New low-VOC, multi-functional additive for coatings based on alkoxylated 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:

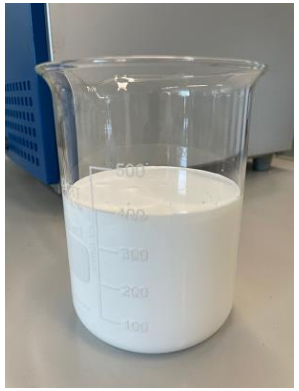
Coalescing aid: Film formation: Ethers, Esters
Glycol: open time, freeze thaw stability

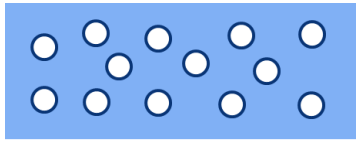
VOC contributors !

Dispersants
Wetting agents
Thickeners
De-foamers
Biocides
…

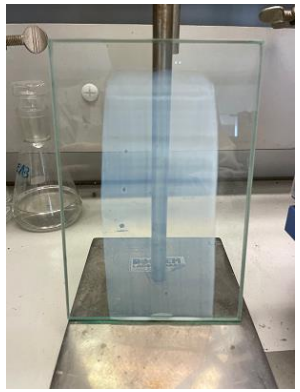
ExxonMobil

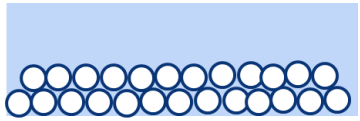
Film formation in polymer dispersion – Coalescing agents



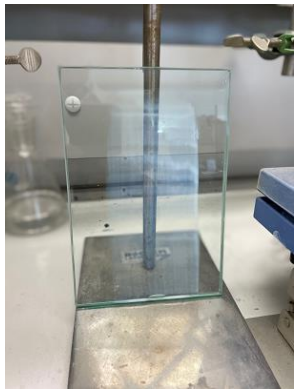


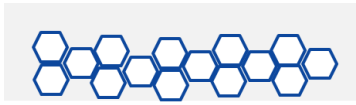
Polymer particles in Water



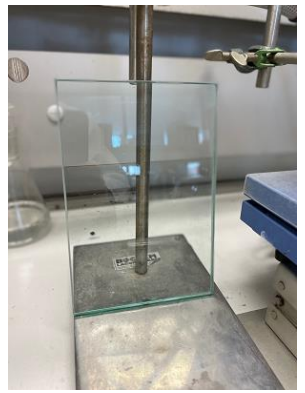


Water loss – closed packed





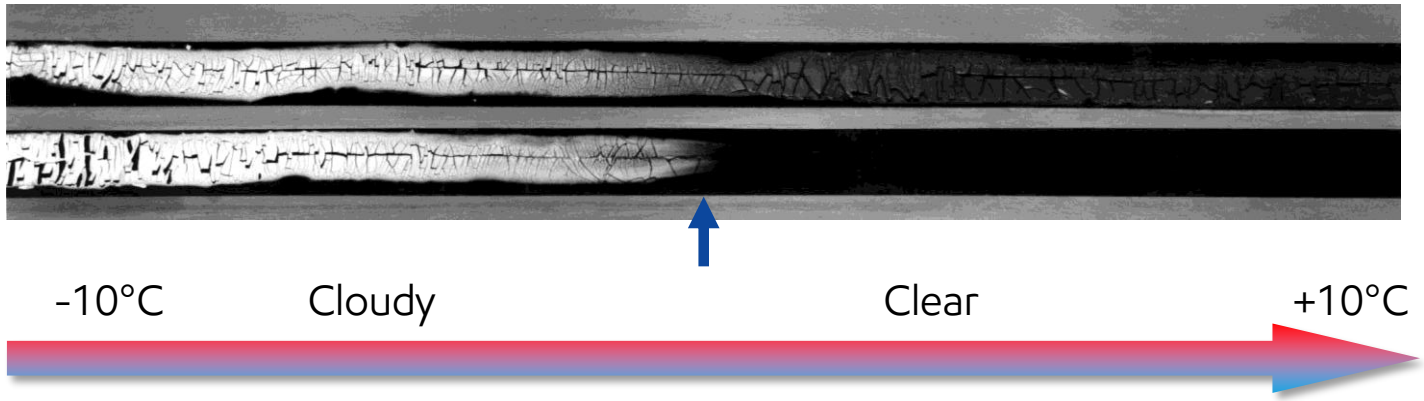
Temp > MFFT – Honey comb



Homogeneous Film

Temp > Tg – Diffusion and Coalescence

Minimum Film Formation Temperature (MFFT)



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

ExxonMobil

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 …

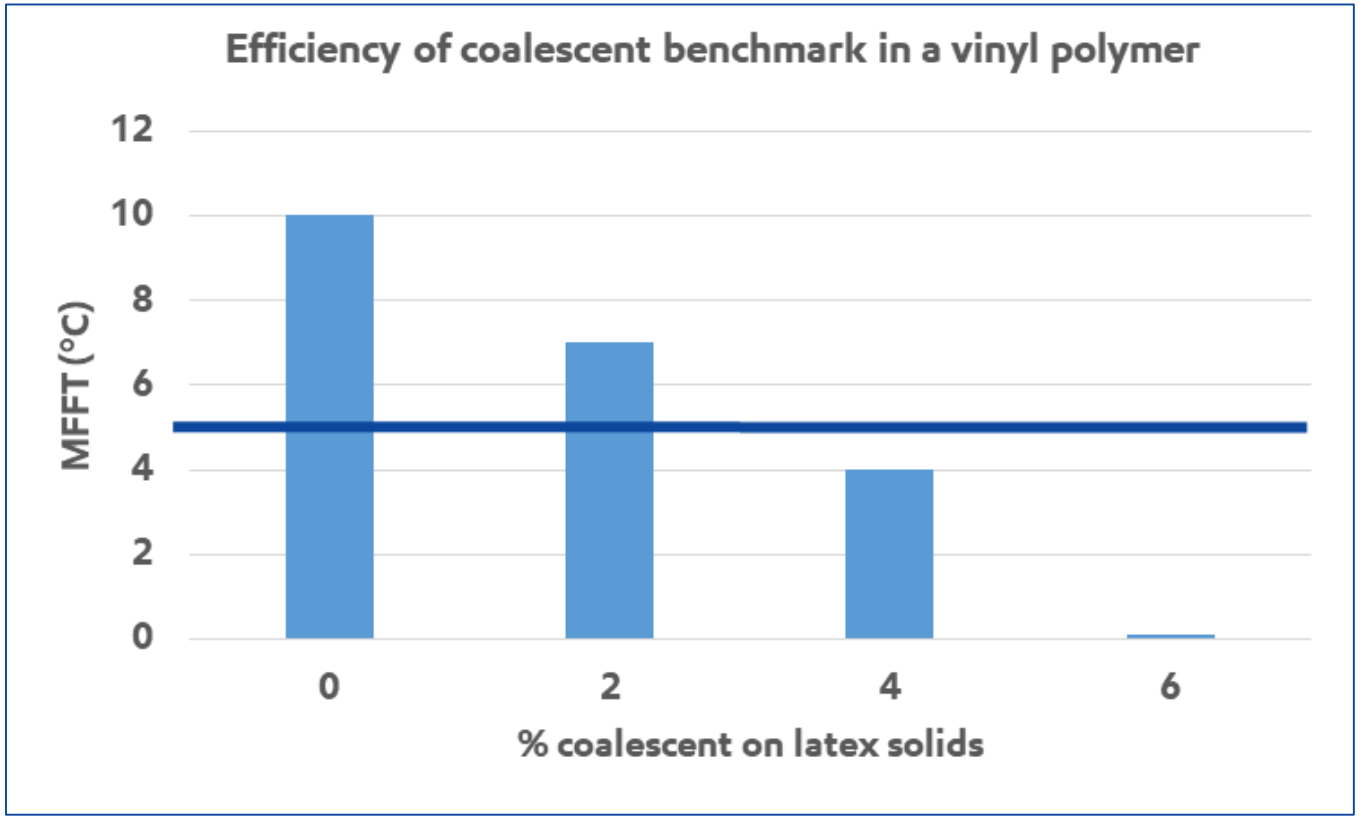
Maximum VOC content limit values for Paints

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

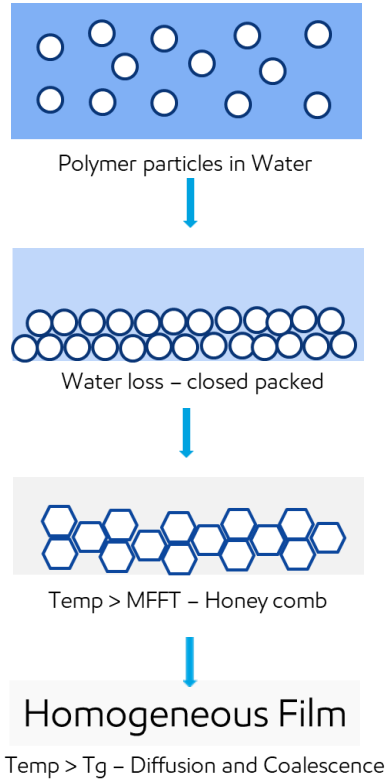
Semi Volatile organic compounds	**S-VOCs**	**> 250 to 400 °C**	**Texanol™, Exxal™ 13, …**

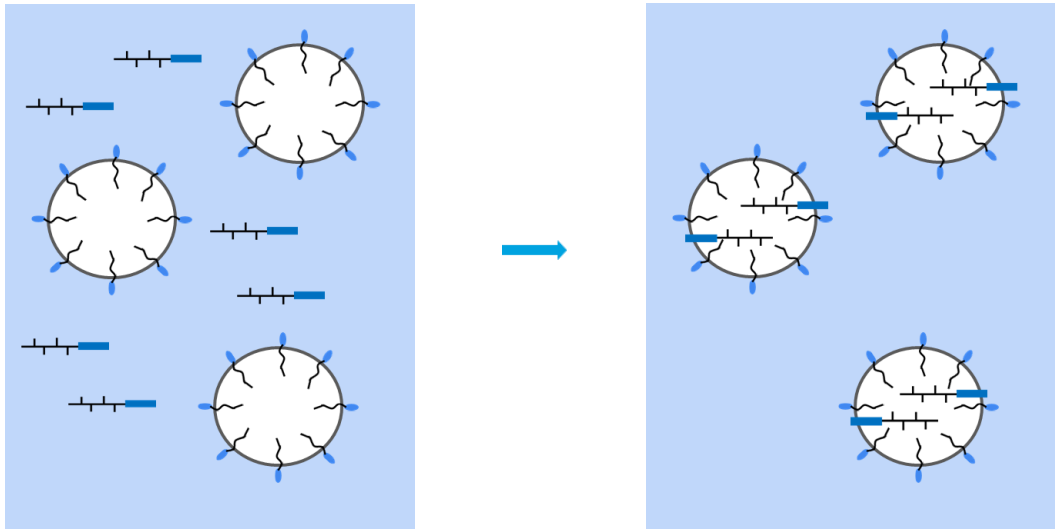
Coalescing agents – other key features

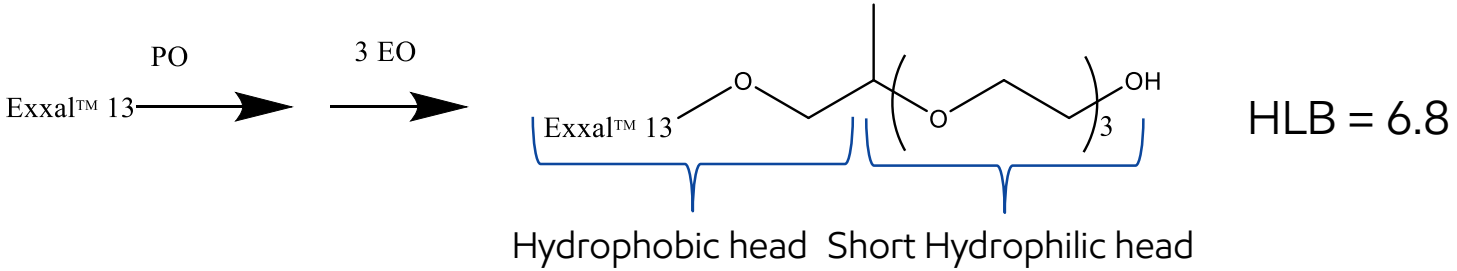
- Good coalescing efficiency and versatility
- Extremely low odor
- Multifunctional additive
- …



Exxal™ alkoxylate: multifunctional additive for low-VOC paints





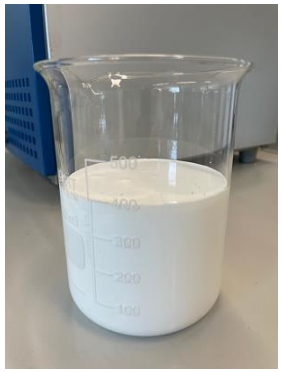


HLB = 6.8

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

ExxonMobil

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)

Water Spot 5

Water Spot 3

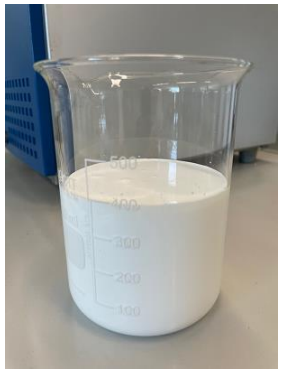
Water Spot 1

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

ExxonMobil

* = determined by HSPiP software – 5th Edition

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 → alkoxylated Exxal™ behaves as a coalescent
- ✓ Storage stability (2 weeks at 50°C): stable viscosity
- ✓ Improved electrolyte stability observed with alkoxylated Exxal™
- ✓ Water whitening resistance: alkoxylated Exxal™ ~ coalescent benchmark

Water Spot 5

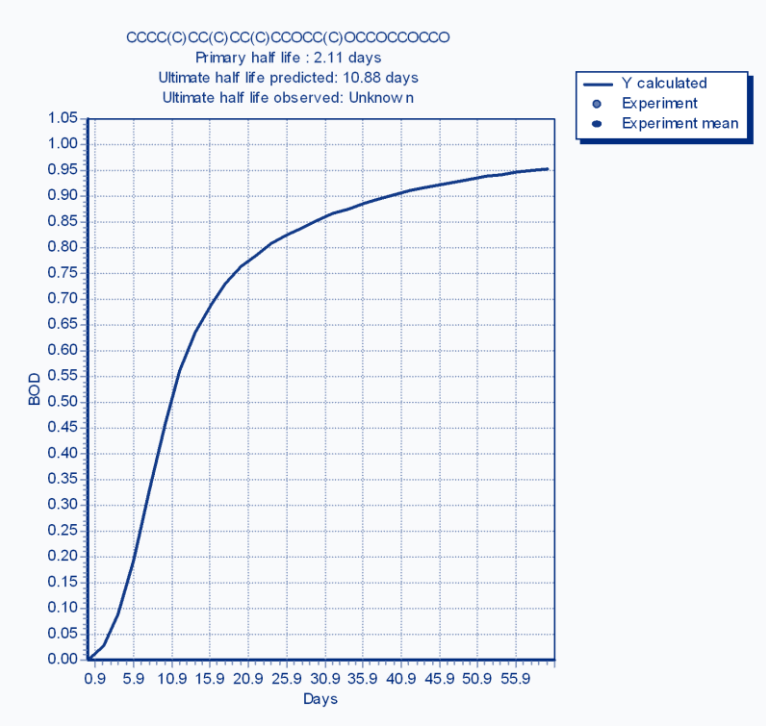
Water Spot 3

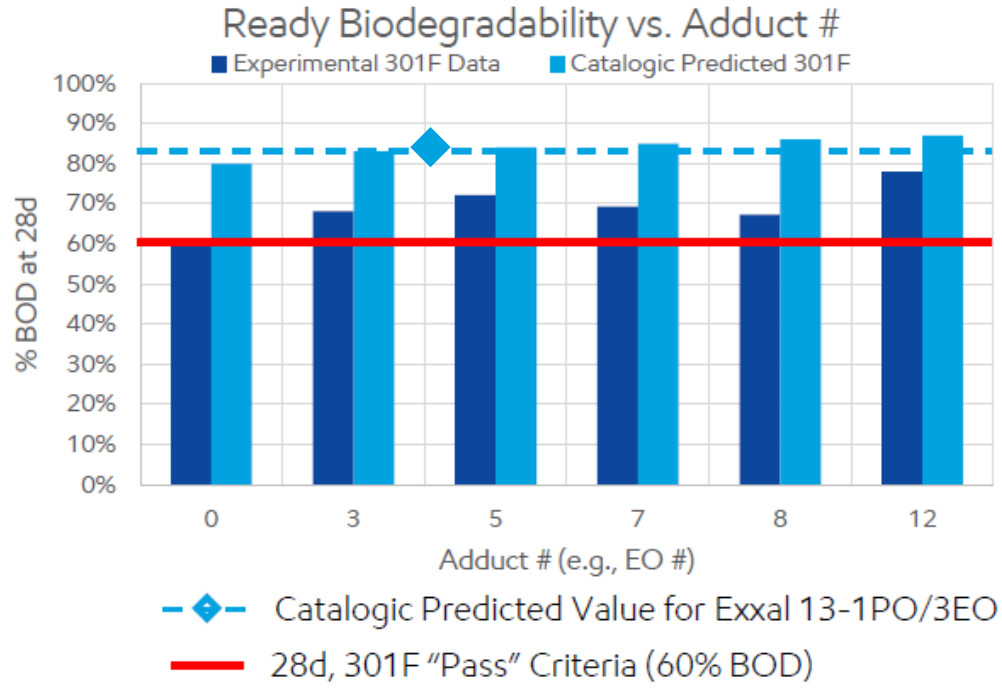
Water Spot 1

ExxonMobil

* = determined by HSPiP software 5th Edition)

Predicted & observed biodegradability for alkoxylated 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 alkoxylated Exxal™ 13 after 28 days

ExxonMobil

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:

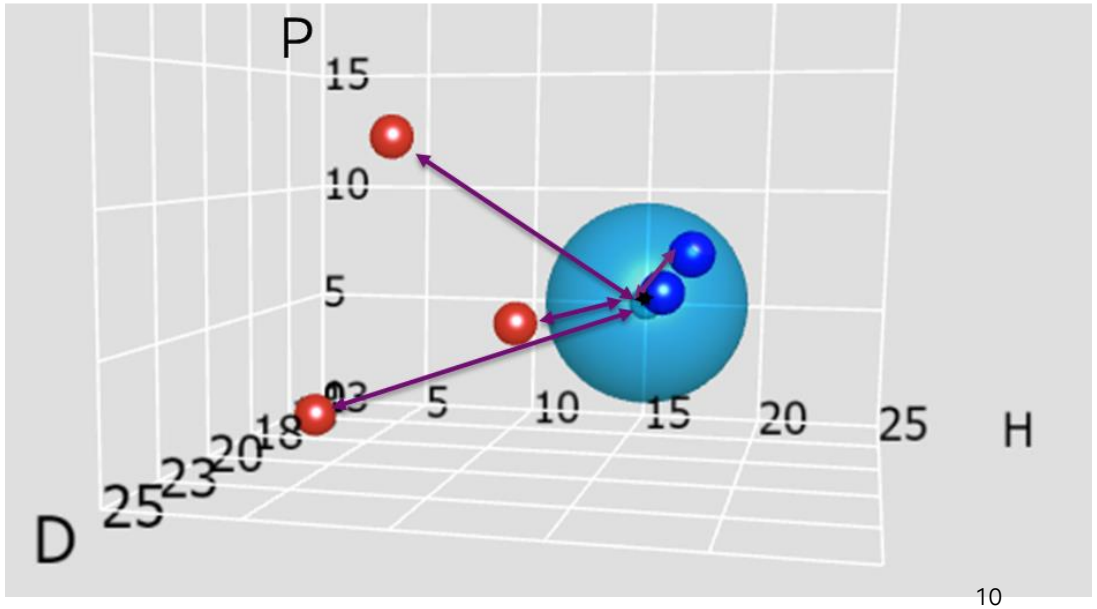
- The energy from dispersion forces between molecules (δD) – δ NON POLAR
- The energy from dipolar intermolecular force between molecules (δP) - δ POLAR
- The energy from hydrogen bonds between molecules (δH) - δ H BONDING

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: ↔

3D-Hansen space



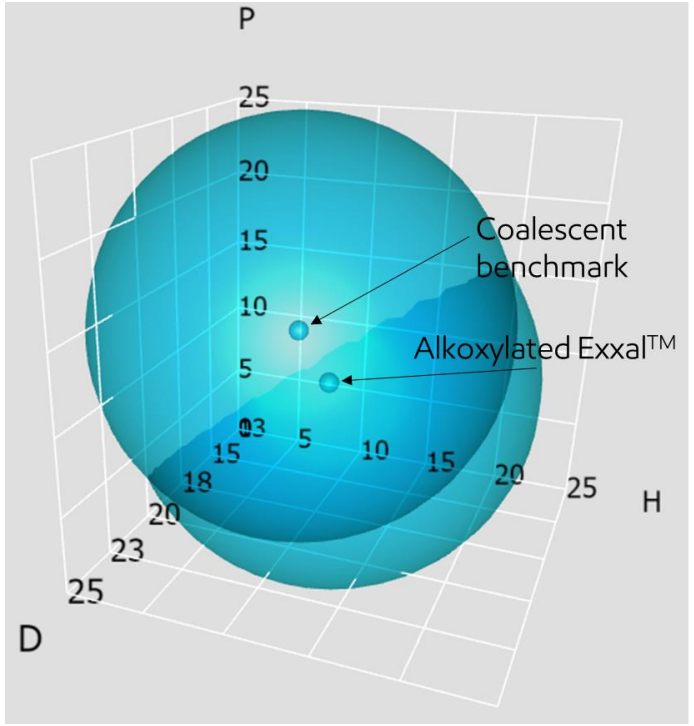
ExxonMobil

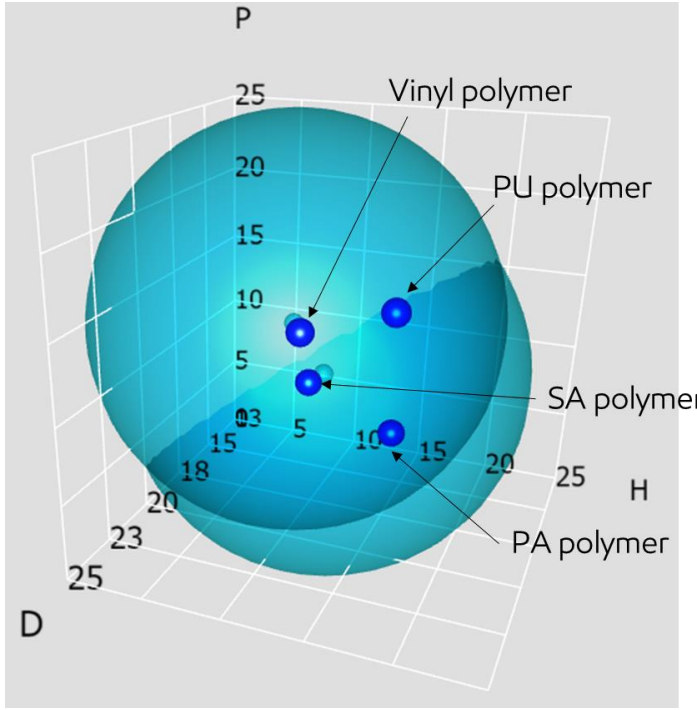
Additive versatility - Hansen Solubility Parameters (HSP)

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): $\mathbf{RED} = \frac{\mathbf{Ra}}{\mathbf{Radius}}$

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





Source: 3D Visualizer from PrediMatch – VLCI (S. van Loon, B. Fricker)

Conclusions

- Promising initial test results of alkoxylated 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

- Alkoxylated 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

THANK YOU

- Contacts:
- francois.simal@exxonmobil.com – Technology
- bram.plessers@exxonmobil.com - Sales