A photograph of two men painting a wall. The man in the foreground is wearing a blue polo shirt and has a beard; he is holding a long-handled roller. The man in the background is wearing a light blue t-shirt and is using a brush. The wall is white and partially painted. The background is a bright, overcast sky.

New low-VOC, multi-functional additive for coatings based on alkoxyated Exxal™ surfactant

Future of Surfactants Summit, 24th May 2022, Barcelona

Francois Simal, ExxonMobil - ETC

ExxonMobil

Waterborne paint/coating additives:

- Polymer dispersion: Binder
- Pigments
- Fillers



Additives:

Coalescing aid: Film formation: Ethers, Esters

Glycol: open time, freeze thaw stability

VOC contributors !

Dispersants

Wetting agents

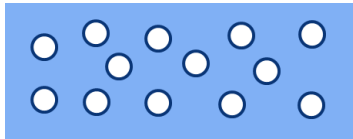
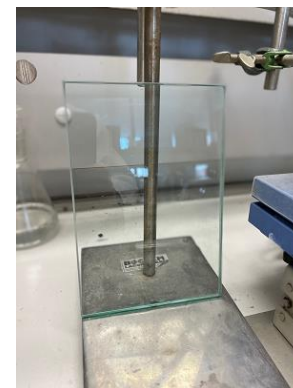
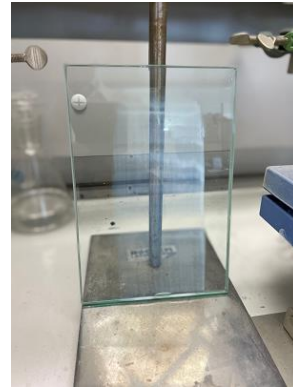
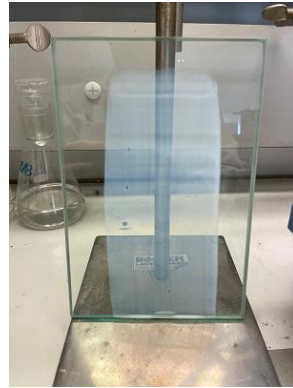
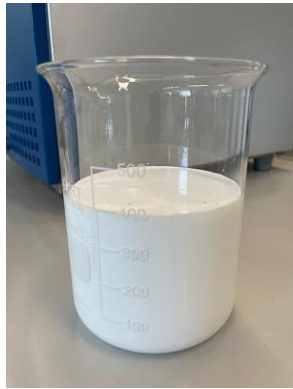
Thickeners

De-foamers

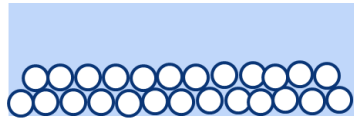
Biocides

...

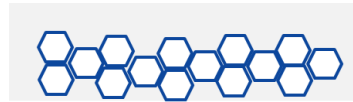
Film formation in polymer dispersion – Coalescing agents



Polymer particles in Water



Water loss – closed packed

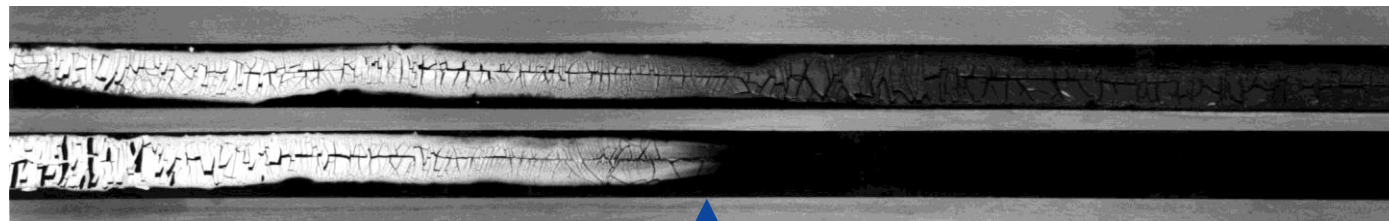


Temp > MFFT – Honey comb

Homogeneous Film

Temp > T_g – Diffusion and Coalescence

Minimum Film Formation Temperature (MFFT)



-10°C

Cloudy

Clear

+10°C



- Coalescing agents are used to reduce the minimum film formation temperature
- Good film formation ensures optimal appearance & mechanical properties

Low VOC paints



With the increasing concerns for the environment and the implementation of deco paint directives, the paint producers tend to compete for the **lowest VOC content** in their products.



Description	Abbreviation	Boiling Point Range (°C)	Example Compounds
Volatile organic compounds	VOCs	< 250	toluene, 2-propanol, Exxal™ 8-11 ...

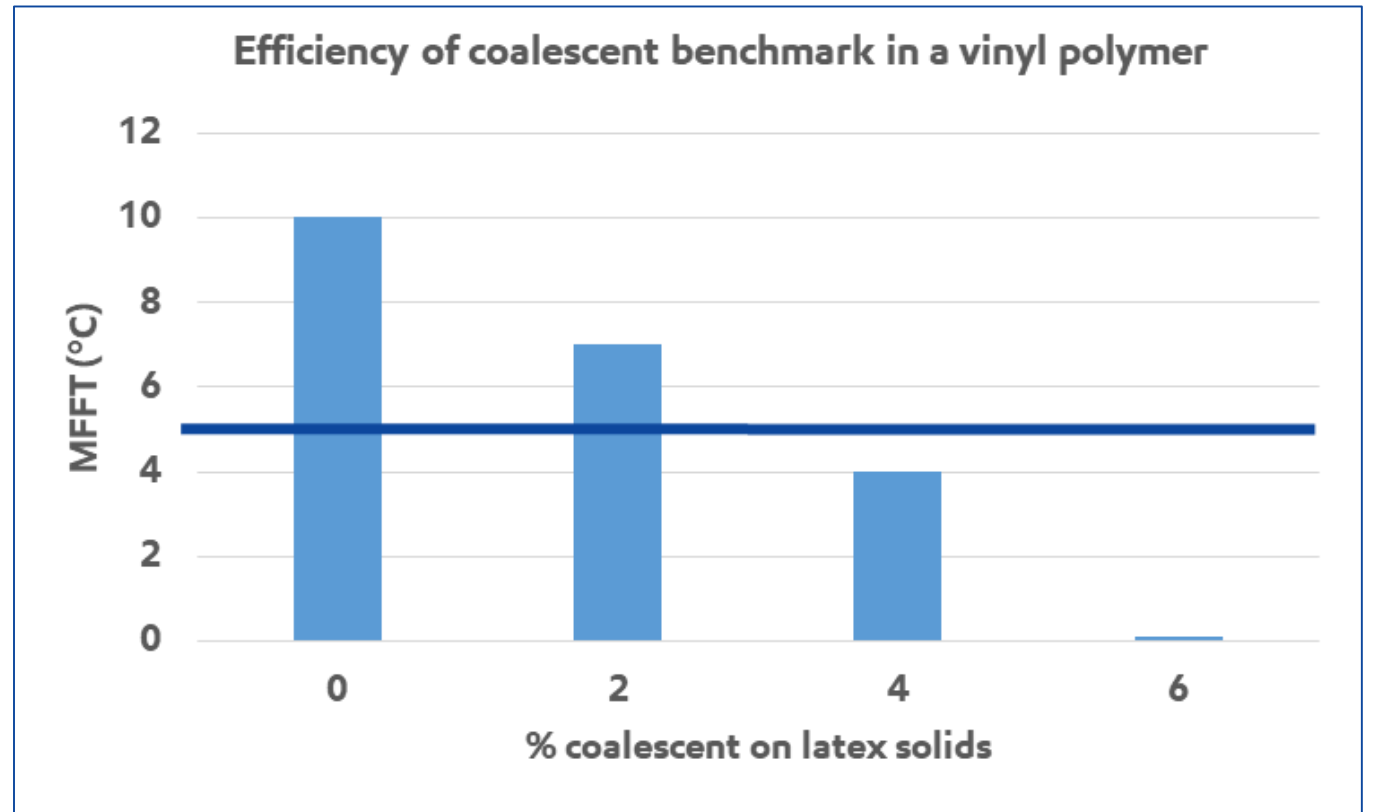
Maximum VOC content limit values for Paints

Product Category	EU Phase I (g/l) 1.1.2007	EU Phase II (g/l) 1.1.2010	Ecolabel (g/l)	Ecolabel New (g/l)
Interior matt walls & ceilings	75	30	15	10
Exterior walls of mineral substrate	75	40	40	25

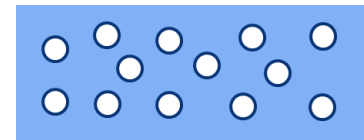
Semi Volatile organic compounds	S-VOCs	> 250 to 400 °C	Texanol™, Exxal™ 13, ...
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Coalescing agents – other key features

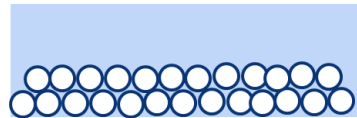
- Good coalescing efficiency and versatility
- Extremely low odor
- Multifunctional additive
- ...



Exxal™ alkoxyate: multifunctional additive for low-VOC paints



Polymer particles in Water



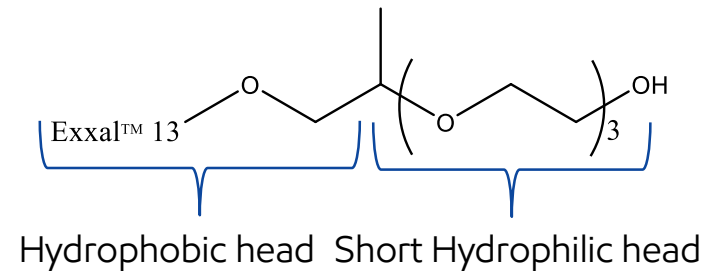
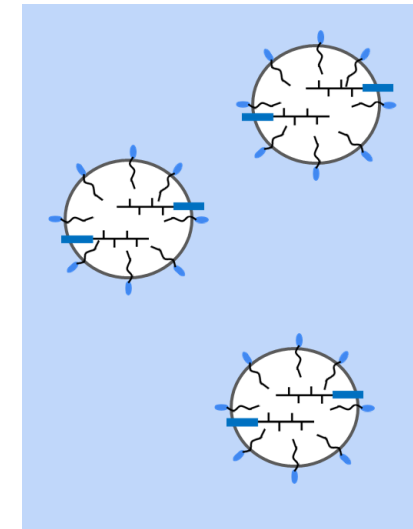
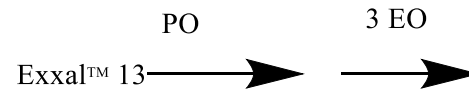
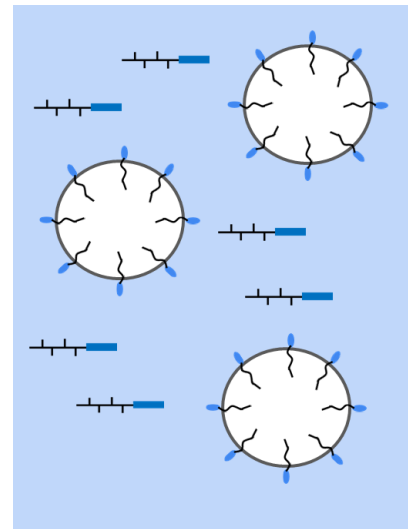
Water loss – closed packed



Temp > MFFT – Honey comb

Homogeneous Film

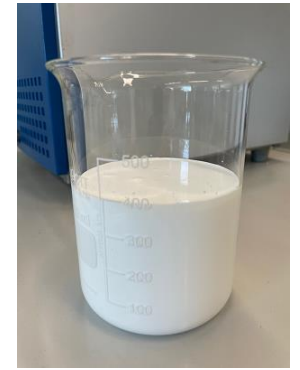
Temp > T_g – Diffusion and Coalescence



HLB = 6.8

- Coalescing agent: Compatibility and particles fusing (film formation)
- Surfactants: Improved stability, high boiling point, low smell, polymer/REACH exempt
- **Multifunctional additive**

Effect of additive on vinyl dispersion



Characteristics	Vinyl polymer dispersion	Exxal™ 13-PO-3EO 4 wt%	Coalescent benchmark 4 wt%
Boiling point (°C)	n.a.	425*	374
MFFT (°C)	10	6	5
Hardness (s, 28 d)	22	8	9
Freeze/Thaw	Not OK	OK	Not OK
Storage stability (viscosity loss %)	28	16	21.5
Electrolytes (Al ³⁺)	Stable	Stable	Stable
Water spot test	4 (24h)	4-5 (24h)	1 (24h)

- ✓ Alkoxyated Exxal™ is non s-VOC
- ✓ MFFT is reduced to ~ 5°C → Alkoxyated Exxal™ behaves as a coalescent
- ✓ No negative effect on film hardness
- ✓ Freeze/Thaw stability improvement observed with Alkoxyated Exxal™
- ✓ Storage stability (2 weeks at 50°C): stable viscosity
- ✓ Water whitening resistance: Alkoxyated Exxal™ >> coalescent benchmark



Water Spot 5

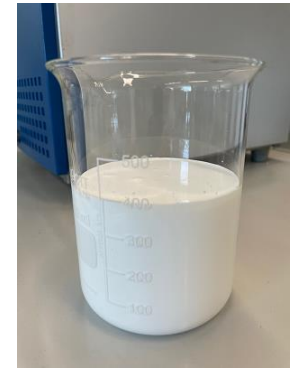


Water Spot 3



Water Spot 1

Effect of additive on styrene/acrylic dispersion



Characteristics	SA polymer dispersion	Exxal™ 13-PO-3EO 8 wt%	Coalescent Benchmark 8 wt%
Boiling point (°C)	n.a.	425*	374
MFFT (°C)	20	6	2
Hardness (s, 28 d)	38	4	3
Freeze-Thaw	not OK	not OK	not OK
Storage stability (viscosity loss %)	5.5	3.0	23.5
Electrolytes (Al ³⁺)	not Stable	Stable	not Stable
Water spot test	5 (24h)	3-4 (24h)	3-4 (24h)

✓ MFFT is reduced to ~ 5°C → alkoxyated Exxal™ behaves as a coalescent

✓ Storage stability (2 weeks at 50°C): stable viscosity

✓ Improved electrolyte stability observed with alkoxyated Exxal™

✓ Water whitening resistance: alkoxyated Exxal™ ~ coalescent benchmark



Water Spot 5

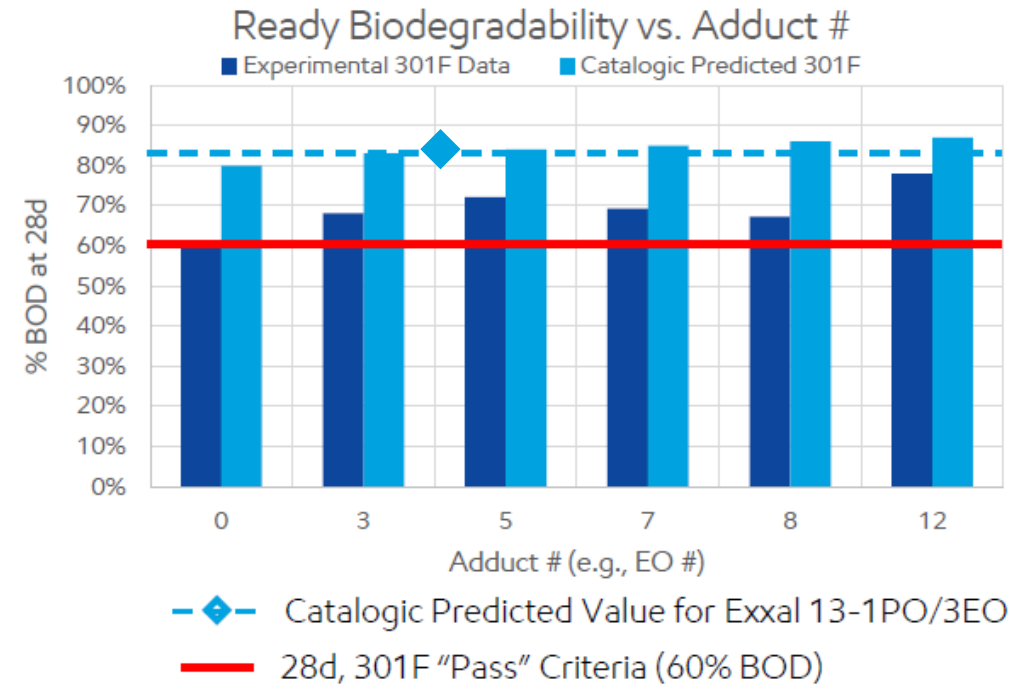
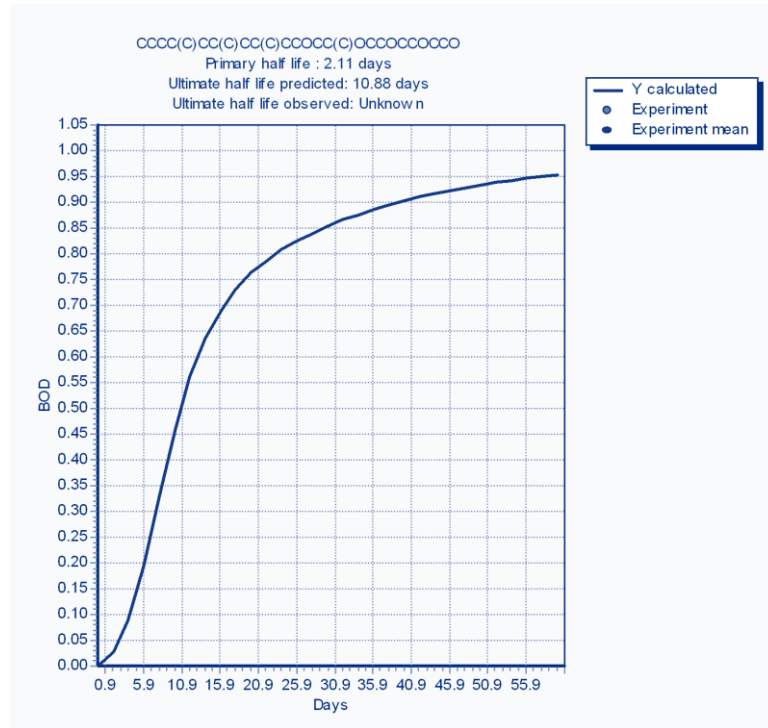


Water Spot 3



Water Spot 1

Predicted & observed biodegradability for alkoxyated Exxal™



- Catalogic predicts ready biodegradability of Exxal™ PO-EO structures
- Minimal steric hindrance from branched PO structure predicted (limited experimental data)
- No obvious red flags from ready biodegradability perspective

- Good agreement between the model results and the experimental data
- The trends (higher EO = slightly better biodeg) as well as the general level of degradability are consistent, however the models are offset (about 15% higher)
- Catalogic 301F predicts 84% of biodegradability for alkoxyated Exxal™ 13 after 28 days

Additive versatility - Hansen Solubility Parameters (HSP)

Hansen solubility parameters: Predictive way to assess if one material will dissolve in another and form a solution

“like dissolves like” concept - i.e. similar types of interactions

Each material is given three Hansen parameters:

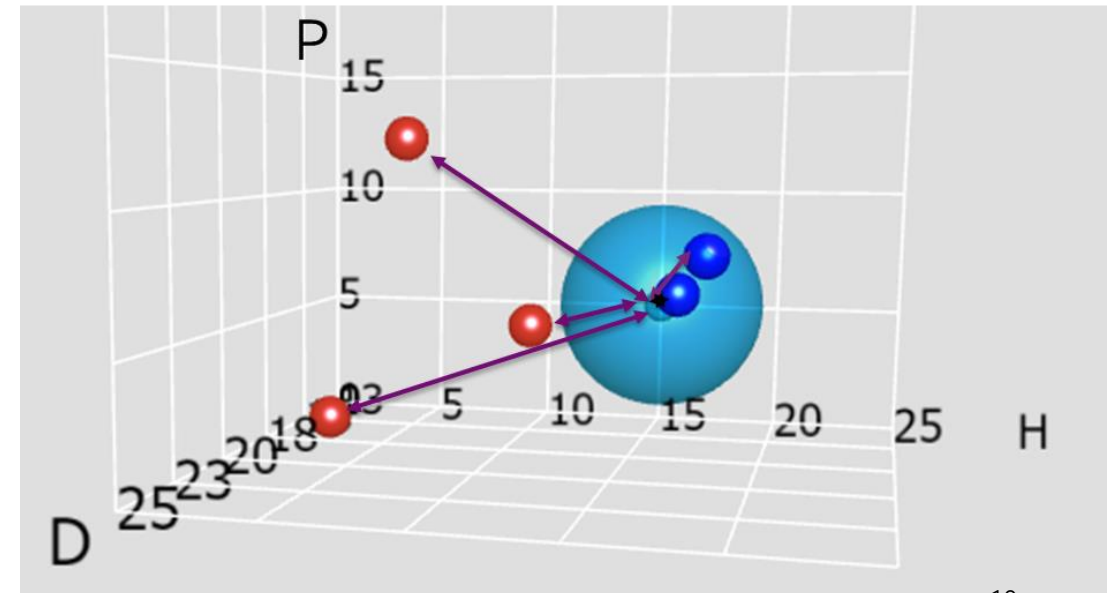
- The energy from dispersion forces between molecules (δD) - δ NON POLAR
- The energy from dipolar intermolecular force between molecules (δP) - δ POLAR
- The energy from hydrogen bonds between molecules (δH) - δ H BONDING

The distance between 2 sets of center HSP (D, P, H) is:

$$Ra = \sqrt{4(\delta D_1 - \delta D_2)^2 + (\delta P_1 - \delta P_2)^2 + (\delta H_1 - \delta H_2)^2}$$

The closer, the better they match, indicated with: \longleftrightarrow

3D-Hansen space



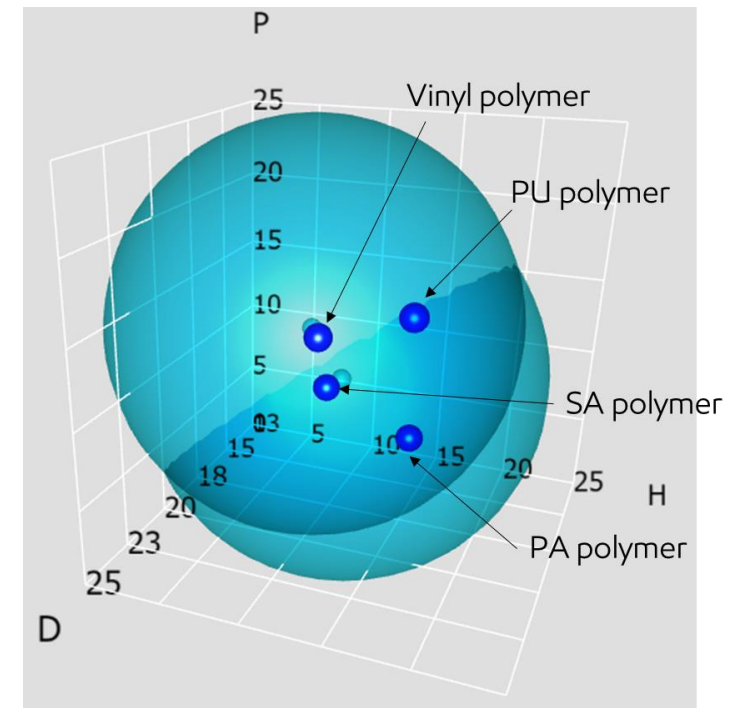
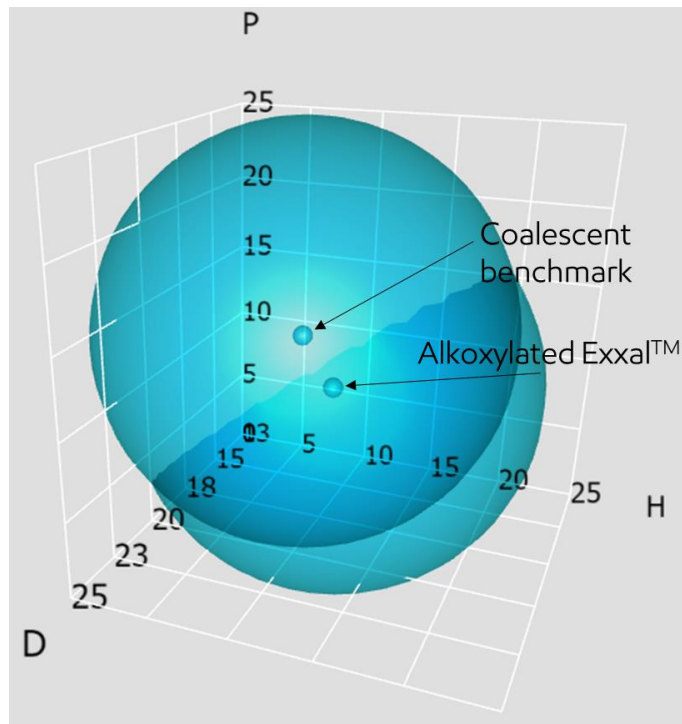
Additive versatility - Hansen Solubility Parameters (HSP)

Characteristics δ NON POLAR δ POLAR δ H BONDING

Alkoxylated Exxal™	16.4	8.5	9.9
Coalescent benchmark	16.0	11.5	7.4

Relative Energy Distance (RED): $RED = \frac{Ra}{Radius}$

Best is $RED < 1$ - indicated with various types of polymers



Conclusions

- Promising initial test results of alkoxyated Exxal™ :
 - ✓ Low viscous, non-VOC, odor-free
 - ✓ REACH exempt (polymer)
 - ✓ Acts as coalescing agent
 - ✓ Provides improved dispersion stability (towards freeze-thaw and electrolytes)
 - ✓ Good biodegradability predicted
 - ✓ Efficient and versatile
- Alkoxyated Exxal™ as non-VOC multifunctional additive for the Coating, Adhesives and Sealants (CASE)

Acknowledgements

- Bernard Leroy and Levi Salaets – ExxonMobil – ETC
- Cecilia Fabris – ExxonMobil – ETC- ESEM
- Craig W. Davis – ExxonMobil – EMBSI
- Beverley Fricker and Sander Van Loon – VLCI

A photograph of two men painting a wall. One man in a blue shirt is in the foreground, holding a long-handled roller. Another man in a light blue shirt is in the background, using a brush. The scene is brightly lit, and the wall is white. The text 'THANK YOU' is overlaid in large white letters.

THANK YOU

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