

Predictive Data for Rheology Modelling



Electric Ant Lab



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- # VLCI & EAL: R&D Digitalization of Formulations
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Electric Ant Lab



VLCI

Practical approach to predictive formulation sciences with HSP and High Throughput screening

EAL

Predictive material research with RheoCube, the virtual lab tool for understanding product behavior with simulation models.

- Cost- and time effective alternative to (wet) lab R&D approach
- Replace trial-and-error approach with predictive data driven solutions
- Acquire more data and (new) insights on your formulations and products



Ingredient Parameter Research

(Van Loon Chemical Innovations B.V., Amsterdam/ NL)

High Throughput screening to obtain HSP data



“**Like seeks like**” principle; likeness measured by the HSP distance metric → compatibility



Provides **intrinsic** and **sustainable** parameter of **many ingredients**: polymers, oils, solvents, pigments, actives...

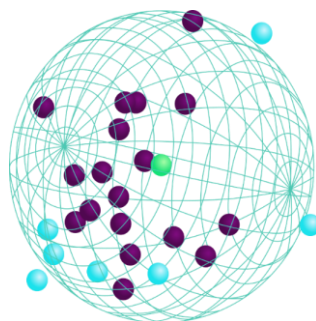


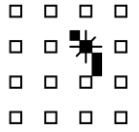
Broad application: **Hansen Solubility Parameters = Similarity**, to compatibilize ingredients which improves stability & efficacy

δD for Dispersion (van der Waals)

δP for Polarity (Dipole Moment)

δH for Hydrogen Bonding





Electric Ant Lab
Scientific Modeling & Simulations



RheoCube
Virtual Complex-Fluids Rheometry

Rheology Simulations & Predictions

(Electric Ant Lab B.V., Amsterdam/ NL)



RheoCube: virtual lab, simulation tool with powerful data visualizations module



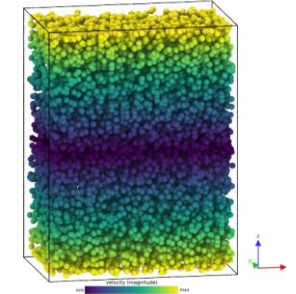
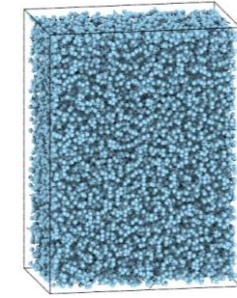
Simulation models based on HSP values of all components in your formulation



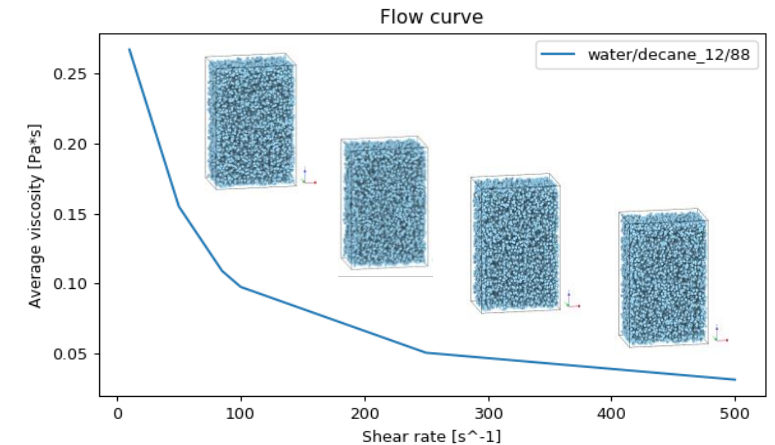
Accelerate your R&D, manage multiple projects and experiments simultaneously



Predict physical behavior of your products with enhanced data



Particles	Fluids	Materials	Samples	States	Experiments	Postprocessing
Demo Particle Allows you to select particles prop...	Demo Fluid Allows you to select fluid properties	Demo Material Mix your particles with your fluid L...	Demo Sample Create a sample	Demo State small sample state	Demo Experiment design your experiment	Postprocessing Postprocessing session
BASF CIP standard BASF CIP particles magnetism and...	AeroShell41 standard AeroShell Oil as used by Ioniga	MRF20 standard A 20 volume percent dispersion of...	MRF20 standard small sample	MRF20 standard small sample state	MRF20 H127k x 1000/s One fixed shear rate (1000 1/s) H...	
BASF CIP particles_Standard BASF CIP particles magnetism and...	AeroShell41_Standard AeroShell Oil as used by Ioniga	MRF20 A 20 volume percent dispersion of...	MRF20-2	MRF20-1-S1	MRF20 H127k y 1000/s One fixed shear rate (1000 1/s)	
			MRF20-B564 Smaller box size for initial check	MRF20-B564-S1 State 1 of the MRF	MRF20 H127k 1/s One fixed shear rate (1000 1/s)	
			MRF20-B596 Same settings as my first attempt ...		MRF20 H64k 1000/s One fixed shear rate (1000 1/s)	
					MRF20 H32k 1000/s One fixed shear rate (1000 1/s)	
					MRF20 H0 1000/s One fixed shear rate (1000 1/s)	



The Road to RheoCube for Chemical R&D

Electric Ant Lab (NL) teamed up with Van Loon Chemical Innovations (NL) for a **new predictive chemistry approach**.

This resulted in a **new product development process** to create simulation models directly from experimental lab data.



6 partners



6 industries



4 countries



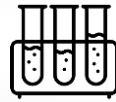
20+ R&D scientists

-
-
-
-

How It Works



YOUR COMPANY
Physical sample(s)



VLCI
HSP and lab data



EAL
Simulation components

- Identify first users in R&D
- Select systems
- Define components
- Ship samples

- HSP determinations for unknown components
- Reporting
- Translate to EAL input data

- Define components in simulation parameters
- Validate system with VLCI
- Onboard your R&D scientists

-
-
-
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Selecting Components

For this HSP/RheoCube approach

After you have defined your first system, the different components will be used as input in RheoCube. You provide the input on the components in your system. VLCl provides the HSP data.



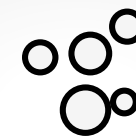
Fluids



Surfactants



Polymers



Particles

-
-
-
-

Measure and Predict

1. HSP is applied to match ingredients, make them compatible and develop stable formulations with utmost efficacy

2. Simulation models are created with HSP values as input, setting up experiments in RheoCube's user-friendly interface

Compatibility Explorer

Quick Start
 This app comes with an HSP database, which will continuously be upgraded. It allows you to: - Compatibilize or replace ingredients of your formulation - Load your own HSP database of ingredients - Select and visualize ingredients which you want to solubilize, disperse or formulate with - Tune with ingredients from the database to find matching ingredients - (more instructions below)

Compatibility Optimiser App

Mouse @
 I1
 Propylene Carbonate = 20, 18, 4.1
 % I2
 I2
 Tetrahydrofuran (THF) = 16.8, 5.7, 8
 Mix HSP
 17.6, 8.7, 7.1
 Mix Ra
 0.8
 Formulate to HSP
 17.8, 8.3, 6.5

Show Targets
 Show Components

Load an Ingredients dataset
 No file chosen

Target Type/Filter

Load a solvents dataset
 No file chosen

Component Type/Filter

Target	GD	GP	GH	R	Type	Dmix	Active
Polystyrene (PS)	18.5	4.5	2.9	4	3		<input checked="" type="checkbox"/>
Polyvinylidene fluoride (PVDF)	17	12.1	10.2	4	3		<input checked="" type="checkbox"/>
Polyethylene (PE)	16.9	0.8	2.8	4	1		<input type="checkbox"/>

R&D project 05

Filter by name

Polymer-X
 Particle-X_500nm
 polymer blend
 polymer blend
 polymer blend
 polymer blend...

Surfactant-X
 Particle-X_2um
 polymer solutio...
 emulsion-y
 emulsion-y-stri...
 polymer blend...

alcohol
 emulsion-x
 polymer solutio...
 emulsion-y-drop
 emulsion-y-drop

Water
 emulsion-y
 polymer solutio...
 polymer sol-x-1%
 emulsion-y-stri...

Surfactant-X2
 Suspension-y
 suspension-y-30...
 suspension-y-20...
 polymer sol-x-1...

suspension-y-20...
 Viscosity
 polymer sol-x-1...

diameter (m)
 0.000002 0.000004 0.000006 0.000008 0.000010

Viscosity (Pa.s)
 0.00 0.01 0.02 0.03 0.04 0.05

Time (s)
 0.00 0.02 0.04 0.06 0.08

Hz
OH
Hz
Hz

- **Results:**
- more data driven research projects and formulations



5-10x more
projects in your
R&D pipeline



40-90%
cost reduction
of R&D process



Predict
behaviour of
end-products



Control your
formulations
with accurate
ingredient data



Intuitive and
cloud-based
collaboration
tool for R&D

- # What We Offer
-
- Receive a specific quotation based on your requirements
-

Example HSP-rheology modelling Trial:

- HSP determinations on main ingredients as a baseline
- RheoCube access 60 days for 5-10 users
- Simulation computing budget to check the influence of various parameters
- Support on implementation from VLCI & EAL scientists



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