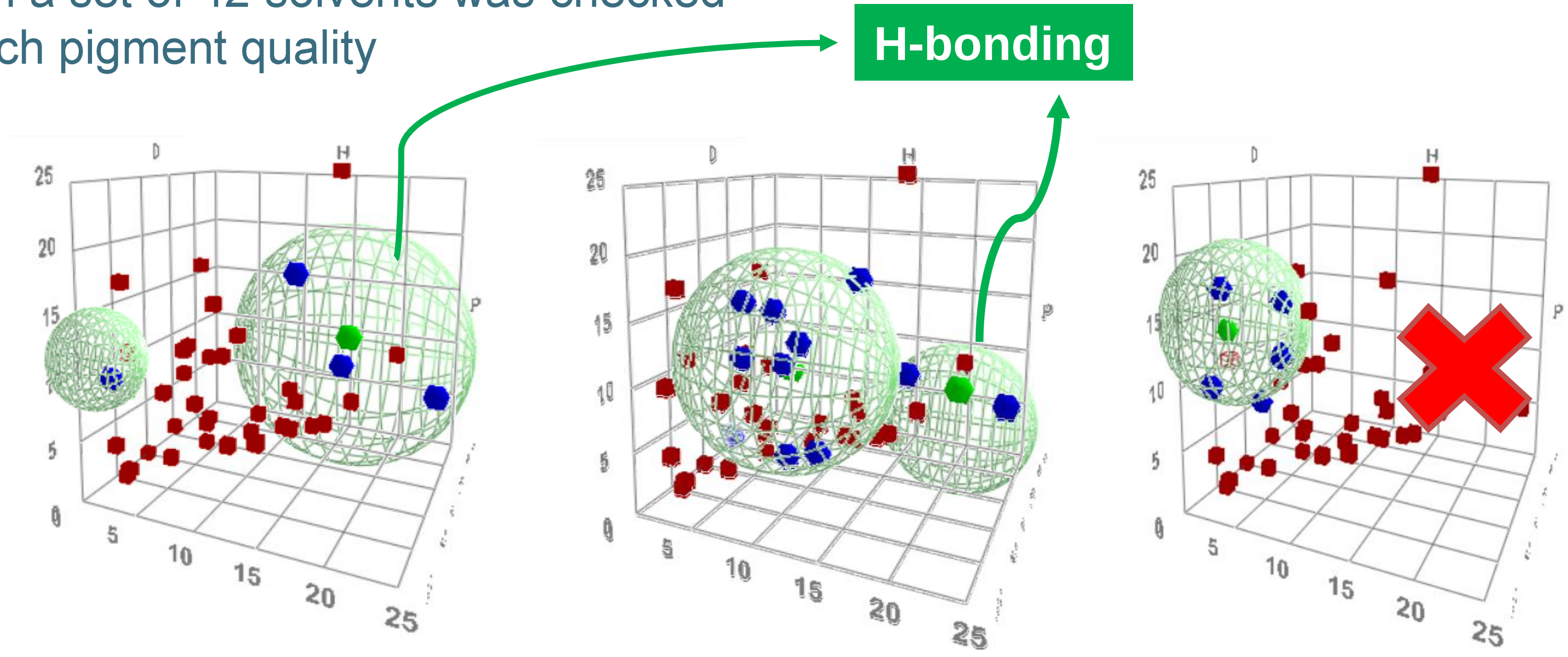
Nano-dispersion stability



PV19 R = H
PR202 R = Cl

Hansen solubility Parameters (HSP) study:
Mixed crystal Magenta 'PV19/PR202'

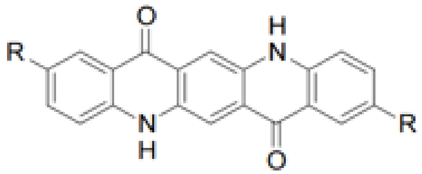
Sedimentation of pigments in a set of 42 solvents was checked
=> Solubility sphere(s) of each pigment quality



Quality A Quality B Quality C

=> Information about the pigment surface characteristics

Nano-dispersion stability



PV19 R = H
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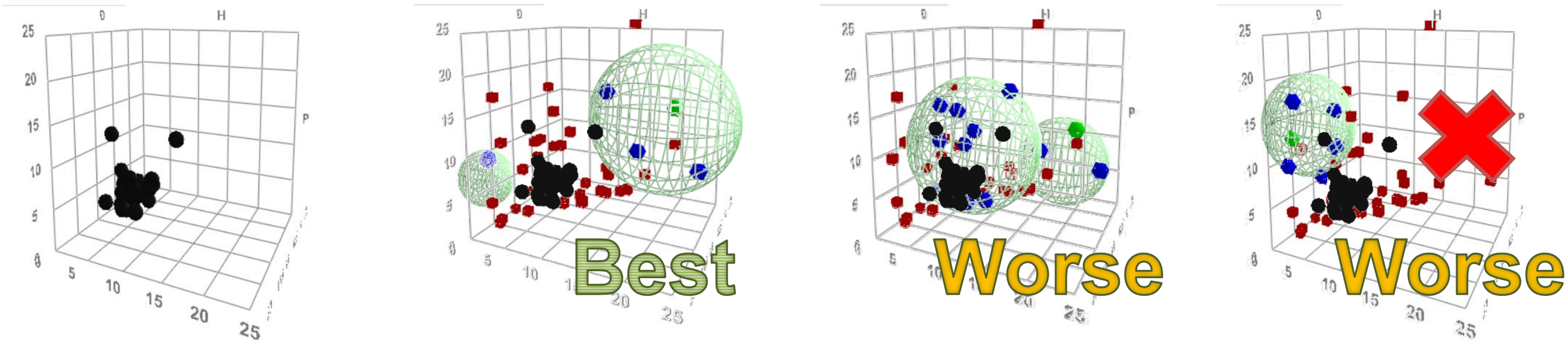
Hansen solubility Parameters (HSP) study:
Mixed crystal Magenta 'PV19/PR202'

Solubility sphere(s) of each pigment quality compared with the position of UV-curable monomers (= classic UV curable ink carrier) in the 3D solubility space



Quality A Quality B Quality C

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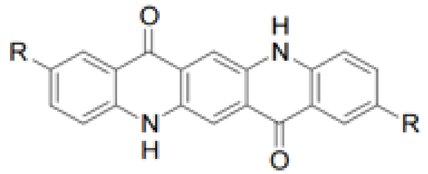
Nano-dispersion stability



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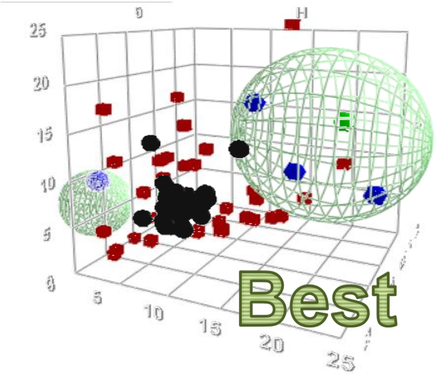
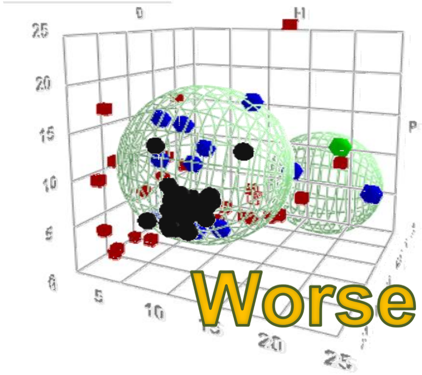
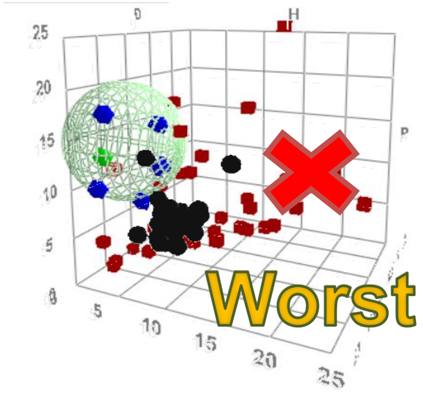
PR202 R = Cl

Hansen solubility Parameters (HSP) study:
Mixed crystal Magenta PV19/PR202







In Practice:

	Dispersions (10% pigment)	CSD01052	CSD01147	CSD001153
	pigment	Quality A	Quality B	Quality C
	physical appearance	liquid	liquid	thick paste
viscosity after filtration	mPa.s @ 25°C	84	105	unable to filter
viscosity after 7d 60°C	mPa.s @ 25°C	86	130	n.d.
viscosity in ink simulation (5% pigment)	fresh (mPa.s @ 25°C)	15,7	26,4	n.d.
	after stability test	17,6	62	n.d.
	% rise in visco	12	135	n.d.

Hansen Solubility Parameters (HSP)

In relation to inkjet printing technology:

Sedimentation of pigments in ink carrier

Nano-dispersion stability

Swelling/attack of polymers in ink carrier

Material compatibility

Hansen Solubility Parameters (HSP)

In relation to inkjet printing technology:

Swelling/attack of polymers in ink carrier

Material compatibility

Material compatibility

Can all materials (printhead, nozzle plate, tubings, etc.) withstand the jetting fluids ?

Material compatibility

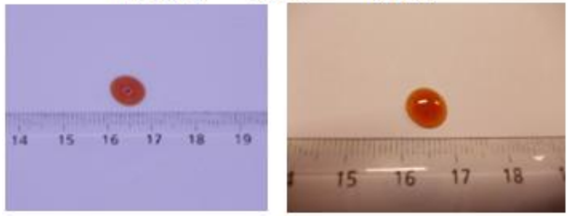
KM1024 compatibility set

Most printhead manufacturers foresee material compatibility tests

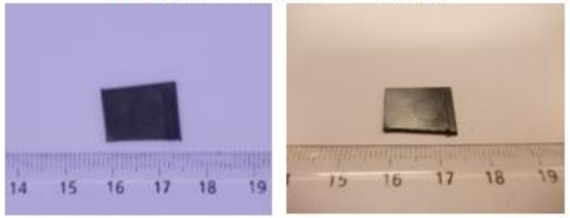
⇒ 'material compatibility kits' + detailed test procedures

- They contain some parts of printheads to test in the ink carrier
- Size and weight are measured before and after soaking

Before HA-2 After



Before HP-1 After



Printhead test SET KM1024	weight (g)	after 7d 60°C in ink carrier	difference in weight (%)
HA-1 Adhesive	0,0978	0,10846	10,9
HA-2 Adhesive	0,10999	0,1117	1,6
HA-3 Adhesive	0,09554	0,10565	10,6
HP-1 Nozzle Plate	0,01918	0,01905	-0,7
HP-2 Head Cover	0,31924	0,32026	0,3
HP-3 Manifold	0,30526	0,30545	0,1

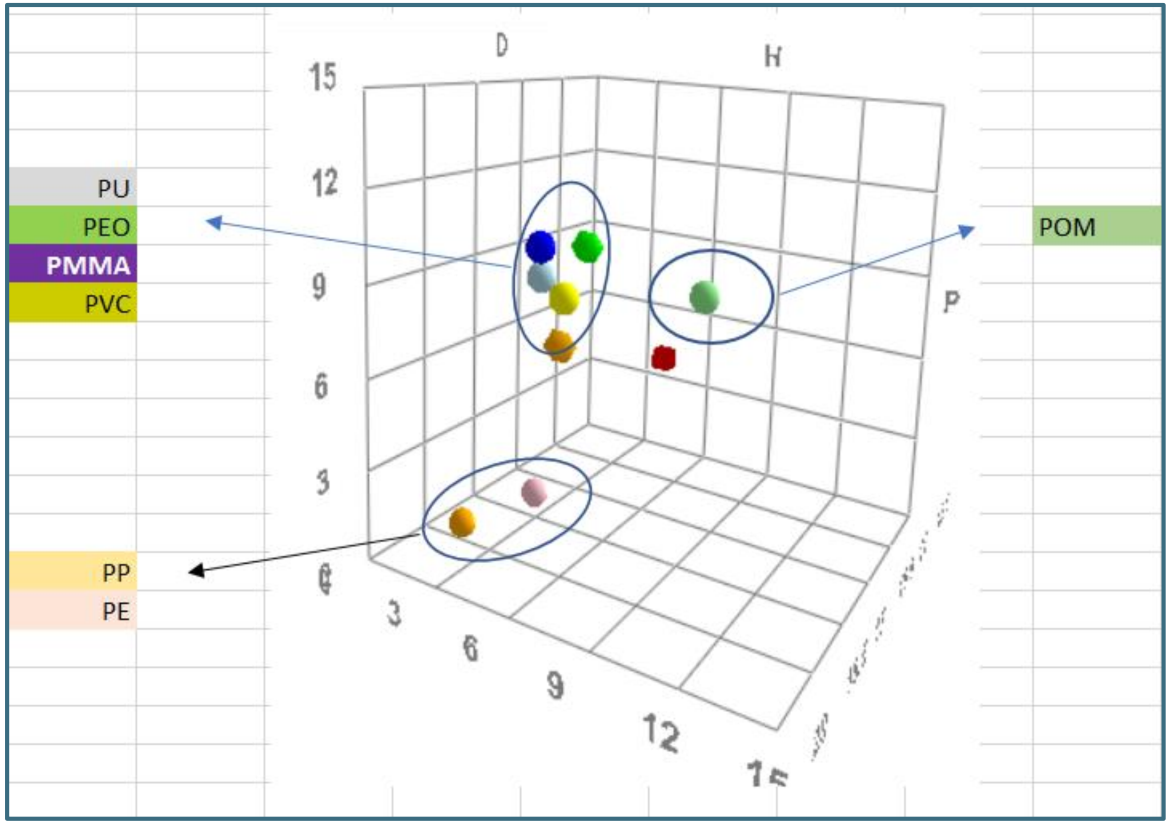
If one knows the nature of those materials => *HSP study can help upfront*

Material compatibility

Hansen solubility Parameters (HSP) study:

Selection of polymers

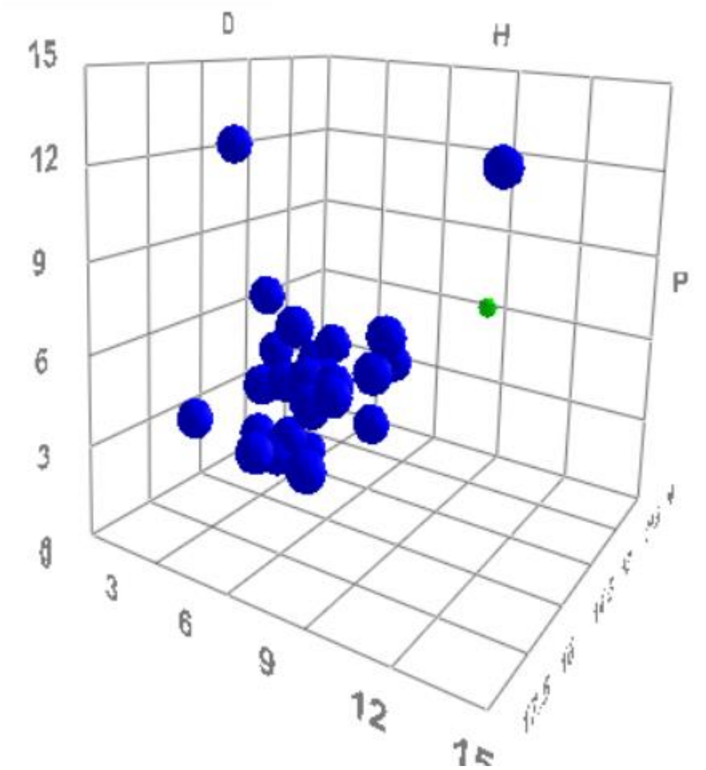
Polymer	dD	dP	dH
Polypropylene (PP)	18	0	1
Polyethylene (PE)	16,9	0,8	2,8
Polyurethane (PU)	18,1	9,3	4,5
Polyethylene oxide (PEO, PEG)	17	10	5
Polymethylmethacrylate (PMMA)	18,6	10,5	5,1
Polyvinylchloride (PVC)	18,8	9,2	6,3
Polyoxymethylene (POM)	17,2	9,2	9,8



Material compatibility

Hansen solubility Parameters (HSP) study:

Selection of 29 commonly used UV-curable monomers



29 different UV-curable monomers in the 3D Hansen solubility space

Material compatibility

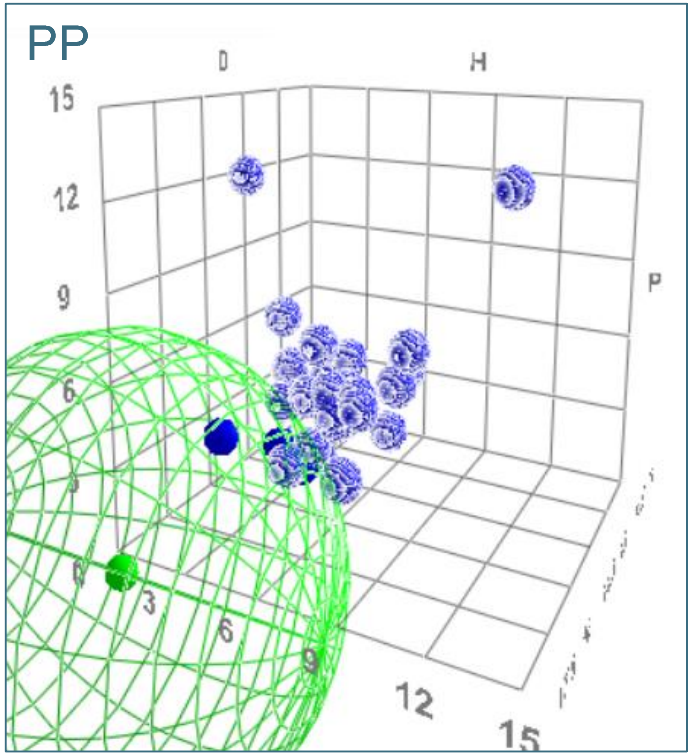
Hansen solubility Parameters (HSP) study:

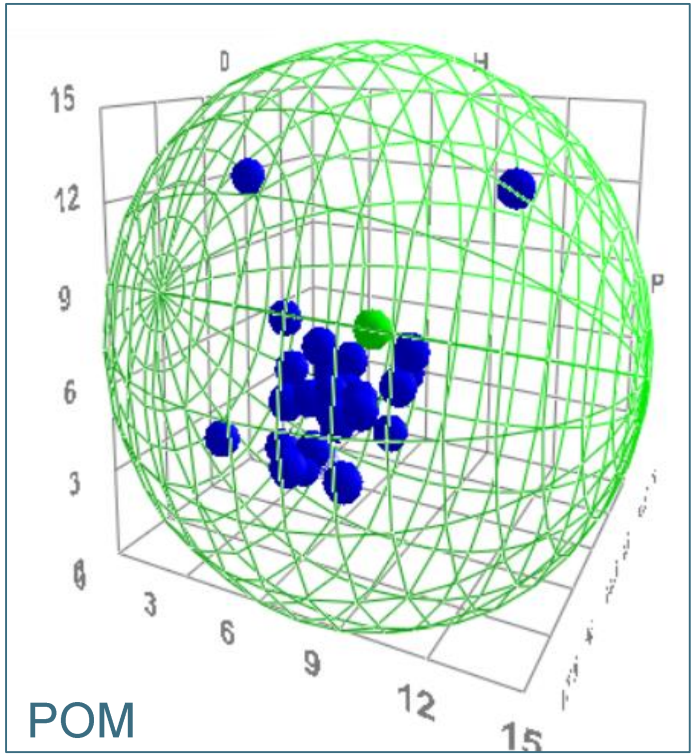
PP and POM in UV curable monomers

Polymer	dD	dP	dH
Polypropylene (PP)	18	0	1
Polyoxymethylene (POM)	17,2	9,2	9,8

PP: very little overlap => very resistant to UV-curable monomers in general

POM: all UV-curable monomers fall into its solubility sphere => not resistant !





Material compatibility

Hansen solubility Parameters (HSP) study:

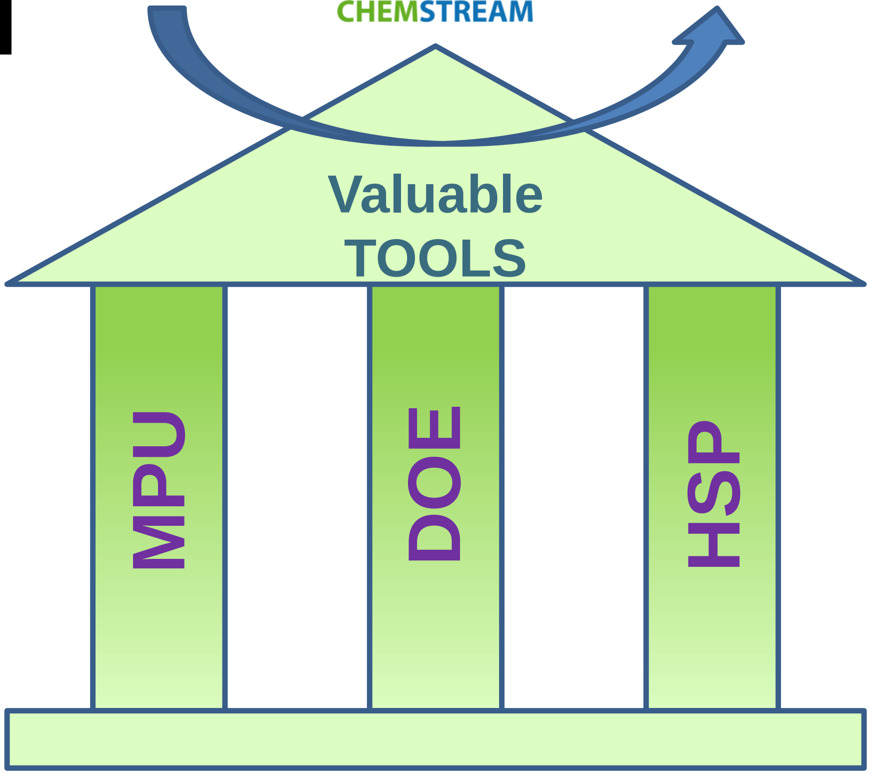
Similar studies can be done for

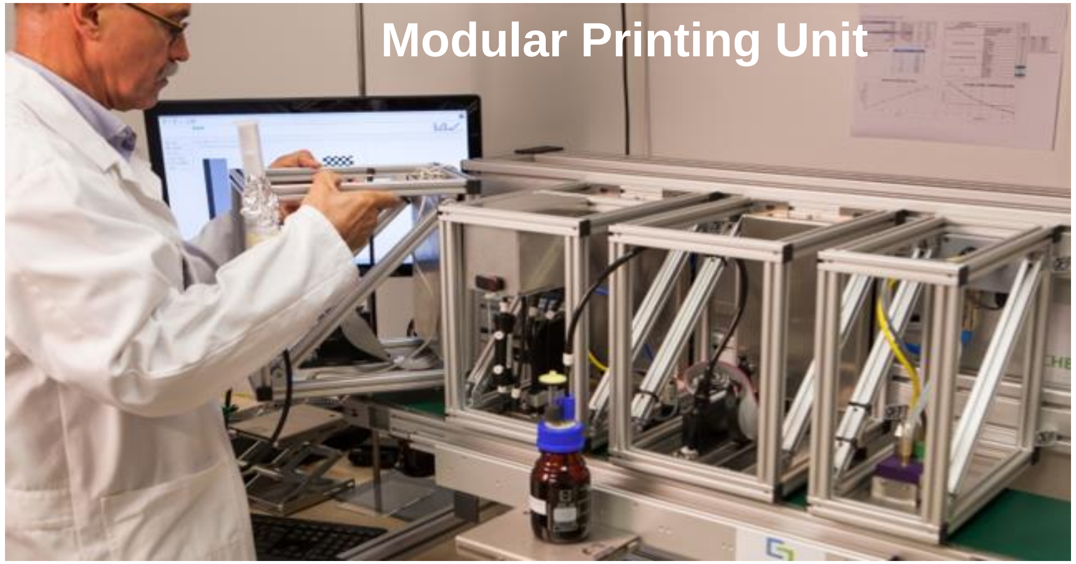
- Tubings
- Ink bottles (packaging)
- Ink cartridges
- Etc.

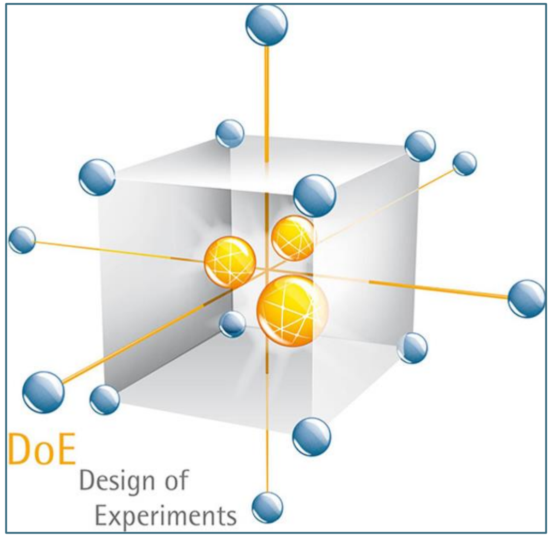
Conclusion

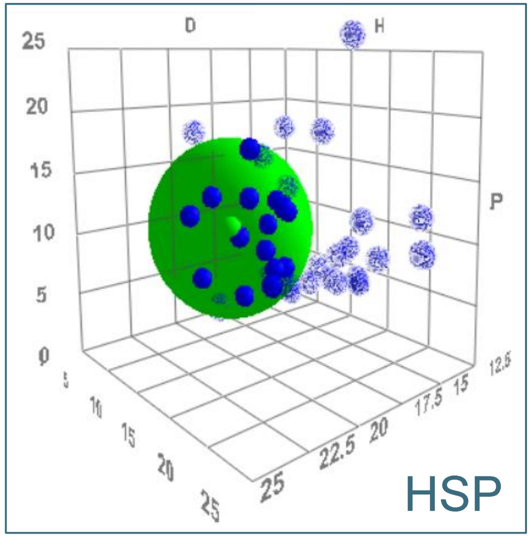
Ink Design

Inkjet inks that fulfill customer requirements









Thanks for listening

You are invited at our booth for further information and discussions:

- ➢Veerle Goossens
- ➢Els Mannekens
- ➢Frank De Voeght

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More info on our website: www.chemstream.be