

# Time is Precious: Using DOE to Get New Products on the Shelf Faster

Presented by  
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Stepan Company  
September 20, 2023





# Agenda

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Ingredient Trends in Personal Care Cleansers  
Introduction to Design of Experiments (DOE)  
Using DOE to Develop a Modern Shampoo

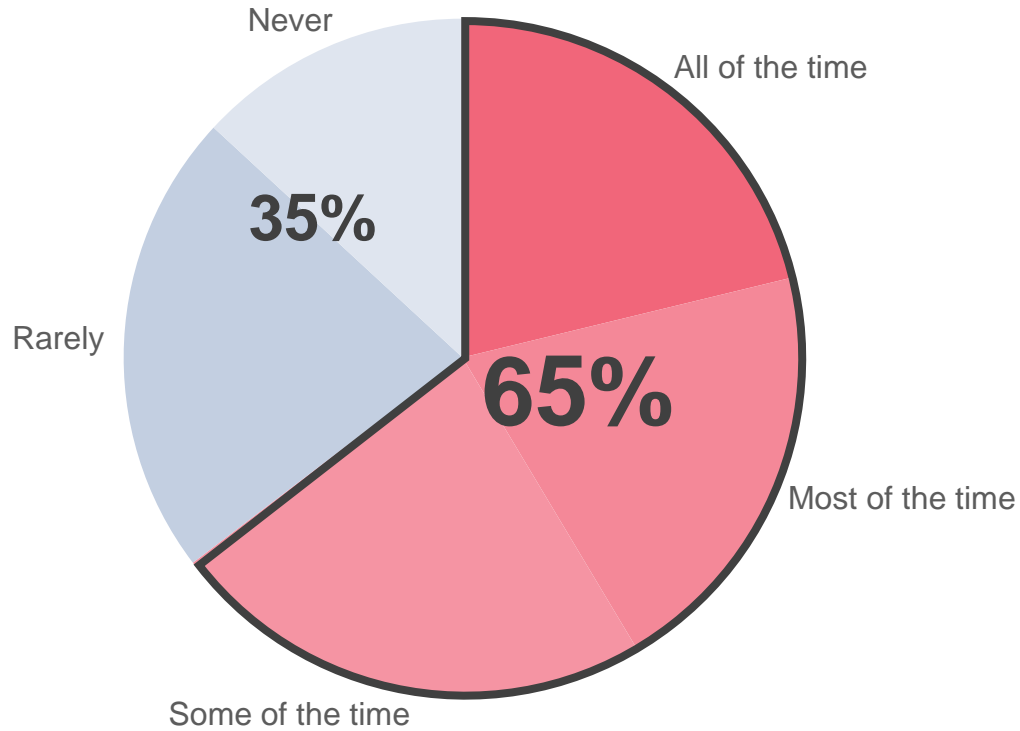


# Ingredient Trends in Personal Care Cleansers

# The Scrutinous Consumer

Consumers regularly research their ingredients by checking the product label.

*"I research the ingredients in my personal care and beauty products..."*



*Product packaging remains the main resource for ingredient information*



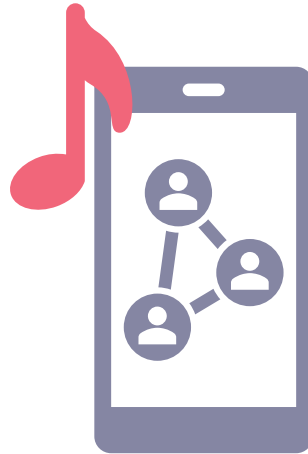
Ingredients: Water, Sodium Lauryl Sulfate, Sodium Laureth Sulfate, Cocamidopropyl Betaine, Glycol Distearate, Dimethicone, Sodium Chloride, Panthenol, Fragrance, Sodium Benzoate, Glycerin, Citric Acid, Tetrasodium EDTA

# Media, Social Attention Leads to Greater Scrutiny

Consumers may take steps to avoid ingredients receiving negative publicity



Retailers' "Banned  
Ingredient" Lists



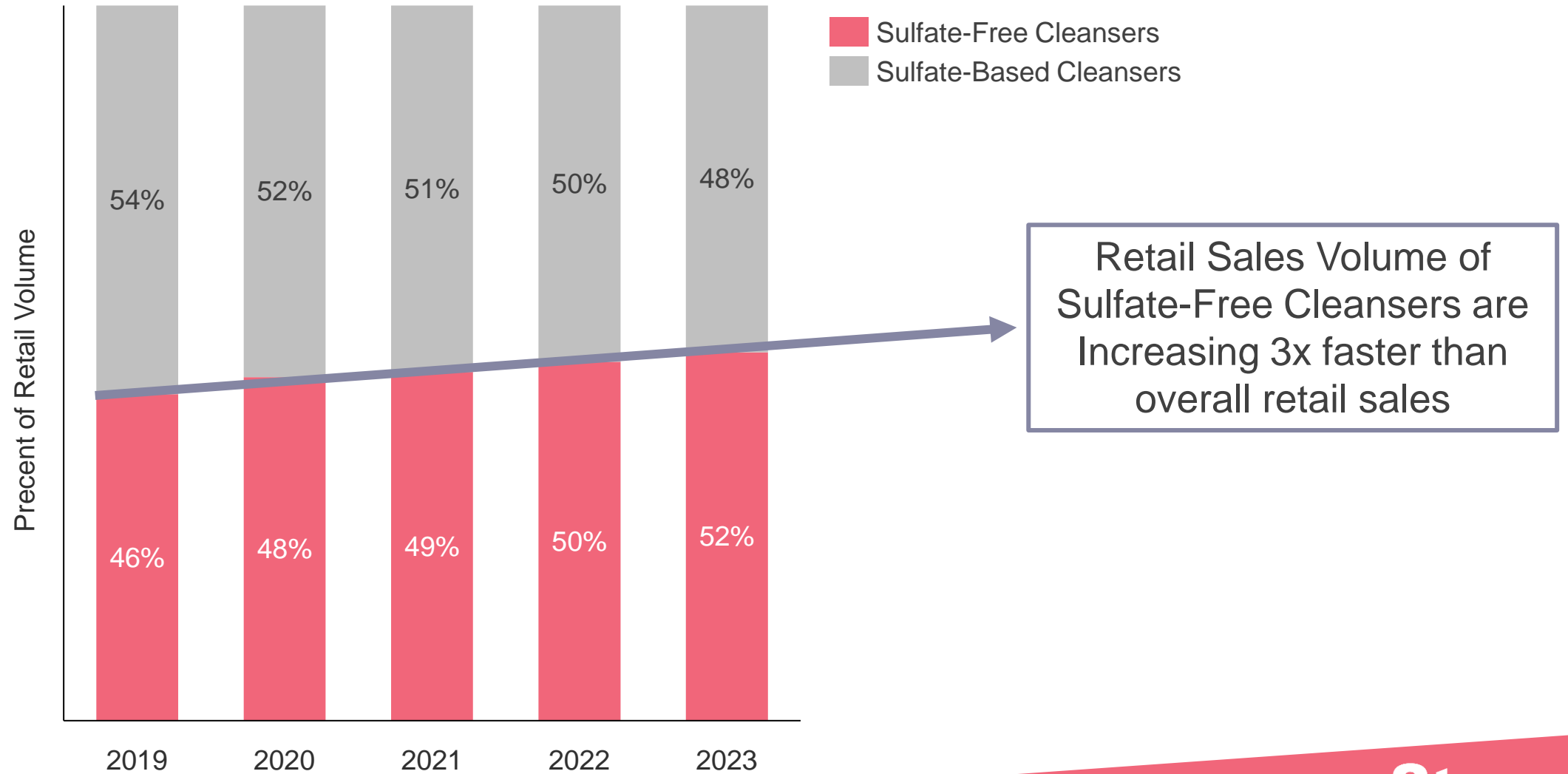
Social  
Media



Government  
Regulations

# Consumers Are Buying Products with Perceived “Safer” Ingredients

For cleansers, retail sales of sulfate-free products continue to overtake traditional sulfate-based products

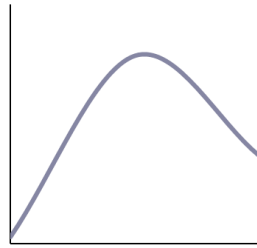


# Formulating Sulfate Free Cleansers Can Be Challenging

High levels of residual salt, poor viscosity building characteristics can lead to an iterative development process

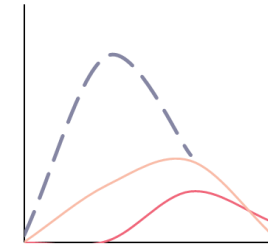
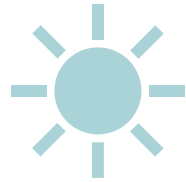
## Sulfate-Based Systems Primary + Secondary Surfactant

Viscosity Response



## Modern Sulfate Free Systems 2+ Co-Surfactants

Clarity, Stability



Development Time



# Modern Formulating Demands Modern Solutions

Mild, powerful secondary surfactants drive performance gains while computer modeling cuts down development time

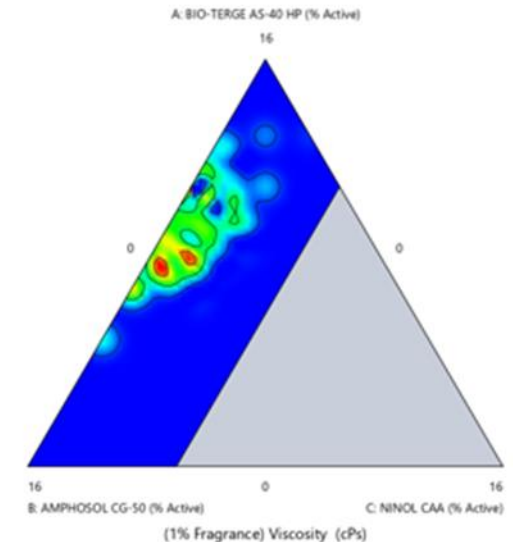
## Overcome Performance Challenges: NINOL<sup>®</sup> CAA

- Maximizes performance
- Enables “no salt added” formulations
- Creates denser, more luxurious foam



## Shorten Development Time: Design of Experiments (DOE)

- Efficient, systematic process
- Can act as a reference for future formulas with similar cleansing ingredients





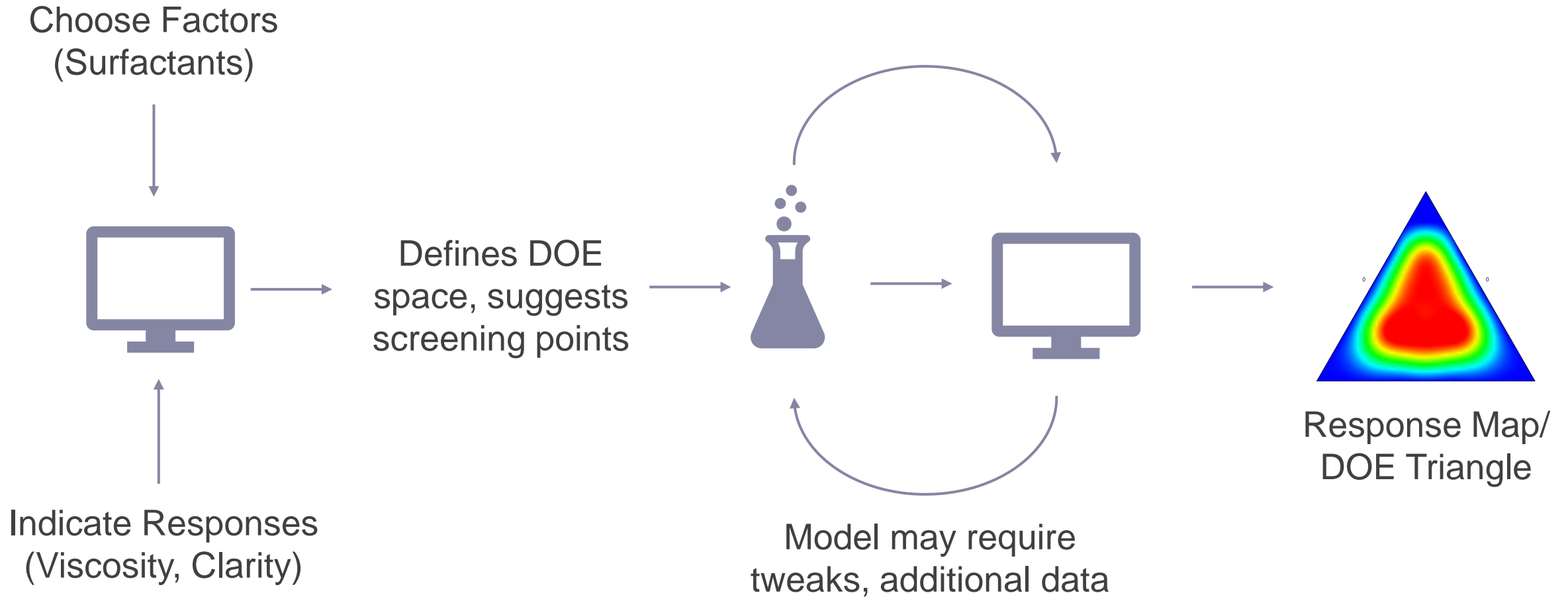


# An Introduction to Design of Experiments (DOE)

# Overview of DOE

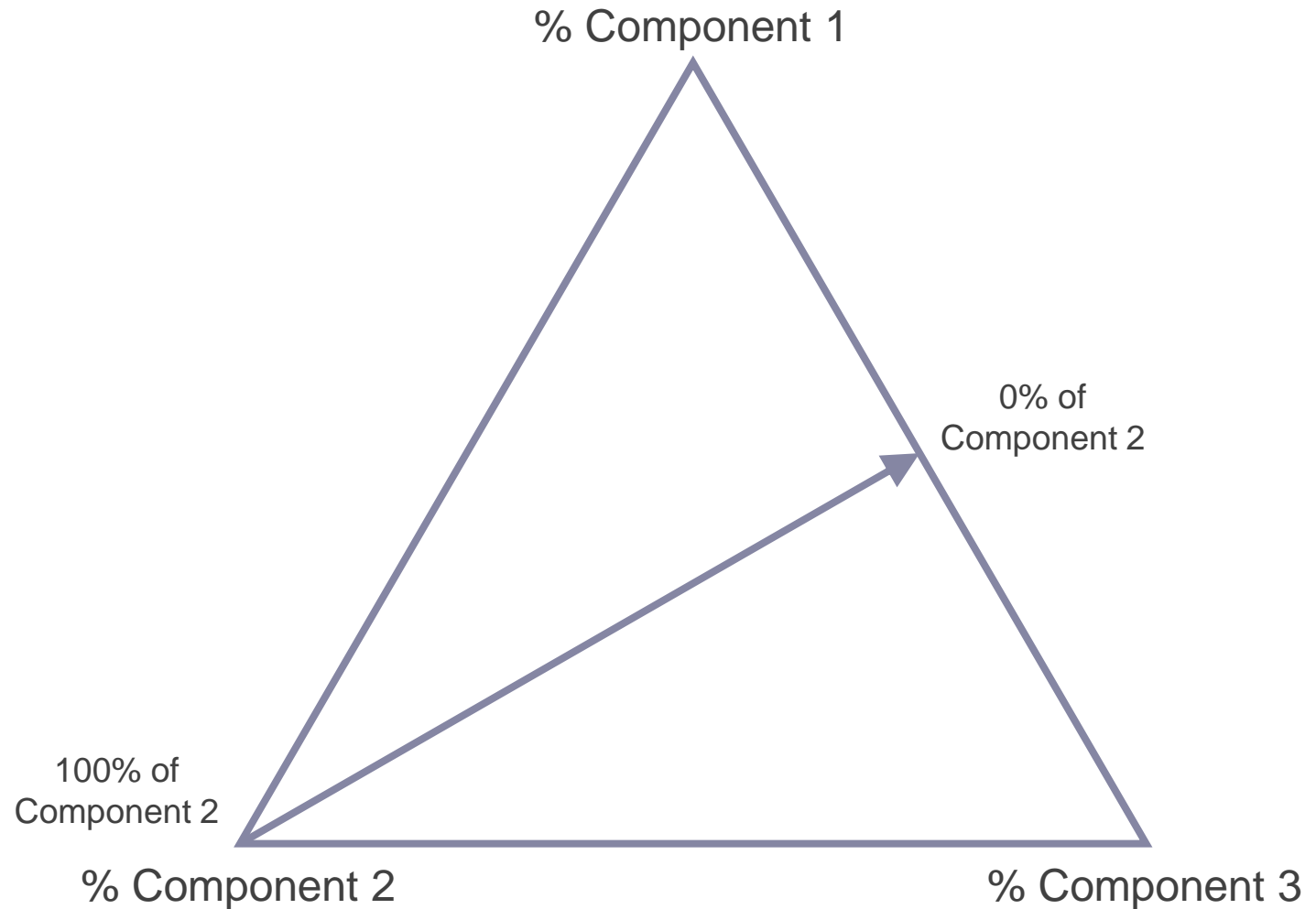
- Design of Experiments: A systematic, efficient methodology that studies the relationship between multiple inputs (factors) and key outputs (responses)
- Factors – surfactants
- Responses – viscosity, clarity, foam, function, etc.
- Multiple programs available for modeling
  - JMP
  - Minitab
  - StatEase

# Process of Using DOE



# Reading a Design Triangle

- Each **COMPONENT** is a modifiable part of the formulation
- Each **VERTEX**, or corner of the triangle, represents 100% of a component (unless otherwise stated)
- As you move away from a vertex, the concentration of that component decreases to 0% (unless otherwise stated)



# Example: Two Co-Surfactants Plus Value-Added Surfactant

Chosen Point Shows:

## Component 1

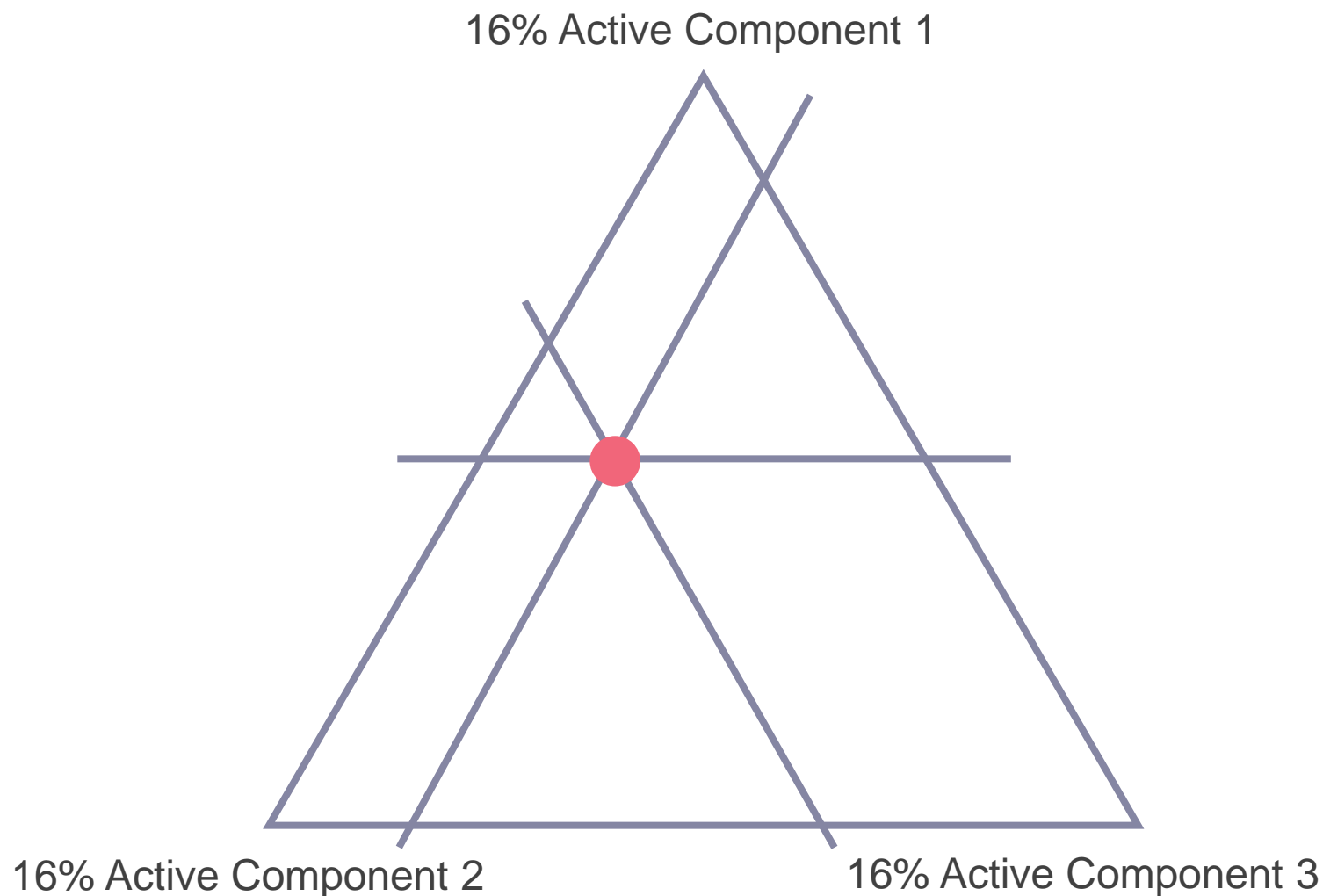
Co-Surfactant: 10% active

## Component 2

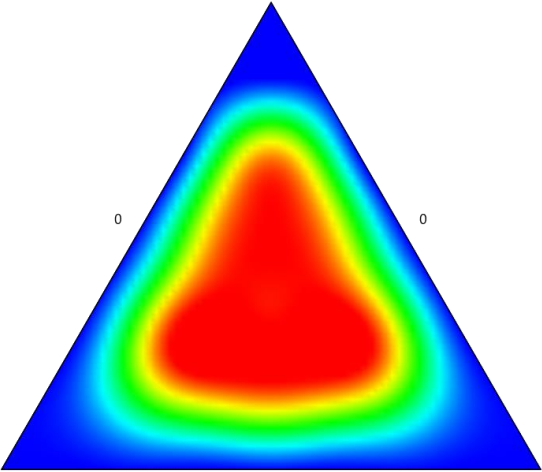
Co-Surfactant: 8% active

## Component 3

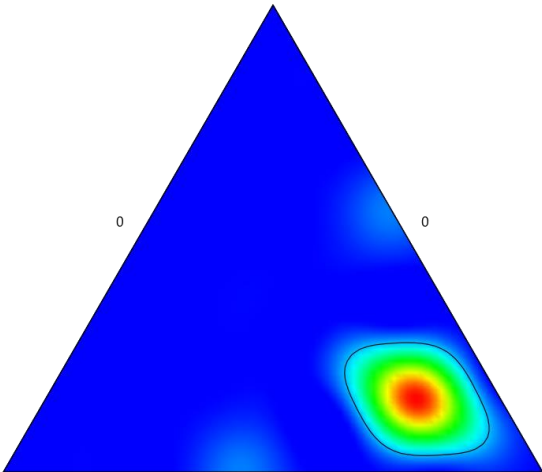
Value-Added Surfactant: 1% active



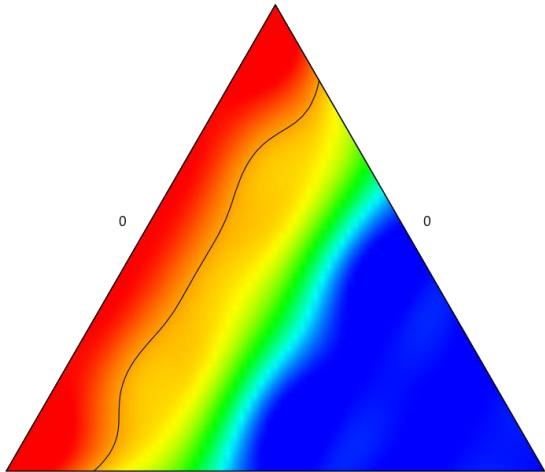
# Interpreting a Design Triangle



Ideal design triangles have medium and high values in the center, low values around the perimeter



Higher values towards a vertex can indicate unique functionality of that specific component



High values along an exterior side indicates the component on the opposing vertex has a depreciating effect



# DOE in Action: Crafting a Modern, Sulfate-Free Shampoo

# Product Development Brief: Modern Shampoo

Product Desired: Modern, Sulfate-Free Shampoo

Benchmarks: OGX

Claims: Sulfate-Free, Volumizing,  
For all hair types,  
No palm/PKO-based ingredients

Characteristics: Clear  
Target viscosity 15,000 cps  
pH 5.5-6.5

Other Ingredients:  
Fragrance: Ocean Fresh WS, 0.5%  
(Belle Aire)  
Preservative: Microcare BDB,  
0.75% (Thor)

Cost: Less than \$0.60/lb for  
cleansing base (actives)

## Factors (Inputs):

- Component 1: BIO-TERGE® AS-40 HP  
(Sodium C14-16 Olefin Sulfonate)
- Component 2: AMPHOSOL® CG-50  
(Cocamidopropyl Betaine)
- Component 3: NINOL CAA  
(Dimethyl Lauramide/Myristamide)

## Responses (Outputs):

- Viscosity
- Clarity
- Formula Cost



# Choosing the Right Ingredients

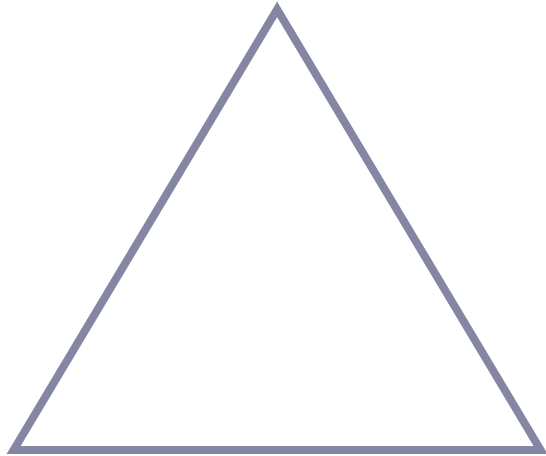
Product Name	INCI Name	Preservative	Active, %	Natural Source	BCI, %
AMPHOSOL CG-50	Cocamidopropyl Betaine	None	43	Coconut	60
BIO-TERGE AS-40 HP	Sodium C14-16 Olefin Sulfonate	None	40	Synthetic	0
NINOL CAA	Dimethyl Lauramide/Myristamide	None	100	Coconut	86

↑  
Preservative flexibility  
for final formulation

↑  
Only coconut as  
natural source

# Setting Up the DOE Triangle - Viscosity

% BIO-TERGE AS-40 HP



% AMPHOSOL CG-50

% NINOL CAA



pH = 5.5

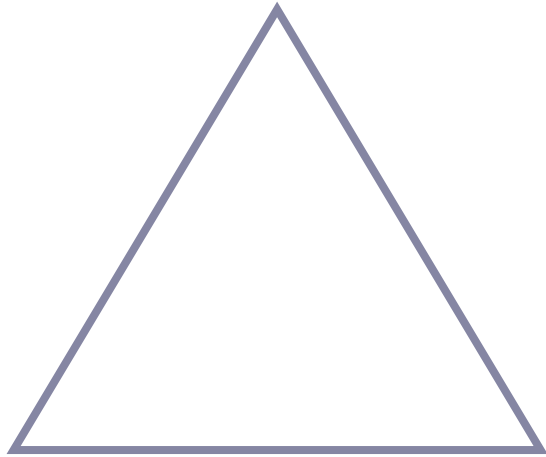
Active = 16%

Response Type: Viscosity

Balance:  
Water, Fragrance,  
Preservative, Other

# Setting Up the DOE Triangle - Viscosity

% BIO-TERGE AS-40 HP



% AMPHOSOL CG-50

% NINOL CAA



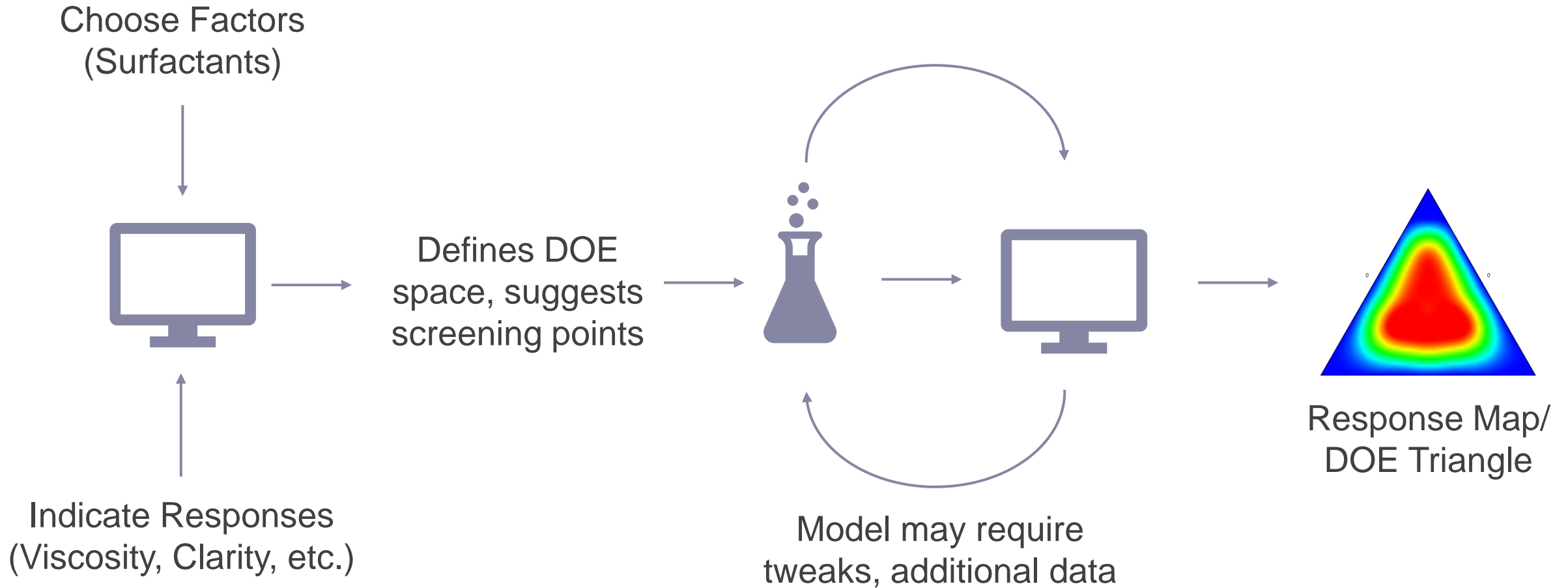
pH = 5.5  
Active = 16%  
Response Type: Viscosity

Balance:  
Water, Fragrance,  
Preservative, Other

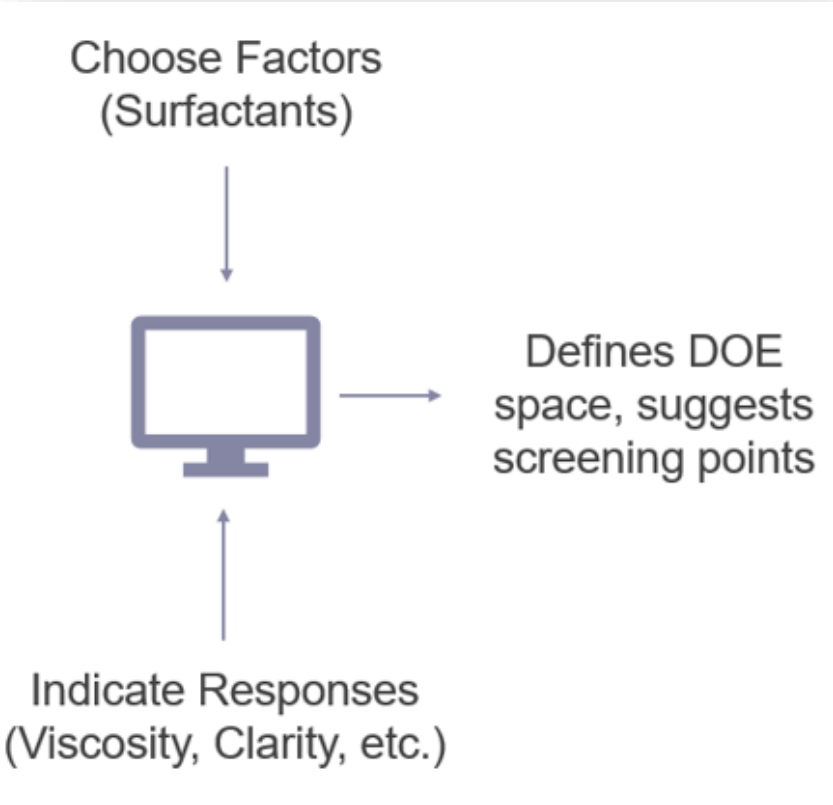


How many datapoints are needed to make a DOE model?

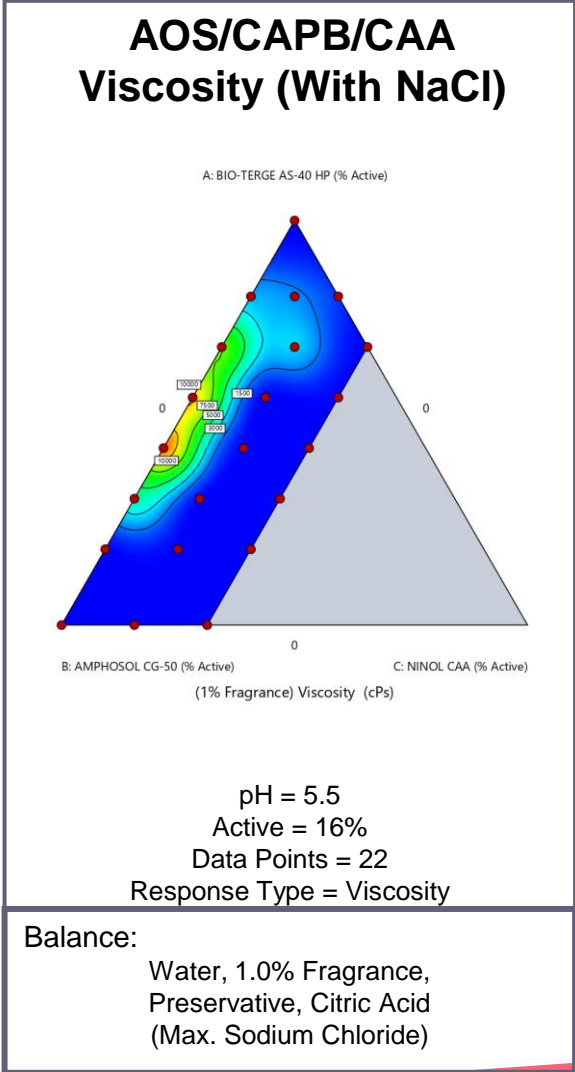
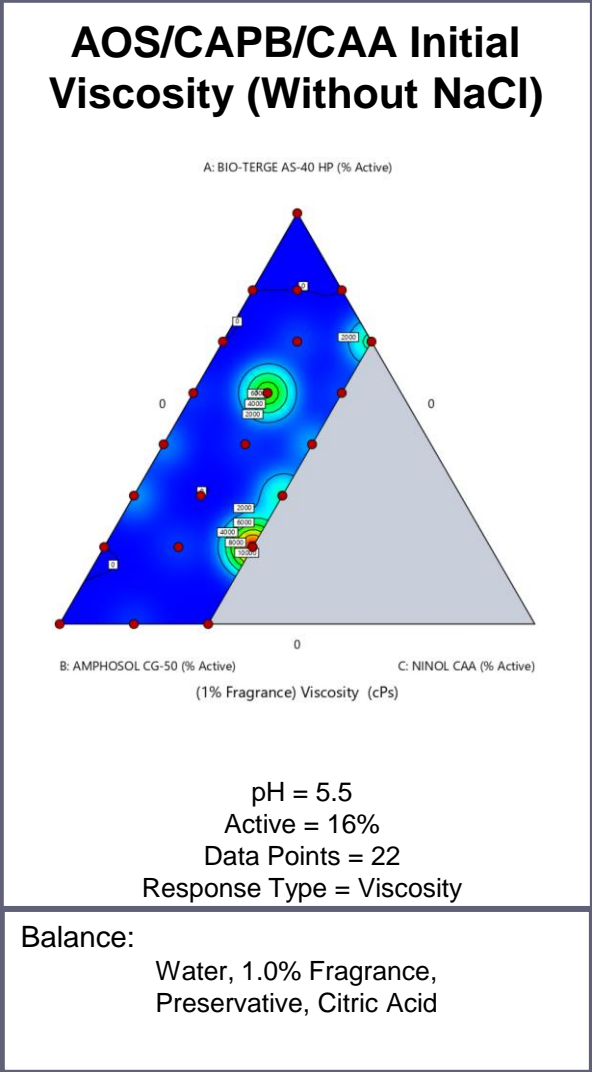
# Process of Using DOE



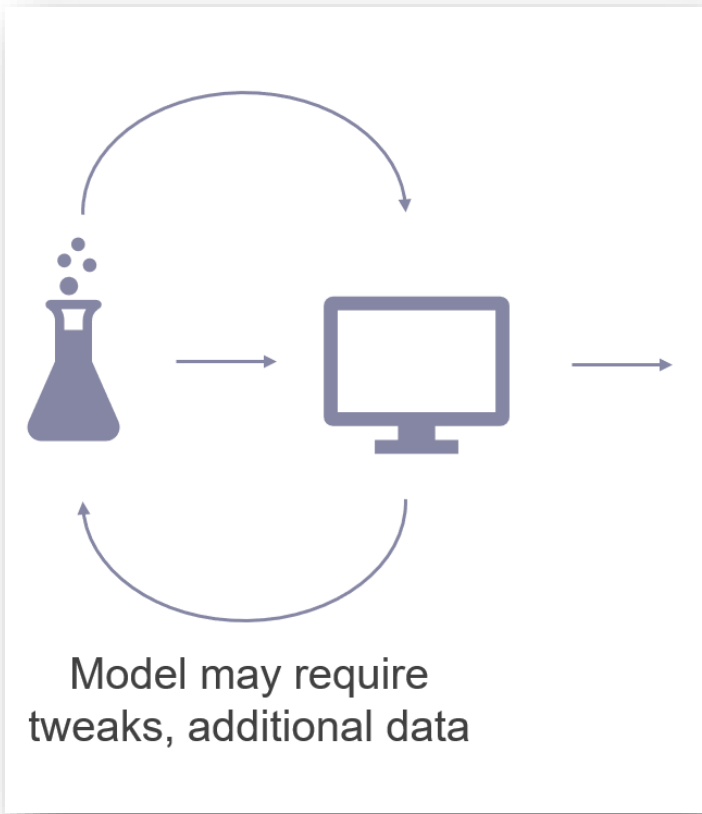
# Shampoo Viscosity Initial Results



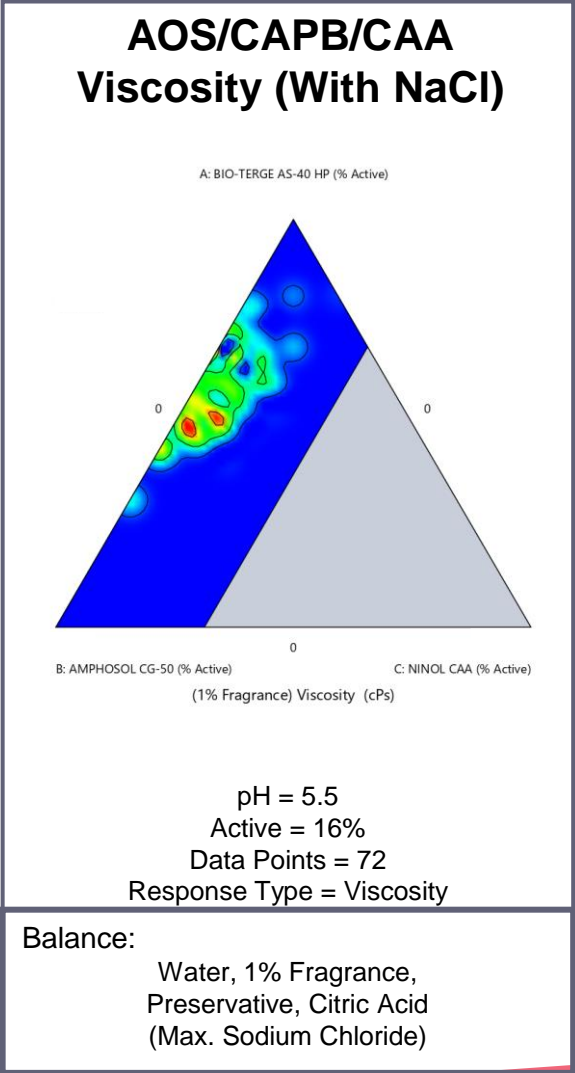
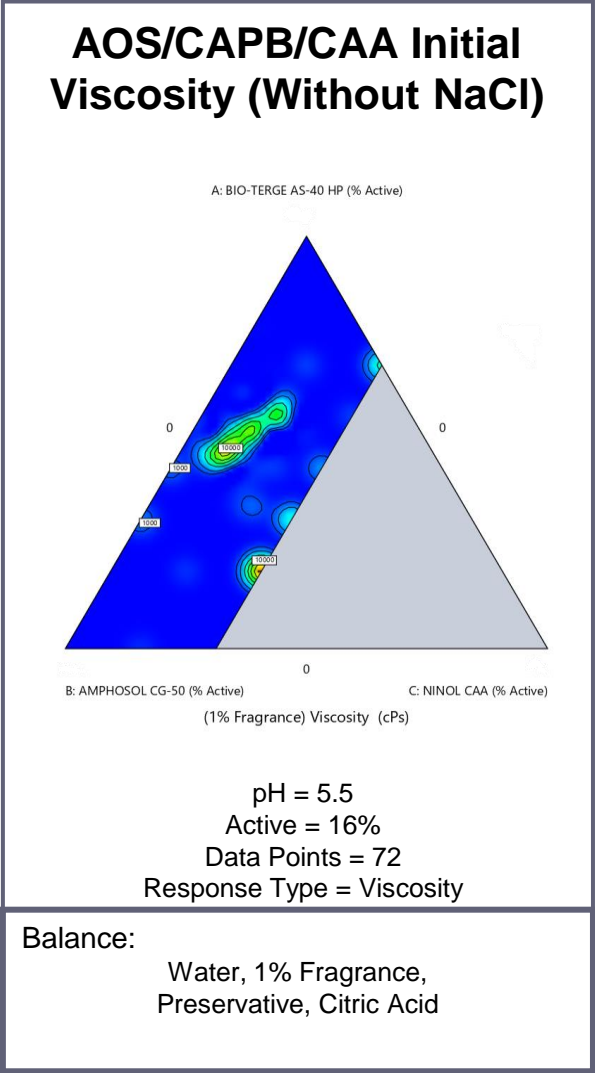
22 points



# Shampoo Viscosity Results with Additional Data



# 72 points

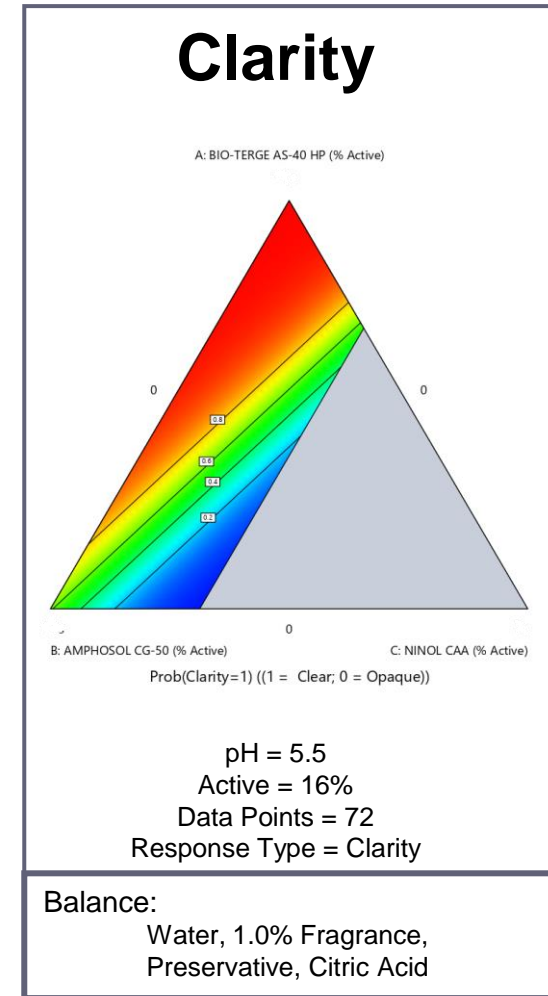


# Maximizing Shampoo Clarity

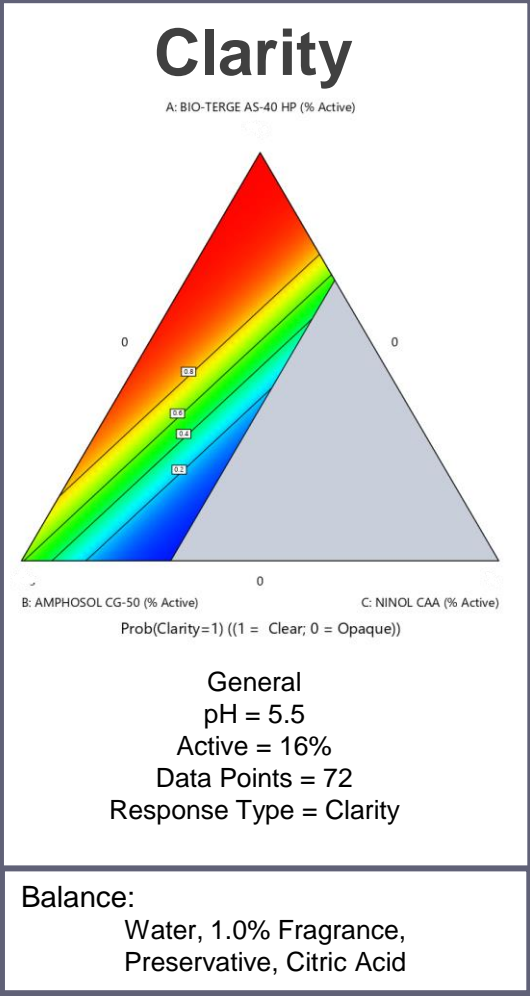
Can use subjective (visual) or objective (turbidity) methods to evaluate clarity

- Visual analysis needs distinct differentiation – responses are designated "1" for crystal clear and "0" for any amount of haze
- Modeling program then shows values between 0 and 1 to reference the highest probability of getting a clear product

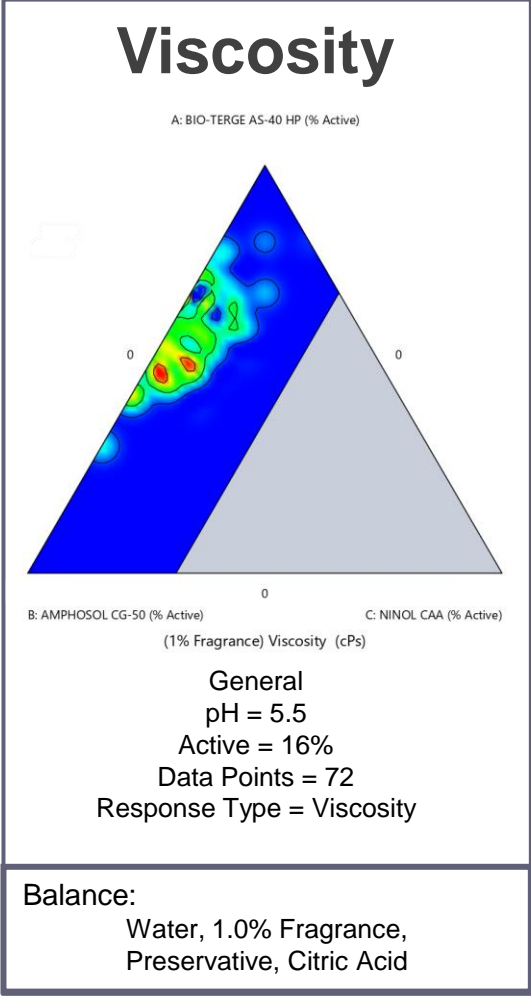
Alternatively, turbidity measurements can be used for response values



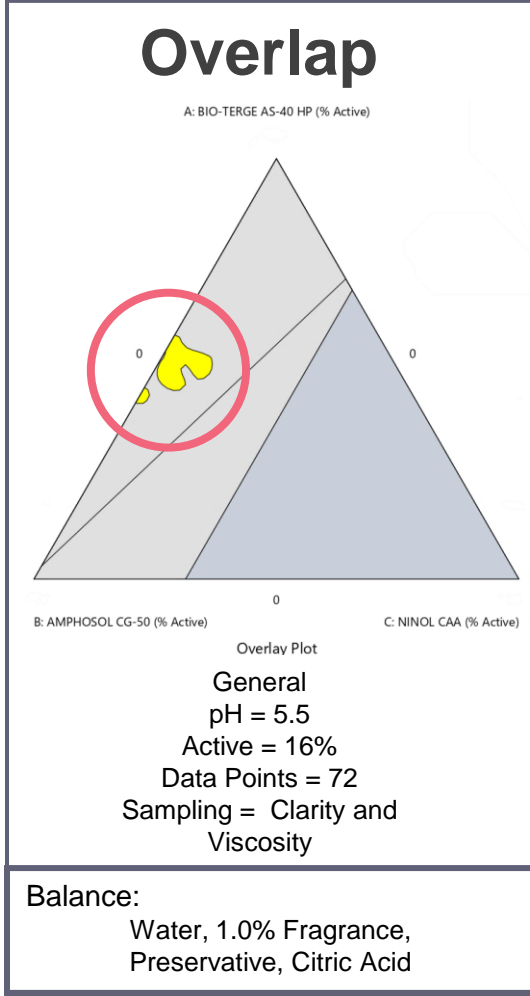
# Combining Clarity & Viscosity to Define Cleansing Base



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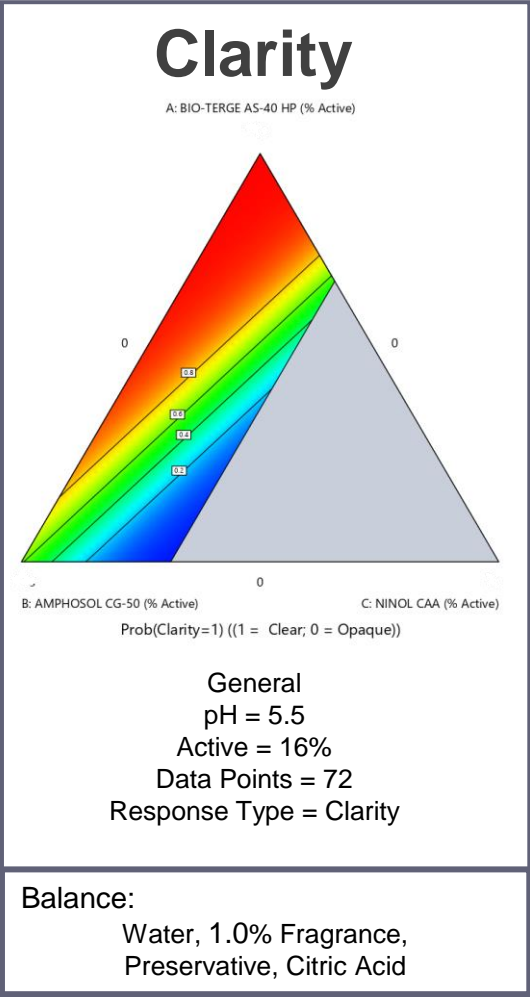


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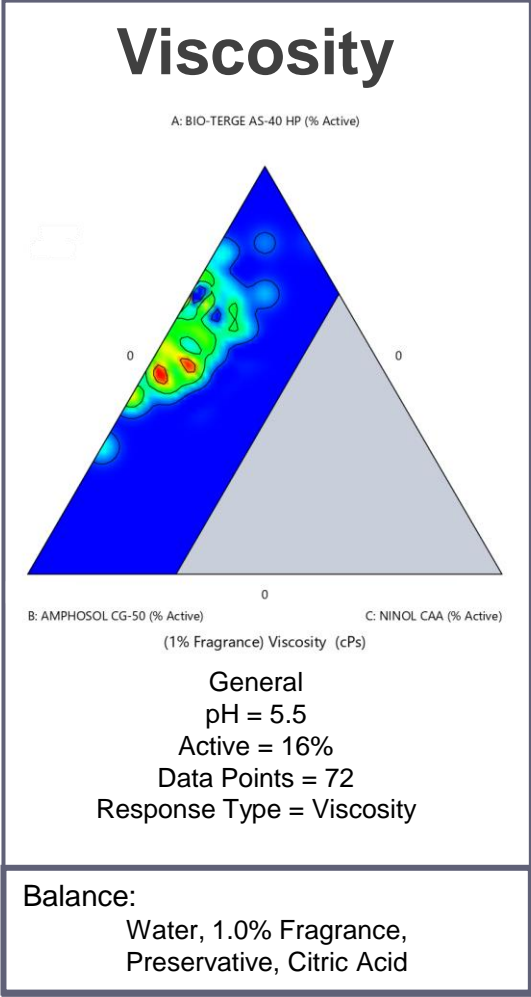




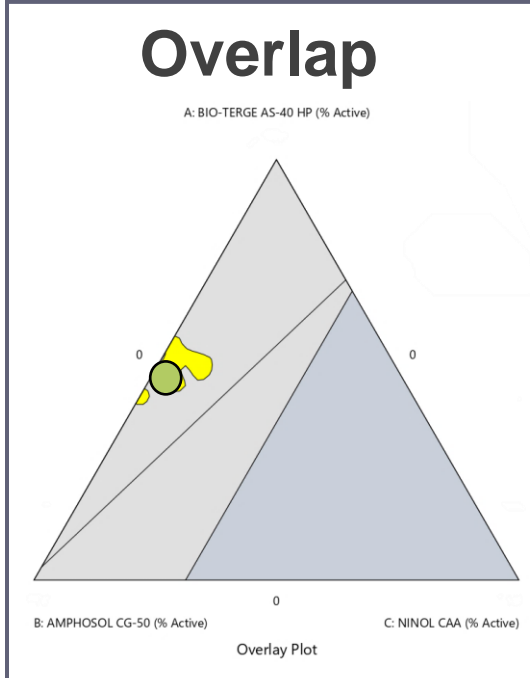
# Combining Clarity & Viscosity to Define Cleansing Base



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Ingredient	DOE Actives Ratio (w/ salt)
<b>BIO-TERGE AS-40 HP</b> <i>Sodium C14-16 Olefin Sulfonate</i>	<b>0.50</b>
<b>AMPHOSOL CG-50</b> <i>Cocamidopropyl Betaine</i>	<b>0.47</b>
<b>NINOL CAA</b> <i>Dimethyl Lauramide/Myristamide</i>	<b>0.03</b>

# Optimizing Shampoo Cost

Ingredient	Price (\$/Lb)* 100% Active
<b>BIO-TERGE AS-40 HP</b> <i>Sodium C14-16 Olefin Sulfonate</i>	\$5.40
<b>AMPHOSOL CG-50</b> <i>Cocamidopropyl Betaine</i>	\$8.85
<b>NINOL CAA</b> <i>Dimethyl Lauramide/Myristamide</i>	\$5.40



Ingredient	DOE Actives Ratio (w/salt)	Optimization Trial 1: 6% Total Actives	Optimization Trial 2: 8% Total Actives
<b>AS-40 HP</b>	<b>0.50</b>	<b>3.00%</b>	<b>4.00%</b>
<b>CG-50</b>	<b>0.47</b>	<b>2.80%</b>	<b>3.75%</b>
<b>CAA</b>	<b>0.03</b>	<b>0.20%</b>	<b>0.25%</b>
<b>Total Cost Per Lb</b>	<b>--</b>	<b>\$0.421</b>	<b>\$0.562</b>
<b>Viscosity, Clarity</b>	<b>--</b>	<b>?</b>	<b>?</b>

## From Brief:

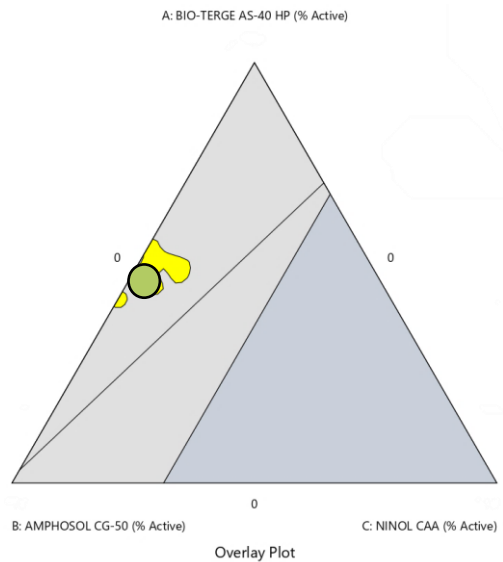
Viscosity of 15,000 cps

Cost <\$0.60/lb for cleansing base (actives)

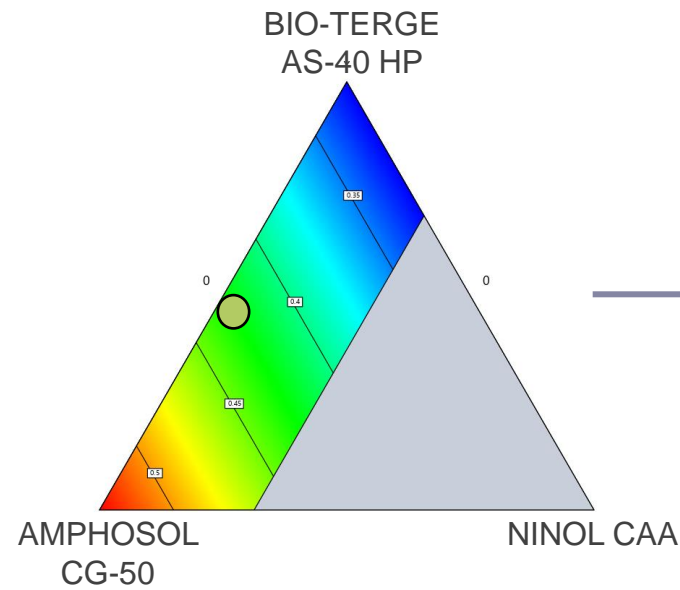
\*Prices indicated are for reference only; please contact your Stepan Sales Representative for an official price quote for any Stepan material.

# DOE Can Optimize Formula Cost

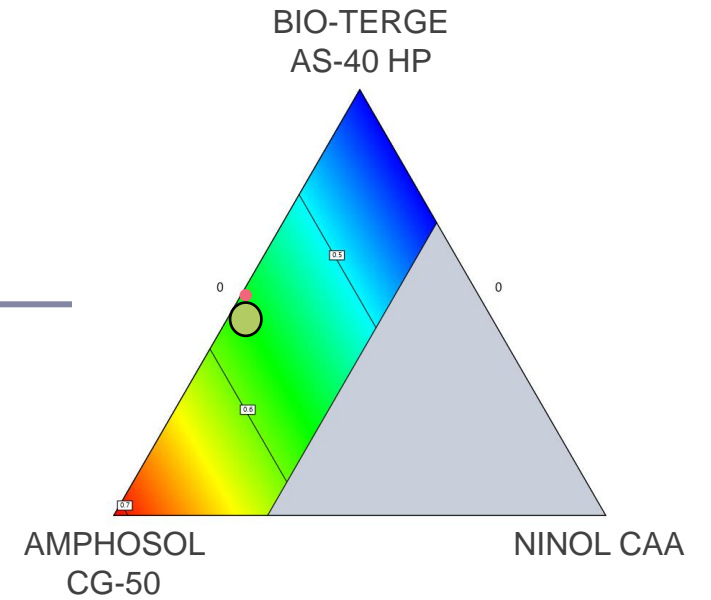
The sum of ratios = 1.0



**Viscosity/Clarity  
Overlap**



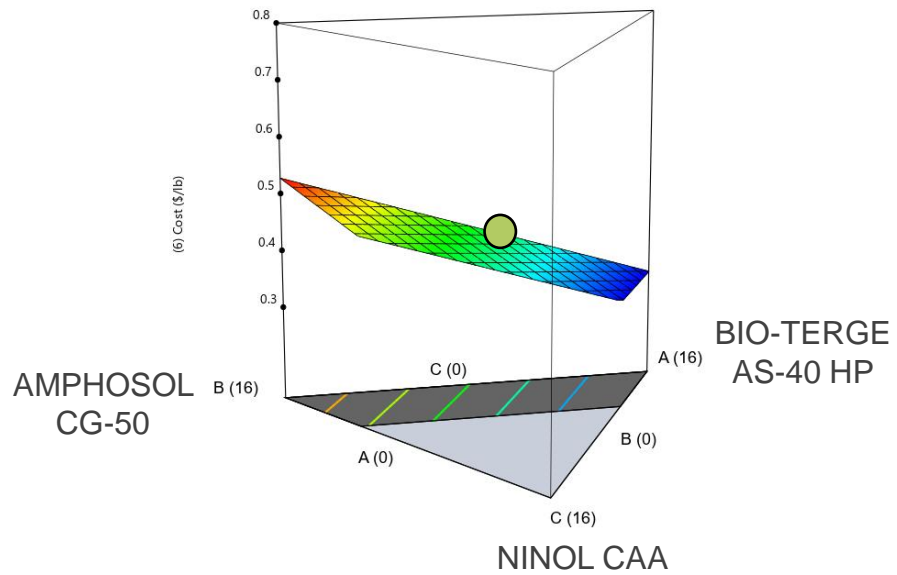
**6% Actives**



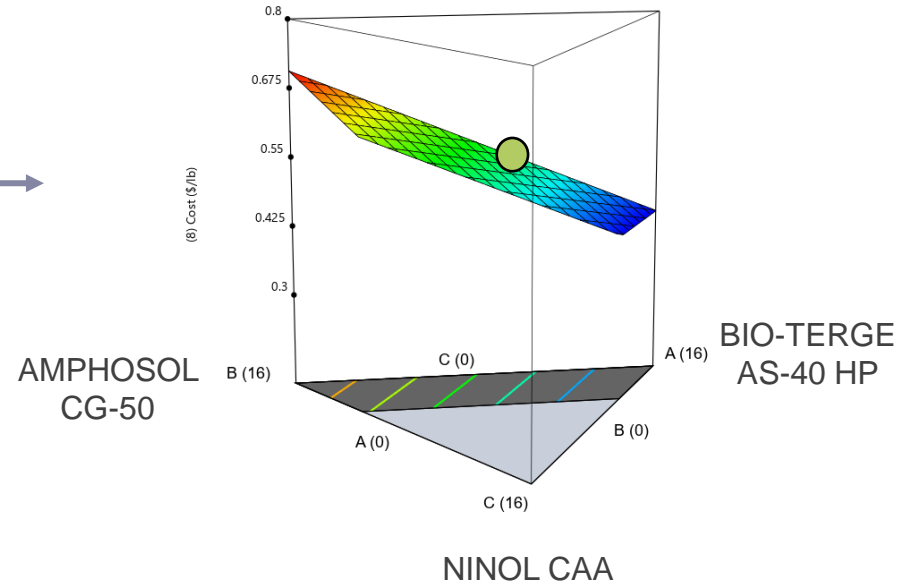
**8% Actives**

# DOE Can Optimize Formula Cost

The sum of ratios = 1.0



**6% Actives**



**8% Actives**

# Optimizing Shampoo Cost



Ingredient	Price (\$/Lb)* 100% Active
<b>BIO-TERGE AS-40 HP</b> <i>Sodium C14-16 Olefin Sulfonate</i>	\$5.40
<b>AMPHOSOL CG-50</b> <i>Cocamidopropyl Betaine</i>	\$8.85
<b>NINOL CAA</b> <i>Dimethyl Lauramide/Myristamide</i>	\$5.40



Ingredient	DOE Actives Ratio (w/salt)	Optimization Trial 1: 6% Total Actives	Optimization Trial 2: 8% Total Actives
<b>AS-40 HP</b>	<b>0.50</b>	<b>3.00%</b>	<b>4.00%</b>
<b>CG-50</b>	<b>0.47</b>	<b>2.80%</b>	<b>3.75%</b>
<b>CAA</b>	<b>0.03</b>	<b>0.20%</b>	<b>0.25%</b>
<b>Total Cost Per Lb</b>	--	<b>\$0.421</b>	<b>\$0.562</b>
<b>Viscosity, Clarity</b>	--	<b>&lt;1,000 cps Clear</b>	<b>16,300 cps Clear</b>

## From Brief:

Viscosity of 15,000 cps

Cost <\$0.60/lb for cleansing base (actives)

\*Prices indicated are for reference only; please contact your Stepan Sales Representative for an official price quote for any Stepan material.

# The Final Result: Modern Sulfate Free Shampoo

Product Desired: Modern, Sulfate-Free Shampoo

Benchmarks: OGX ✓

Claims: Sulfate-Free, Volumizing,  
For all hair types,  
No palm/PKO-based ingredients ✓

Characteristics: Clear ✓  
Target viscosity 15,000 cps ✓  
pH 5.5-6.5 ✓

Other Ingredients:  
Fragrance: Ocean Fresh WS, 0.5%  
(Belle Aire)  
Preservative: Microcare BDB,  
0.75% (Thor)

Cost: Less than \$0.60/lb for  
cleansing base (actives) ✓

## Final Steps:

- Minor formula adjustments to achieve marketing targets
- Verify accelerated, long-term and elevated temperature stability
- Verify performance claims with panel and/or consumer testing
- Component stability
- Scale up and processing

Using DOE response triangles can expedite range expansion – new fragrances, additives

Finished project  
after making  
only 2 formulas

# Stepan Has Done the Hard Work For You

Stepan's expertise in DOE can accelerate your new product development

DOE summaries with surfactant ratios, viscosity response maps available for various sulfate free systems, more to come

Simply multiply each surfactant ratio by desired total actives to start formulating!

Mild & Gentle Body Wash with Glutamate Stepan Personal Care

Mild & Gentle Shampoo with Sarcosinate Stepan Personal Care

Naturally Derived, Sulfate Free Cleansing Base Stepan Personal Care

Modern Sulfate Free Shampoo Stepan Personal Care

Stepan Surfactant	Without Salt	With Salt
BIO-TERGE AS-40 HP <i>Sodium C14-16 Olefin Sulfonate</i>	0.50	0.50
AMPHOSOL CG-50 <i>Cocamidopropyl Betaine</i>	0.41	0.47
NINOL CAA <i>Dimethyl Lauramide/Myristamide</i>	0.09	0.03

Table 1: Predicted ideal surfactant ratios. Multiply each factor by desired actives.

**Multiply the total actives concentration for your formula by the multiplier ratios to get a product with viscosity!**

(Convert to % by weight as needed)

**AOS/CAPB/CAA Viscosity (Without NaCl)**

A: BIO-TERGE AS-40 HP (IN ACTIVE)  
B: AMPHOSOL CG-50 (IN ACTIVE)  
C: NINOL CAA (IN ACTIVE)

(7% Fragrance) Viscosity

pH = 5.5  
Active = 16%  
Data Points = 72  
Sampling = Standard

Balance: Water, 1% Fragrance, Preservative, Citric Acid

**AOS/CAPB/CAA Viscosity (With NaCl)**

A: BIO-TERGE AS-40 HP (IN ACTIVE)  
B: AMPHOSOL CG-50 (IN ACTIVE)  
C: NINOL CAA (IN ACTIVE)

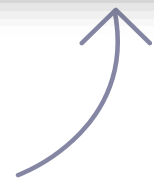
(7% Fragrance) Viscosity (SPS)

pH = 5.5  
Active = 16%  
Data Points = 72  
Sampling = Standard

Balance: Water, 1% Fragrance, Preservative, Citric Acid

Interested in receiving one of these summaries?

Leave a note in the chat!



# In Summary:

- Consumer-desired, sulfate free cleansers can require lengthy development processes due to performance challenges
- DOE provides a systematic approach to product development, streamlining the process and creating comprehensive foundation for SKU expansion
- Stepan has created viscosity response maps for multiple sulfate free systems to put you steps ahead in the development process

What sulfate free surfactants are giving you trouble?  
Let us know in the chat!

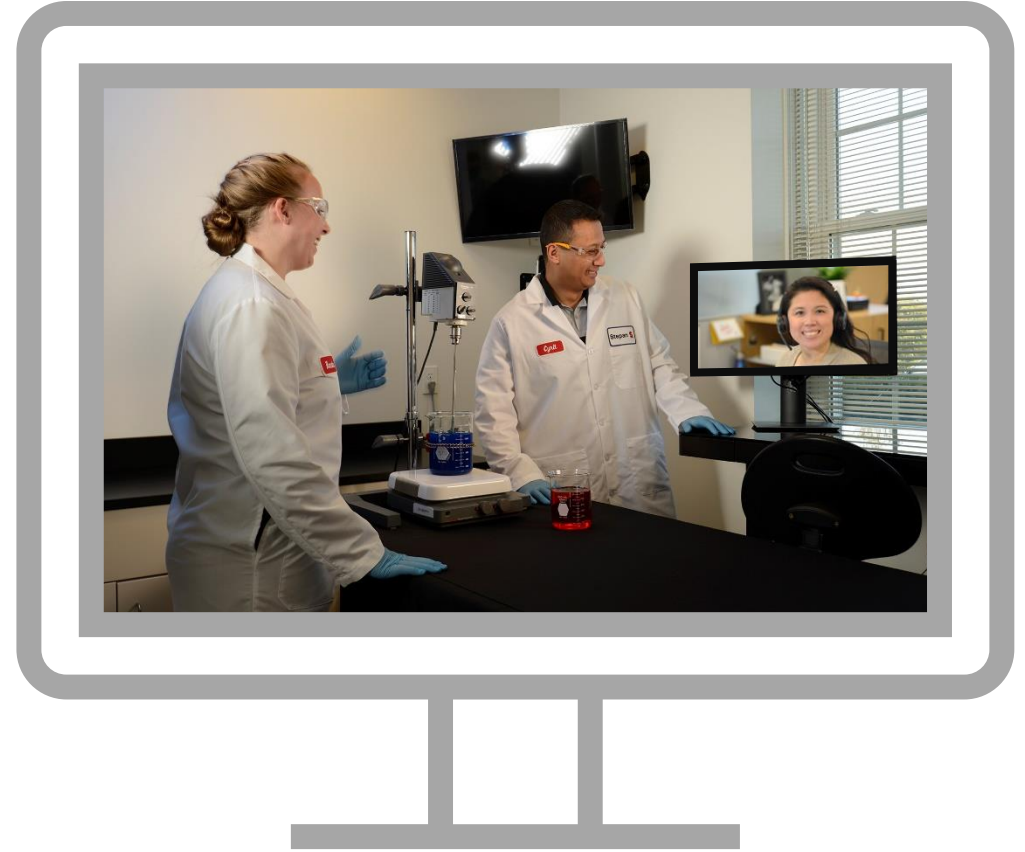


# Struggling with a Sulfate Free Cleanser?

Take advantage of Stepan's Virtual Lab

Stepan's **Virtual Collaboration Lab** is available to you for live demonstrations or formulation troubleshooting!

- Reach out to your local sales representative
- Contact us through UL Prospector





**Stepan**   
Personal Care

**Thank you!**

Visit [stepan.com/personalcare](https://stepan.com/personalcare)  
for more information.

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