EVONIK - PU Additives

Novel Additive Technology Designed to Optimize the use of Natural Oil Polyols in Support of the Construction market

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Agenda

1. **Introduction**
2. The Challenge
3. Foam Performance
    a. Spray Foam
    b. Boardstock
4. Conclusions

Construction Market goes "green"

- The global construction market continues to grow but does face some serious challenges
- Conservative estimation calculate that > 50% of all energy needs are consumed for the heating and cooling of building structures
- Today's builders are looking for products that increase energy efficiency…..yet are also sustainable for the future generations
- Fortunately, insulating polyurethane foam is one of today's most effective insulation materials

Increasing Renewable Content

- Bio-based materials such as sugar, glycerin and sorbitiol have been used for many years now in the production of polyols
- But the polyurethane industry is looking more and more into increasing its renewable content
- New Natural Oil Polyols have been developed in an attempt in increase the renewable content in the finished PU foam
- To date, NOP technology has been proven in many PU construction applications
- But what is the limit? How much petroleum-based Polyol can be replaced by NOPs?

Natural Oil Polyols Limitations in PU Applications

The Pros:

- Technology exists
- Variety of new structures in polyols
- “Sustainable”
- Offers a solution to a growing demand for Eco-Friendly Products

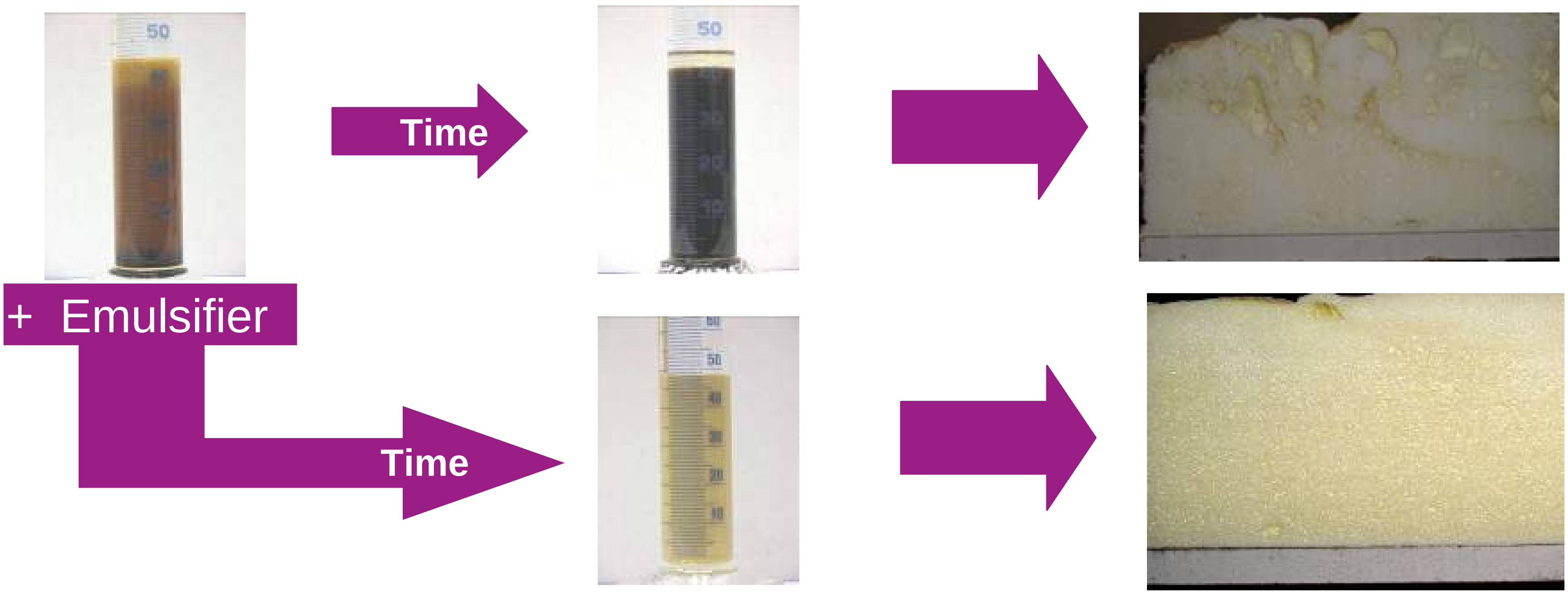
The Cons:

- Composition may vary from geographic area, weather conditions
- Relatively low hydroxyl functionality and lower OH values
- Limited compatibility with conventional polyols
- ….Resulting in poor foam performance

What Role Can Additives Play?

Emuslifier

……..WILL NOT make NOPs more homogeneous
……..WILL NOT increase NOPs hydroxyl functionality
……..CAN maximize NOP usage by creating a stable emulsion



Resulting in acceptable foam performance
…with maximum renewable content!

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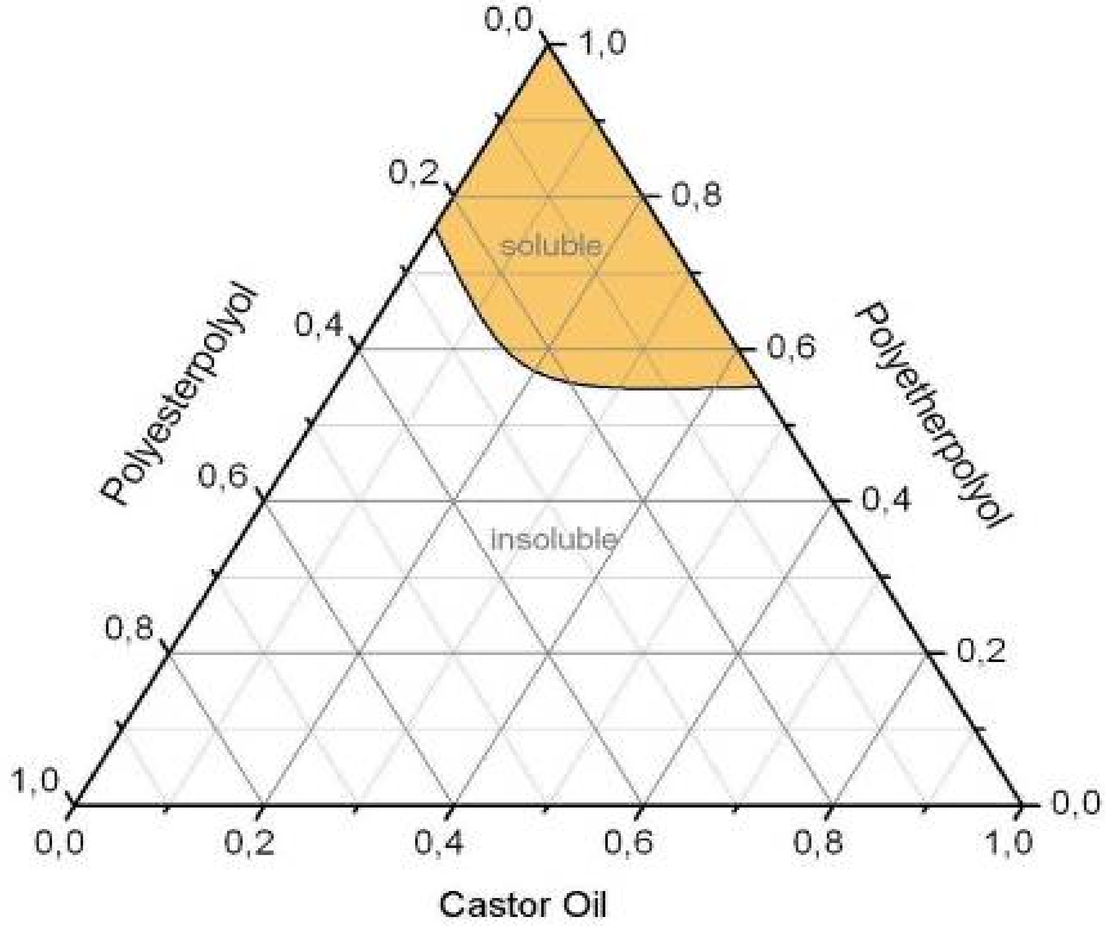
Unmodified NOP's and Polyesterpolyols Create a Challenge

Unmodified NOP's are Not Soluble in Aromatic Polyesterpolyols

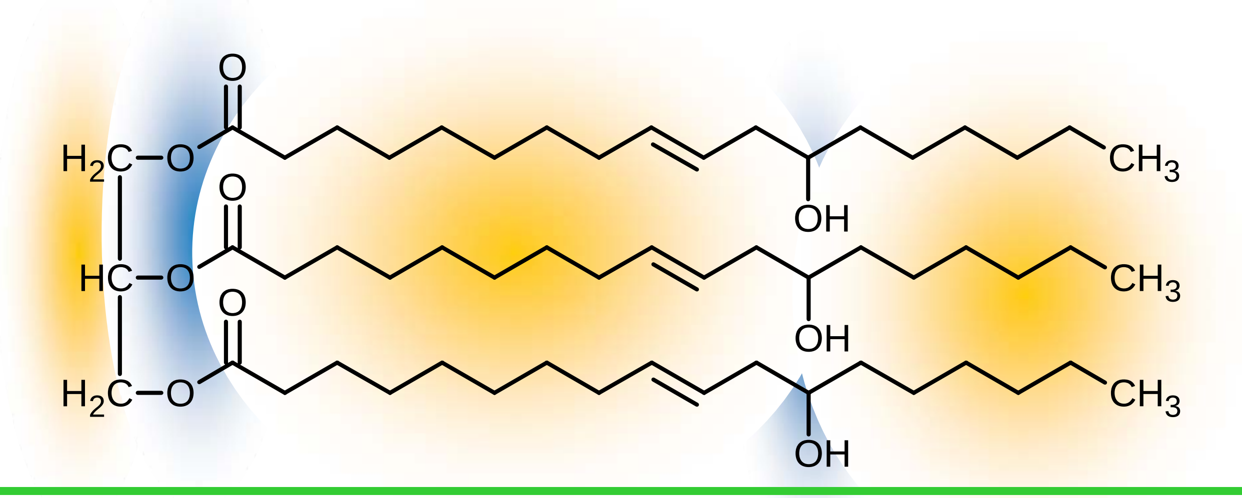


Even Modified NOP's Display Limited Solubility!

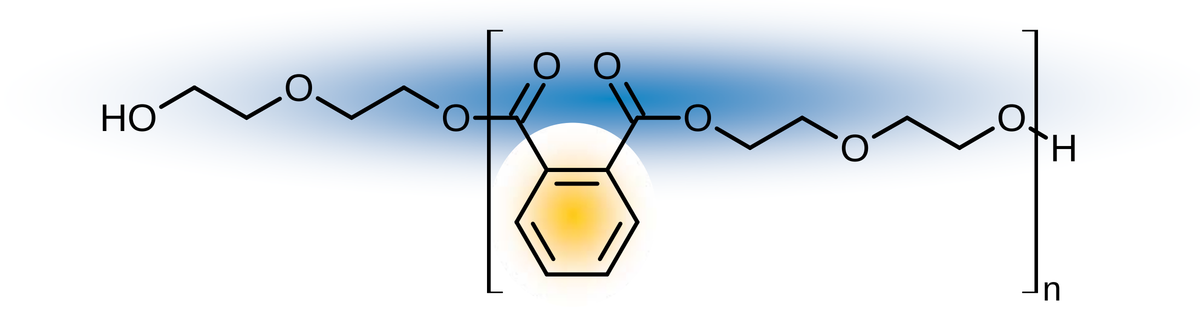
	Polyester-polyol	99:1	95:5	90:10	80:20	50:50	NOP	Type
Phthalic Anhydride	PA 1	+					A	Castor Oil
	PA1						B	mod. Soybean Oil
	PA1	+					B'	mod. Soybean Oil
	PA1	+	+	+	+		C	mod. Soybean Oil
	PA1	+	+	+	+	+	C'	mod. Soybean Oil
DMT-based	DMT 1	+					A	Castor Oil
	DMT 1						B	mod. Soybean Oil
	DMT 1						B'	mod. Soybean Oil
	DMT 1	+					C	mod. Soybean Oil
	DMT 1	+					C'	mod. Soybean Oil
PET- based	PET 1						A	Castor Oil
	PET 1						B	mod. Soybean Oil
	PET 1						B'	mod. Soybean Oil
	PET 1						C	mod. Soybean Oil
	PET 1						C'	mod. Soybean Oil

Polarity Differences Result in Poor Compatibility

Castor oil - hydrophobic



Aromatic polyester polyol - hydrophilic



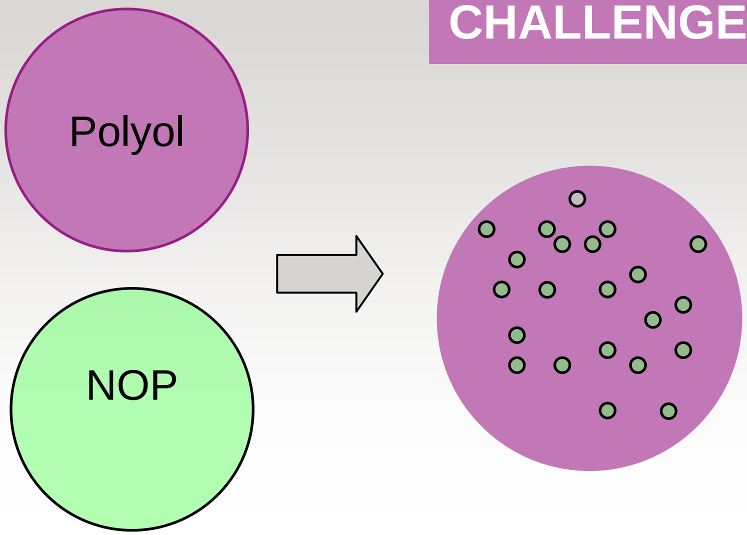
hydrophilic segments

hydrophobic segments

Lack of Solubility Requires Excellent Emulsification !

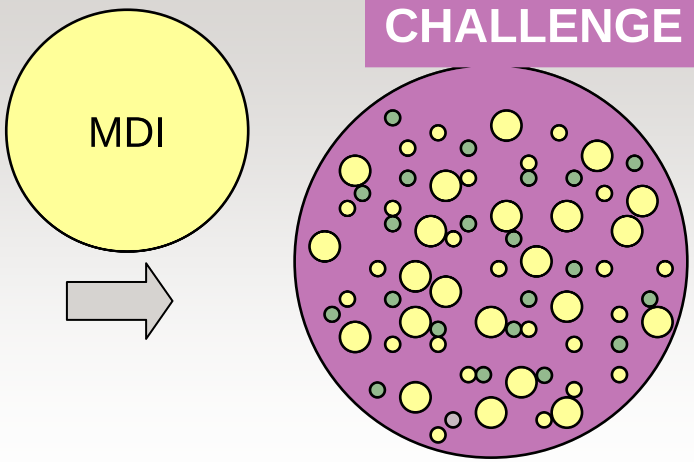
Fine & Stable Polyol Premix / System

CHALLENGE 1



Homog. & Stable Reaction Mixture

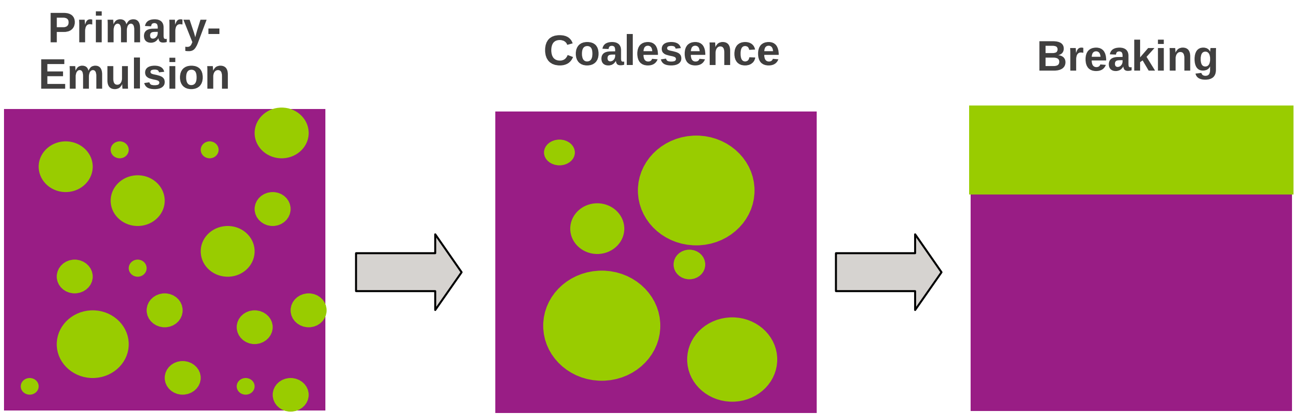
CHALLENGE 2



Insufficient emulsification would result in:

- Instability of the reaction premixes
- Inhomogeneous reaction profile
- Foam imperfections
- Inhomogeneous distribution of foam properties

Emulsifier Support Stable Emulsions

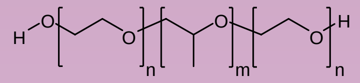
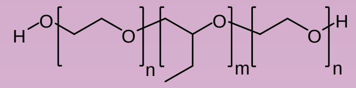
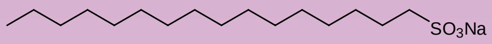
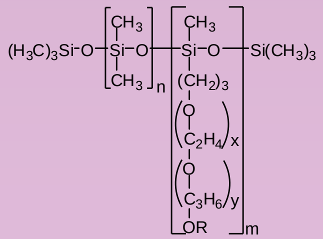


Emulsifier impact on the emulsification process:

- Coalescence is prohibited by a protecting layer of surfactant molecules at the interface

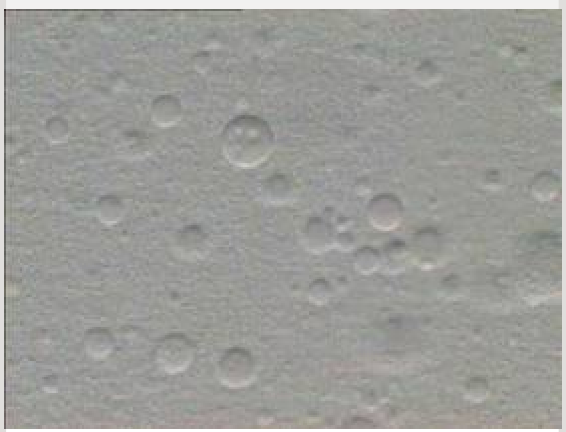
- Emulsification requires
  - less mixing energy,
  - is faster and finer and
  - the emulsion stability is increased !

Conventional Emulsifiers Fail to Stabilize !

Mixtures with	20% NOP A 76% PA 1 4% Emulsifier	(Castor Oil), (Ester Polyol)	
Emulsifier / Surfactant	**Structure**	at 40°C	at RT
EO-PO-EO		< 4h	< 1 d
EO-BO-EO		< 4h	< 1 d
Alkylsulfonate		< 4h	< 1 d
PES		< 4h	< 1 d
EP-S-140		20-24 h	> 14 d

NOP & Polyester Blend Stability
- Freshly Mixed -

None

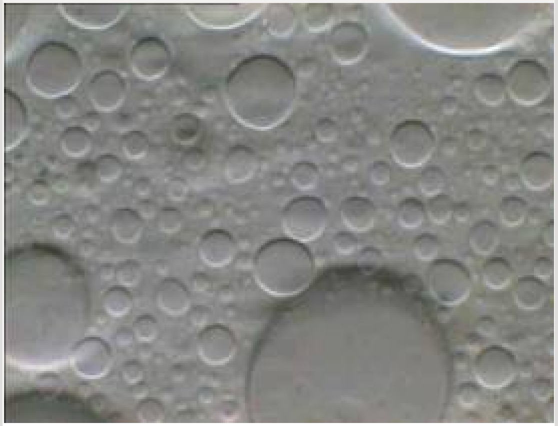


EO-PO-EO

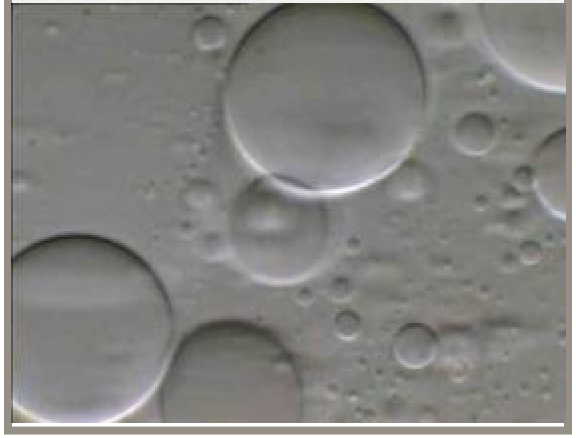
EP-S-140

NOP & Polyester Blend Stability
- 1 h after mixing -

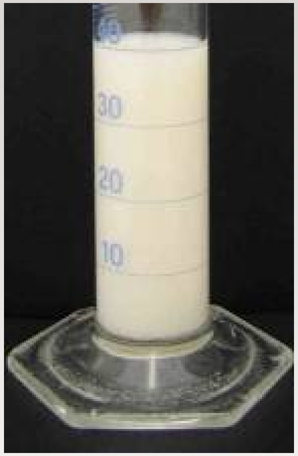
None

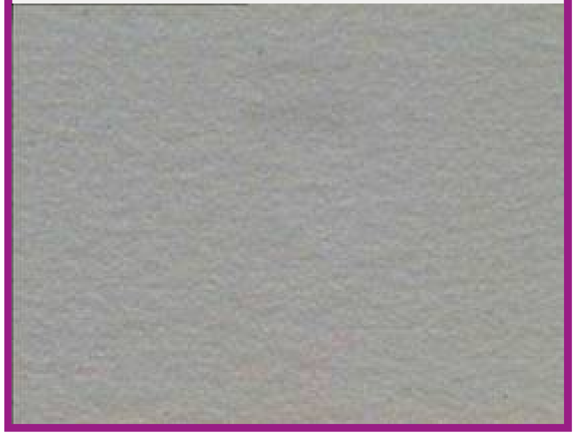


EO-PO-EO



EP-S-140

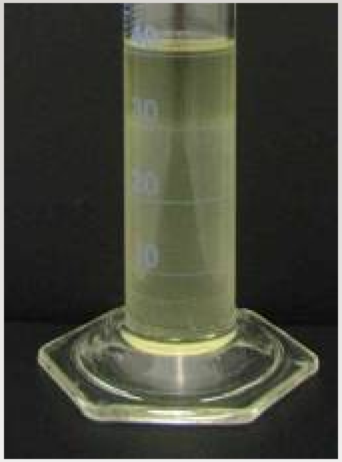




NOP & Polyester Blend Stability
- <u>2h after mixing</u> -

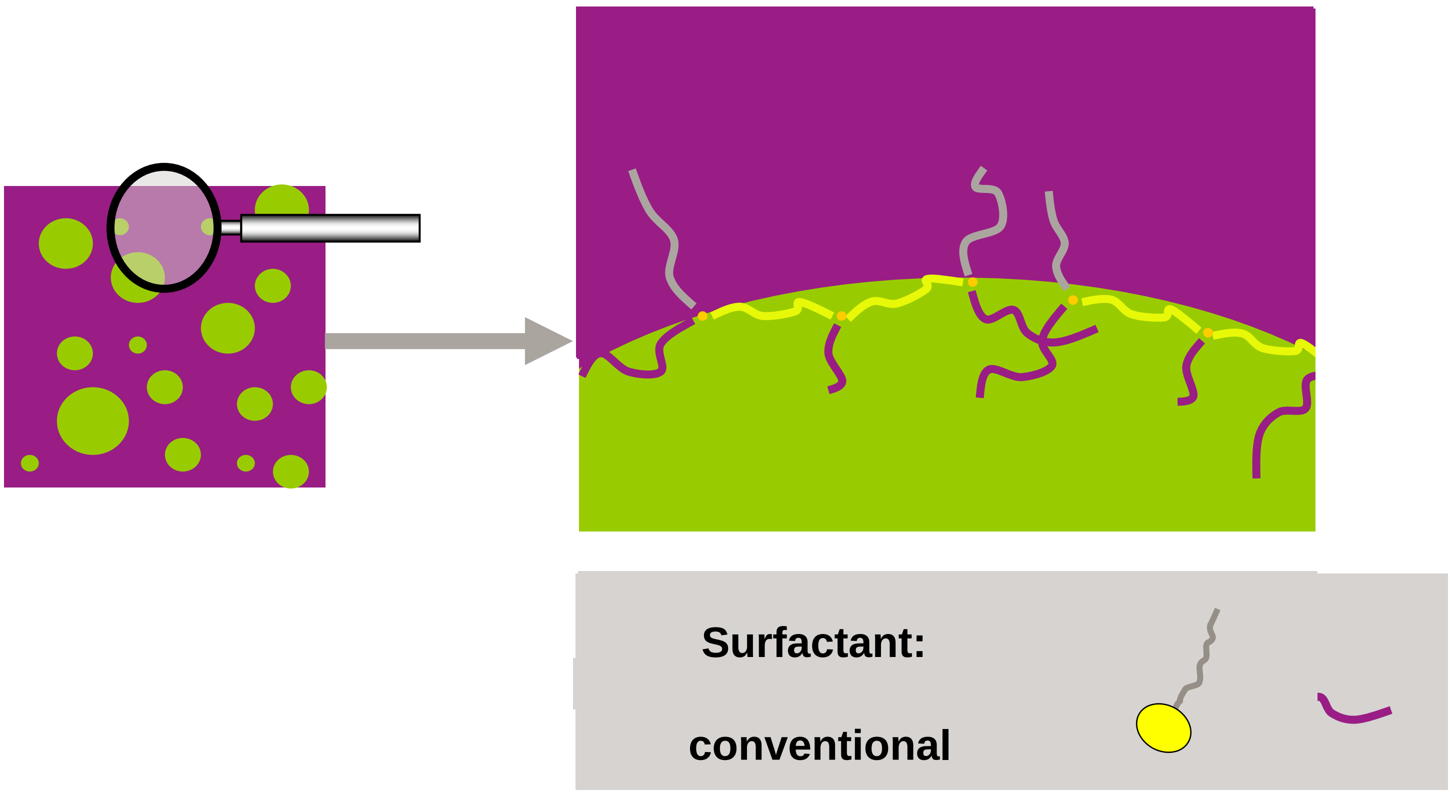
None

EO-PO-EO

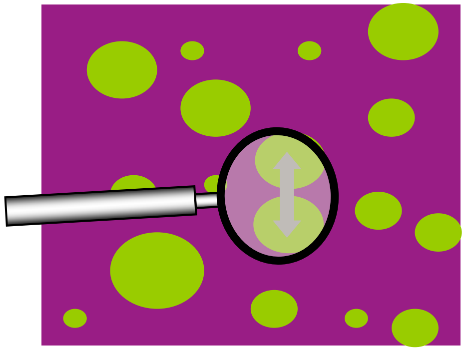


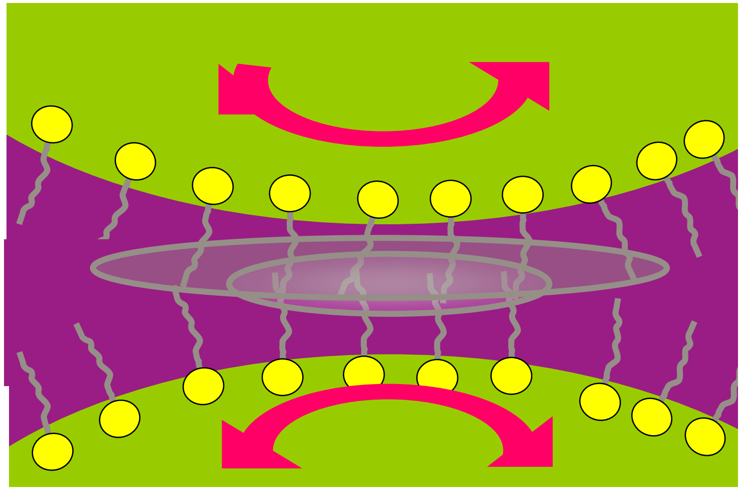
EP-S-140

Novel Surfactant Boost Emulsion Stability



Conventional Emulsifiers Lack Coalescence Prevention

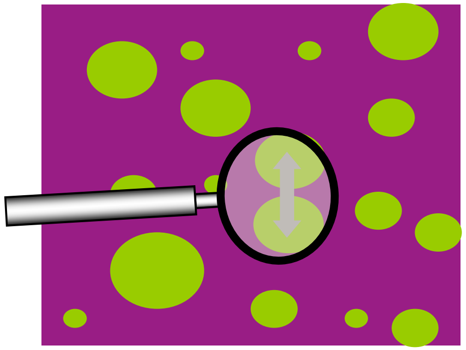


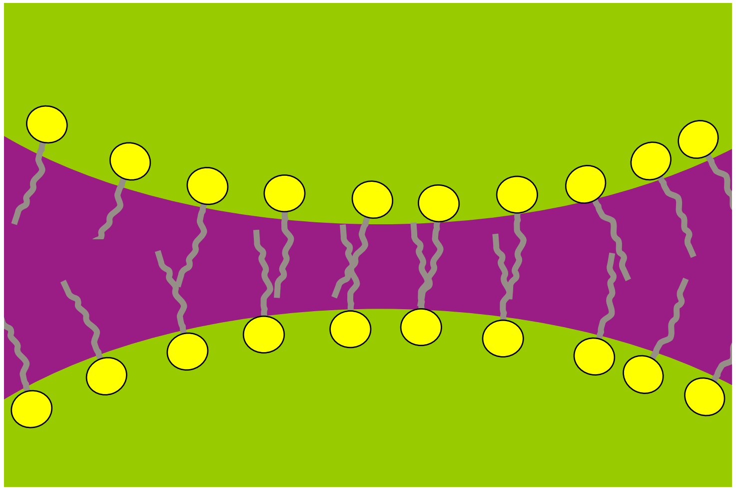


The physiochemical background:

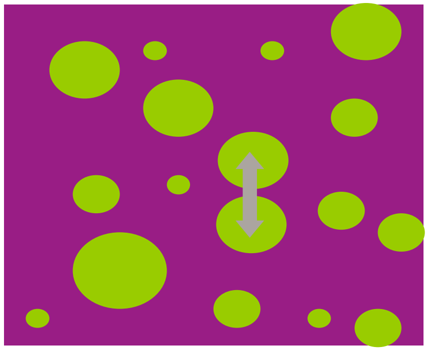
Repulsive forces pull surfactants with “mobility” to lower stress areas

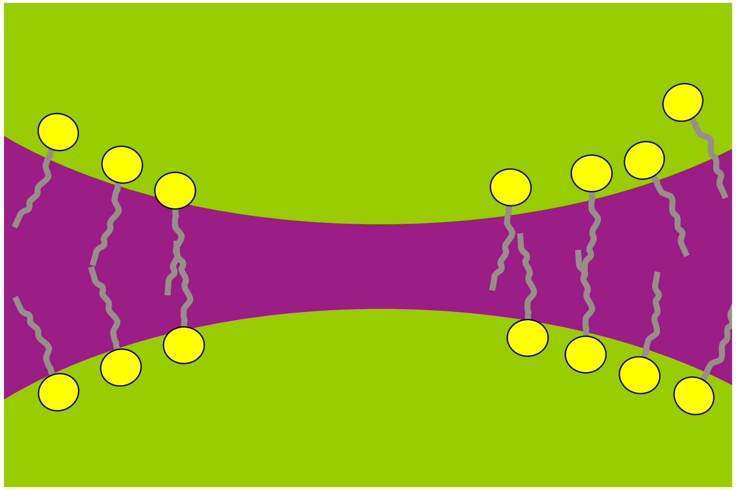
Conventional Emulsifiers Lack Coalescence Prevention



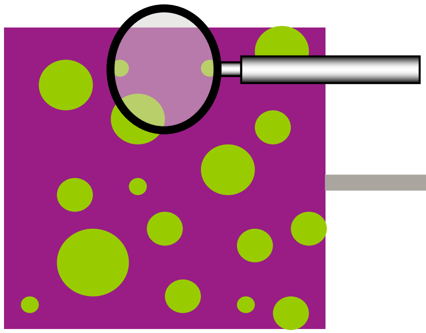


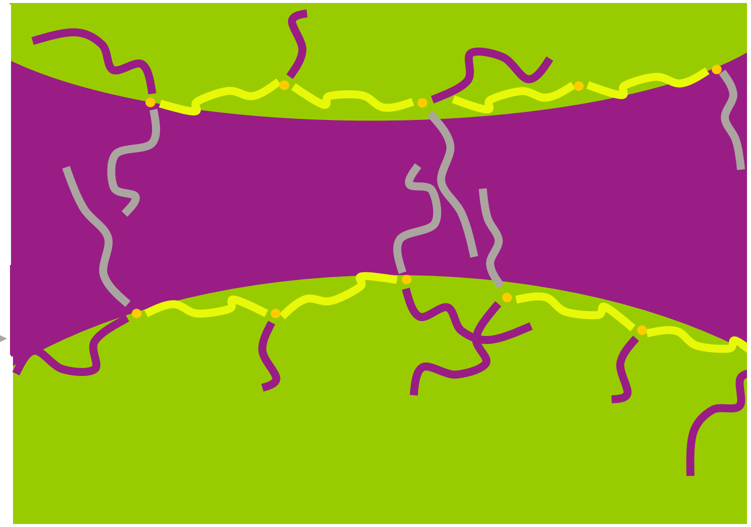
Conventional Emulsifiers Lack Coalescence Prevention





New Emulsifier Technology Clusters to Reduce Coalenscence !





The physicochemical background:

EP-S-140 features high surface activity & substantially reduced mobility

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    a. **Spray Foam**
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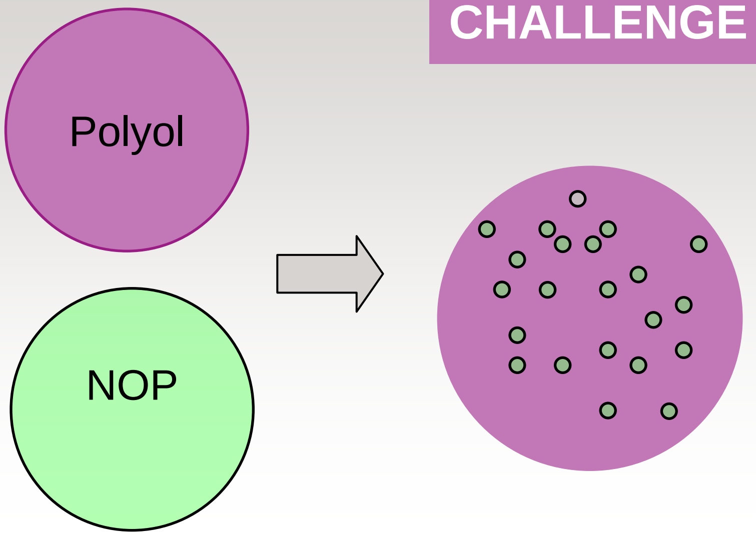
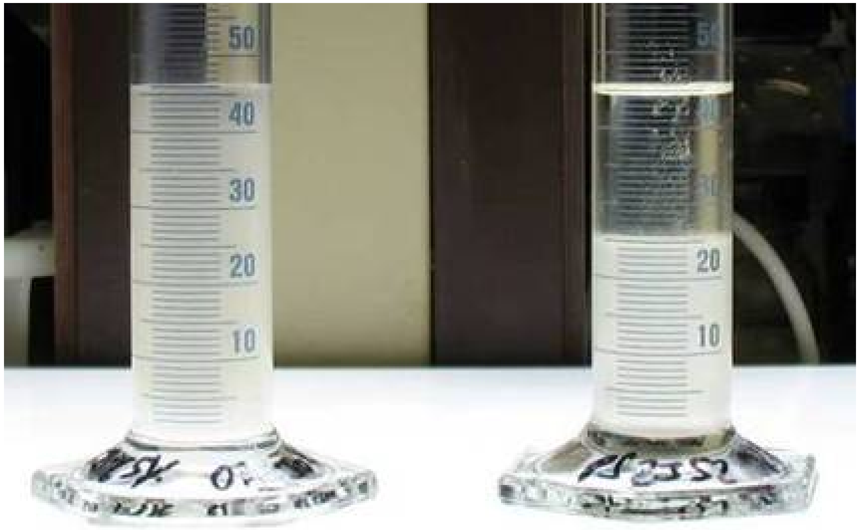
System Stability a Challenge for Spray Foam Applications

Fine & Stable Polyol Premix / System

CHALLENGE 1





Example: 0.5pcf Wall Spray Foam

The Experimental Setup

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Spray System #1 – PET based	
Polyethylene Terephthalate Polyester	25.0
Mannich-based Polyether Polyol	10.0
Sucrose Initiated Polyether Polyol	5.0
Flame Retardants	30.0
Catalysts	8.5
Tegostab B8589	2.5
Water	19.0
Polymeric MDI	1:1 ratio

Spray System #2 – PA based	
Phthalic Anhydide Polyester	25.0
Mannich-based Polyether Polyol	10.0
Sucrose Initiated Polyether Polyol	5.0
Flame Retardants	30.0
Catalysts	8.5
Tegostab B8589	2.5
Water	19.0
Polymeric MDI	1:1 ratio

NOP	Vegetable oil	Chemical modification	OH number	functionality
A	Castor oil	NO	200 -250	3
B	Soybean oil	YES	200 -230	>3
C	Soybean oil	YES	220 -250	>3

Low System Solubility with NOP's

Solubility Limit of Resin Blends

Spray System #1 with 0 - 20% PET-polyester replaced by NOP's after 4h

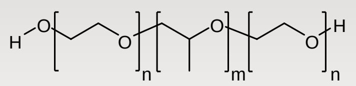
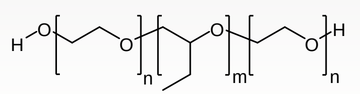
Even without NOP, phase separation occurs

NOP A	NOP B	NOP C

Establishing New Limits with EP-S-140

< 30 Day Resin Side Stability >

Spray System # 1

	Emulsifier	Chemical Structure
I	EP-S-140	trade secret
II	EO-PO-EO	
III	ethoxylathed phenol	
IV	EO-BO-EO	

NOP	Surfactant (Tegostab B8589)	Emulsifier (2.0 pphp)	Max % replacement of Polyester
None	2.0 pphp	None	None
A	None	None	< 5%
A	2.0 pphp	None	< 5%
A	2.0 pphp	EP-S-140	45%
A	2.0 pphp	II	10%
A	2.0 pphp	III	< 5%
A	2.0 pphp	IV	< 5%

Establishing New Limits with EP-S-140

< 30 Day Resin Side Stability >

Spray System	NOP	Surfactant (Tegostab B8589)	Emulsifier	Max % replacement of Polyester
#1	none	2.0 pphp	None	< 5%
	A	2.0 pphp	EP-S-140	45%
	A	2.0 pphp	II	10%
	A	2.0 pphp	III	< 5%
	A	2.0 pphp	IV	< 5%
	none	2.0 pphp	None	< 5%
	B	2.0 pphp	EP-S-140	25%
	B	2.0 pphp	II	< 5%
	B	2.0 pphp	III	< 5%
	B	2.0 pphp	IV	< 5%
	none	2.0 pphp	None	< 5%
	C	2.0 pphp	EP-S-140	30%
	C	2.0 pphp	II	10%
	C	2.0 pphp	III	< 5%
	C	2.0 pphp	IV	< 5%

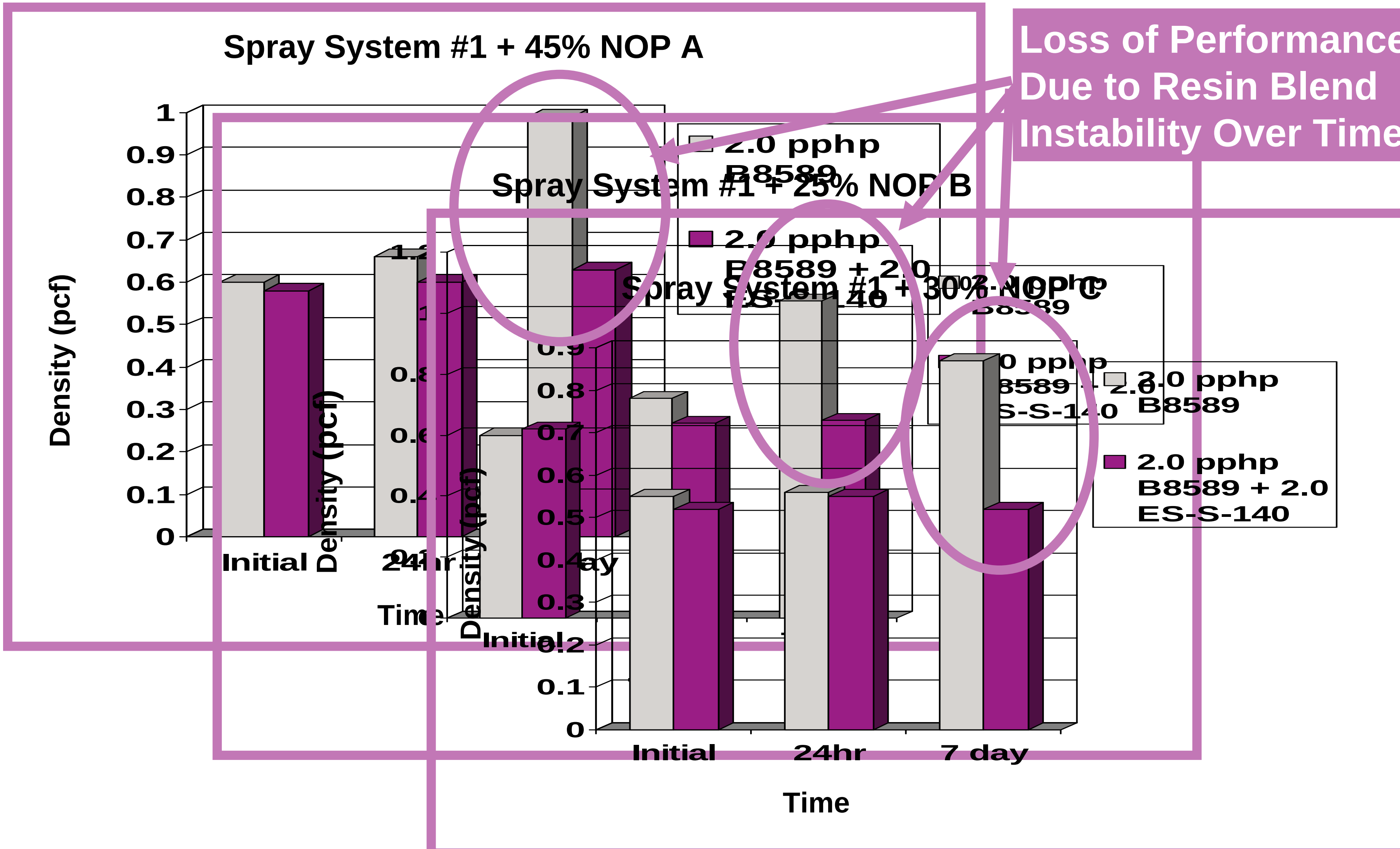
Establishing New Limits with EP-S-140

< 30 Day Resin Side Stability >

Spray System	NOP	Surfactant (Tegostab B8589)	Emulsifier	Max % replacement of Polyester
#2	none	2.0 pphp	None	< 5%
	A	2.0 pphp	EP-S-140	15%
	A	2.0 pphp	II	10%
	A	2.0 pphp	III	< 5%
	A	2.0 pphp	IV	< 5%
	none	2.0 pphp	None	< 5%
	B	2.0 pphp	EP-S-140	25%
	B	2.0 pphp	II	< 5%
	B	2.0 pphp	III	< 5%
	B	2.0 pphp	IV	< 5%
	none	2.0 pphp	None	< 5%
	C	2.0 pphp	EP-S-140	15%
	C	2.0 pphp	II	< 5%
	C	2.0 pphp	III	< 5%
	C	2.0 pphp	IV	< 5%

ES-S-140 Impact on Aged Resin Blends

Loss of Performance Due to Resin Blend Instability Over Time



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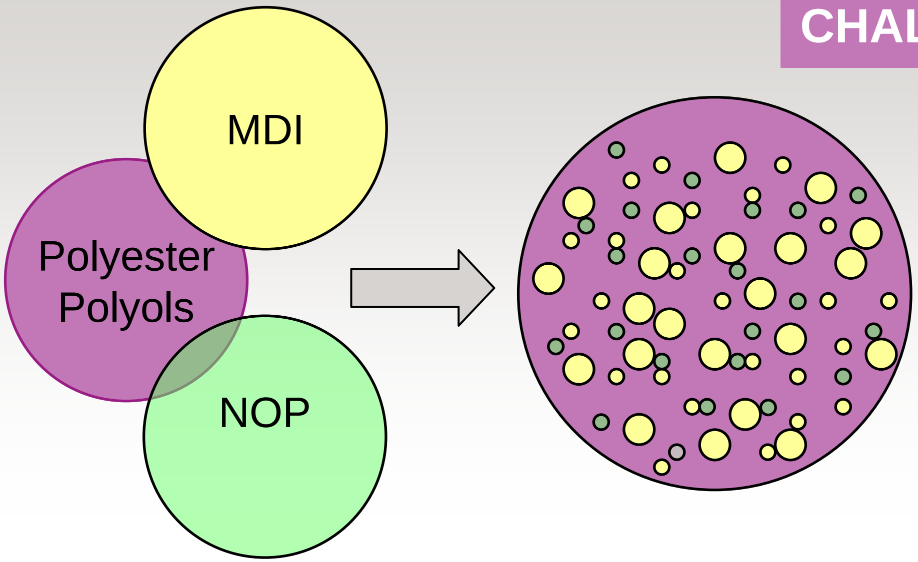
Stable Reaction Mixture a Challenge for Boardstock Applications ?

Homog. & Stable Reaction Mixture

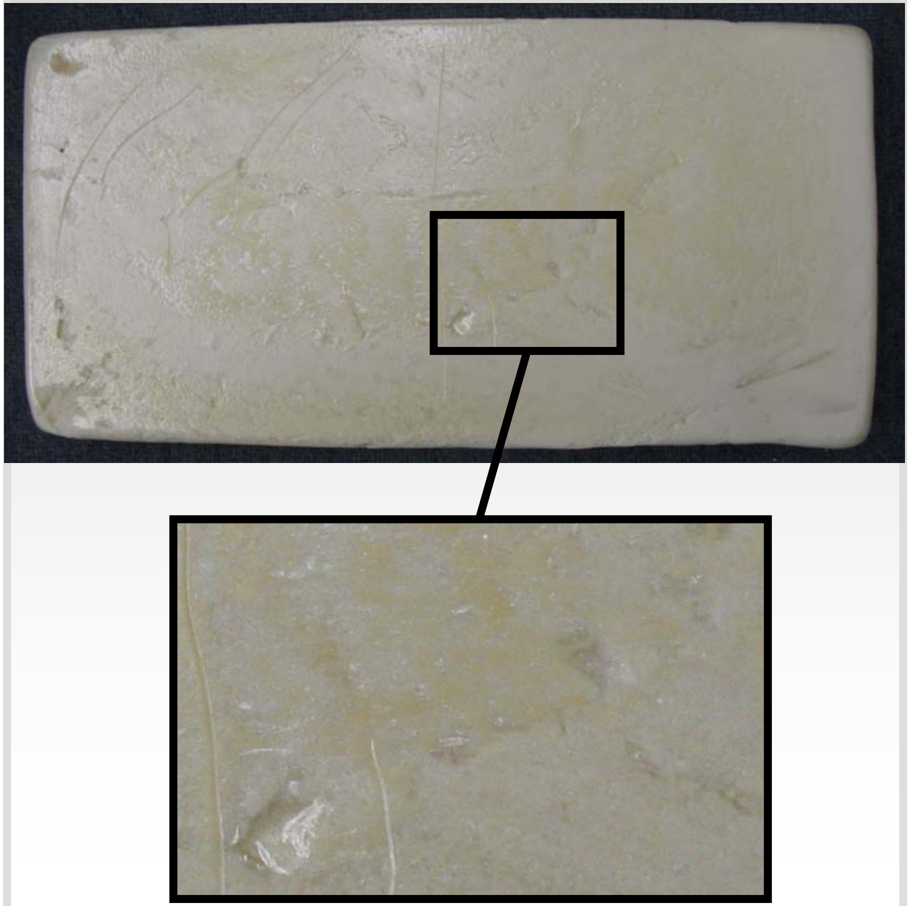
CHALLENGE 2



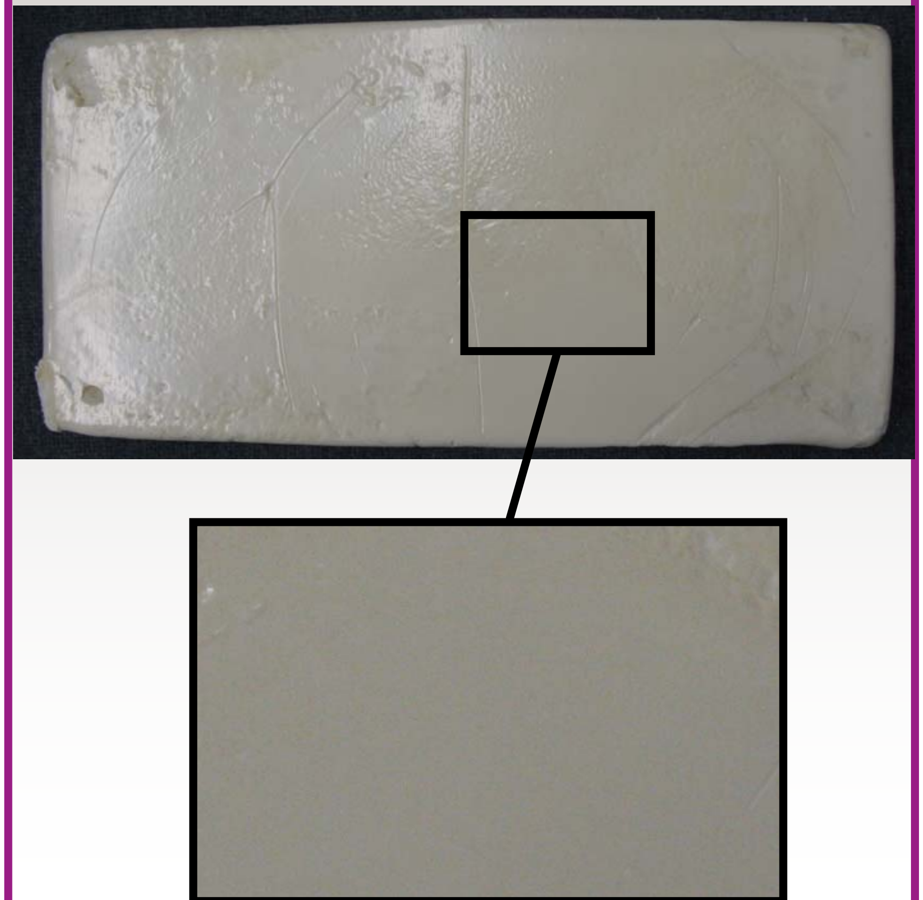
EP-S-140 Stabilize the Reaction Mixture

Boardstock Formulation: 80% PA1 + 20% NOP A

without emulsifier



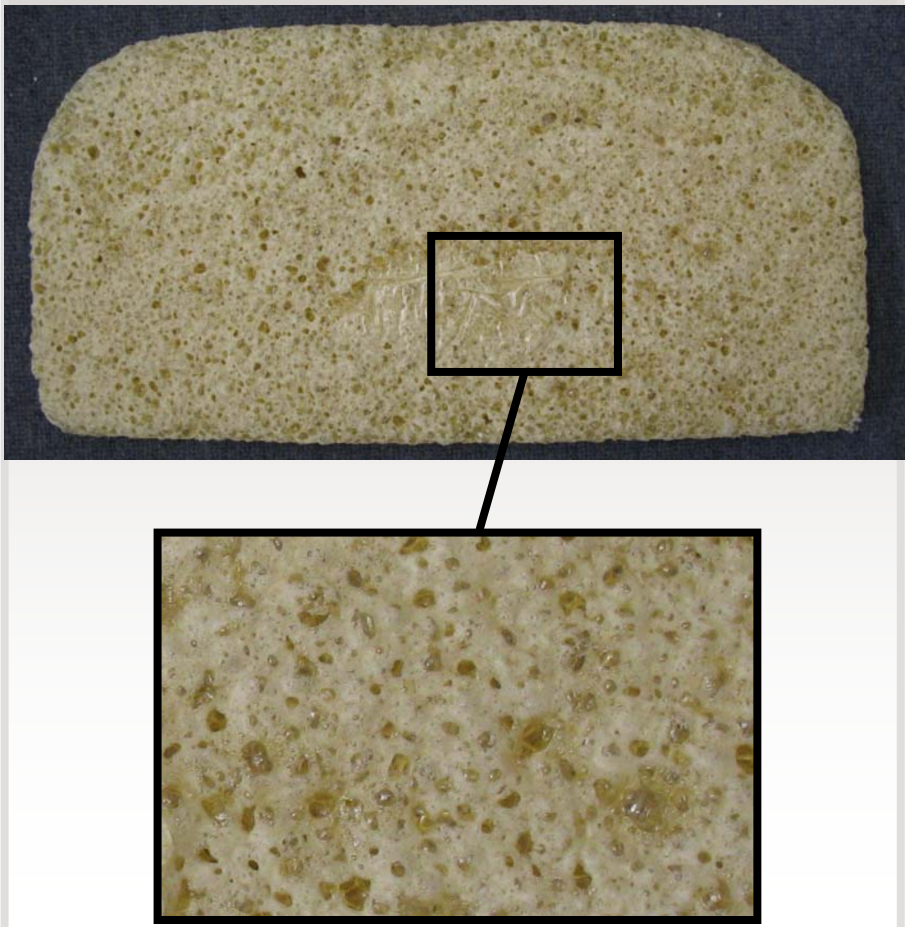
with 1% EP-S-140



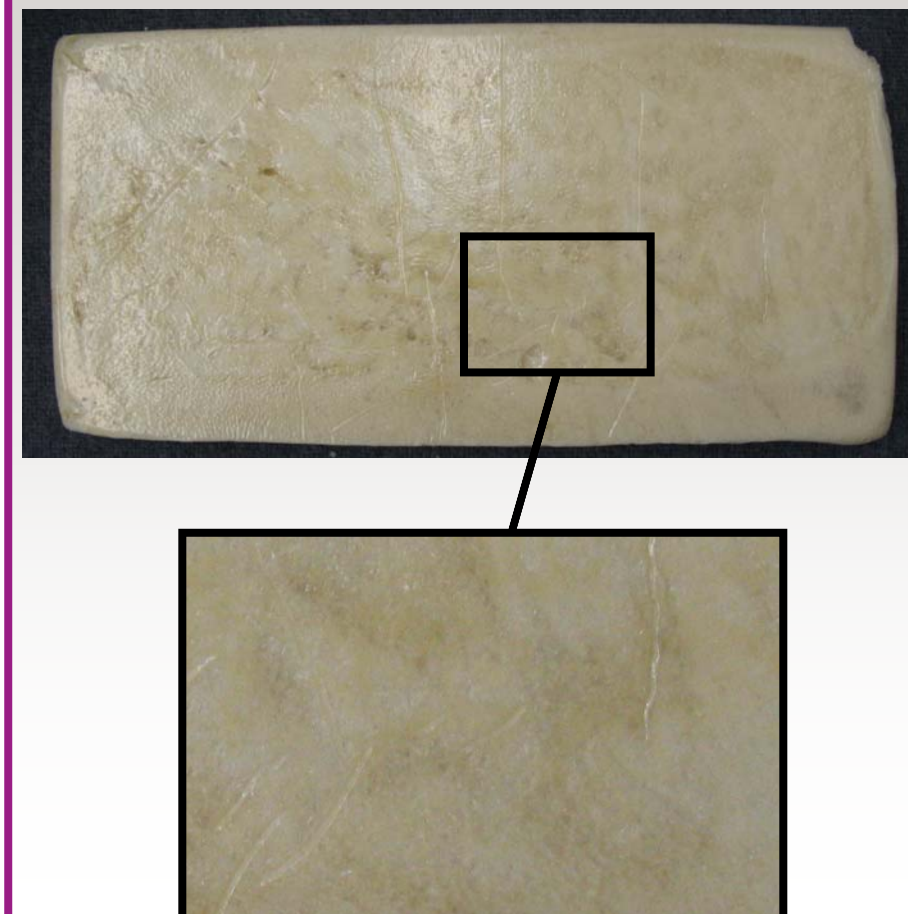
EP-S-140 Stabilize the Reaction Mixture in Critical Formulations

Boardstock Formulation: 70% PA1 + 30% NOP A

without emulsifier



with 2% EP-S-140



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Conclusions:

- The solubility & compatibility limitations of NOPs are real and can have a profound impact on final foam performance.
- Even “modified-NOPs” have their limitations.
- To better utilize NOP technology one must first create a uniform state (resin blend/reaction mixture).
- EP-S-140 helps to enable the use of NOP technology by:
  - Helping to create a uniform resin blend (fine & homogeneous emulsion)
  - Improved resin blend stability (days not hours)
  - Promotes improved A/(B + NOP) mixing,

    resulting in acceptable foam performance
  - Maximize NOP usage – from a system compatibility standpoint

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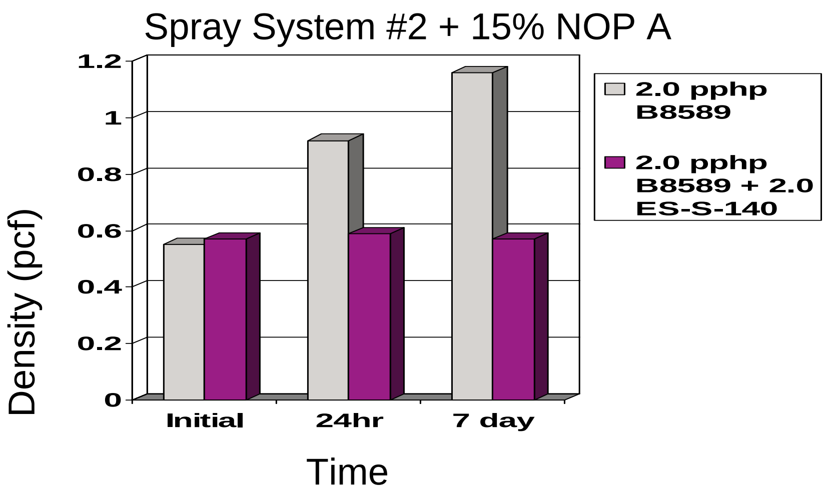
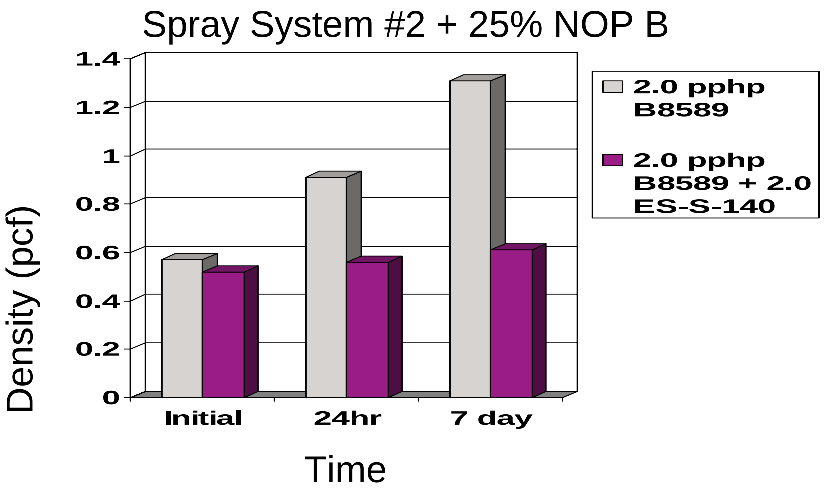
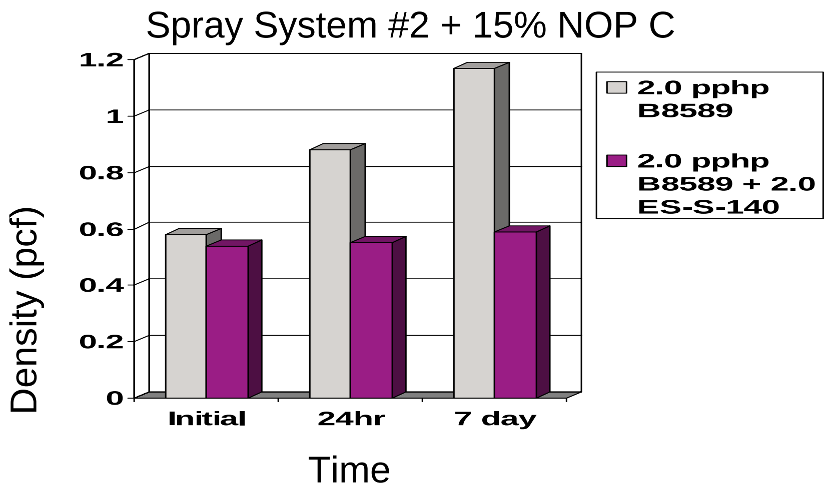

Spray System #2 + 15% NOP A
Density (pcf)
1.2
1
0.8
0.6
0.4
0.2
0
Initial
24hr
7 day
Time
2.0 pphp B8589
2.0 pphp B8589 + 2.0 ES-S-140


Spray System #2 + 25% NOP B
Density (pcf)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Initial
24hr
7 day
Time
2.0 pphp B8589
2.0 pphp B8589 + 2.0 ES-S-140


Spray System #2 + 15% NOP C
Density (pcf)
1.2
1
0.8
0.6
0.4
0.2
0
Initial
24hr
7 day
Time
2.0 pphp B8589
2.0 pphp B8589 + 2.0 ES-S-140