A Comprehensive View of Surfactant Irritation Potential

Dennis Abbeduto, Colonial Chemical, Inc.

Colonial Chemical

A Comprehensive View of Surfactant Irritation Potential

Dennis Abbeduto, Colonial Chemical, Inc.

Overview

As modern consumers continue to seek new and improved ways to optimize their cleansing routines, one trend stands out over others: the need for more gentle cleansing. And as animal testing for irritation has been replaced by a wide array of in-vitro tests, each with its own result scale and inherent challenges, it has become difficult to compare results across a broad array of products. Vegan-compliant lab scale zein testing has been conducted on over 60 individual surfactant ingredients and commercial cleansing products, covering traditional chemistry as well as new innovations in all major surfactant types: anionic, cationic, amphoteric, and nonionic.

The same method is used to benchmark and evaluate formulation modifications with the goal of reducing the potential for irritation in vivo.

1. Introduction

Consumer safety is the most vital component of sustainable product development. Until recently, predicting skin and eye irritation in consumers was done primarily with animal models. Recognizing the potential for suffering in mammals, efforts have been made to develop humane animal-free models with good prediction power. Today, a large variety of test protocols are available, which has achieved the goal of reducing animal suffering. Unfortunately, it has also created challenges in comparing products.

Various globally recognized OECD methods all have specific nuances in how they react to irritants, from the closest animal analog, the Bovine Corneal Opacity and Permeability Assay (BCOP) to Hen's Egg Test – Chorioallantoic Membrane (HET-CAM) to propriety cell models like MatTek EpiDerm™ and EpiOcular™ to in chemico models like InVitro International's Irritection® and now *in silico* "AI" models.

Zein, a corn protein that is similar to keratin present in the skin and hair, is insoluble in water unless it is denatured. Protein denaturation is considered to be a good predictor of skin and eye irritation *in vivo*[1] and the use of zein as a proxy for human proteins and irritation potential as been well established[2,3], demonstrating acceptable correlation, though generally insufficient to achieve global acceptance for regulatory bodies.

The goal of this study is to develop a single, large body of zein data using a modified zein method that offers good repeatability with almost no specialized equipment necessary.

2. Materials

Surfactants and surfactant mixtures, with the exceptions of those noted were supplied by Colonial Chemical, Inc, South Pittsburg, TN. Zein protein was purchased from Spectrum Chemical, New Brunswick, NJ. Whatman filter papers were purchased from VWR, Radnor, PA. Additional surfactants and mixtures are Genamin® CTAC 50 (Cetrimonium Chloride), Plantapon® ACG HC (Sodium Cocoyl Glutamate), Pureact I-78 C (Sodium Cocoyl Isethionate), Iselux® LQ-CLR (Sodium Lauroyl Methyl Isethionate), Hamposyl™ L30K (Sodium Lauroyl Sarcosinate), and Pureact WS Conc (Sodium Methyl Cocoyl Taurate).

3. Methodology

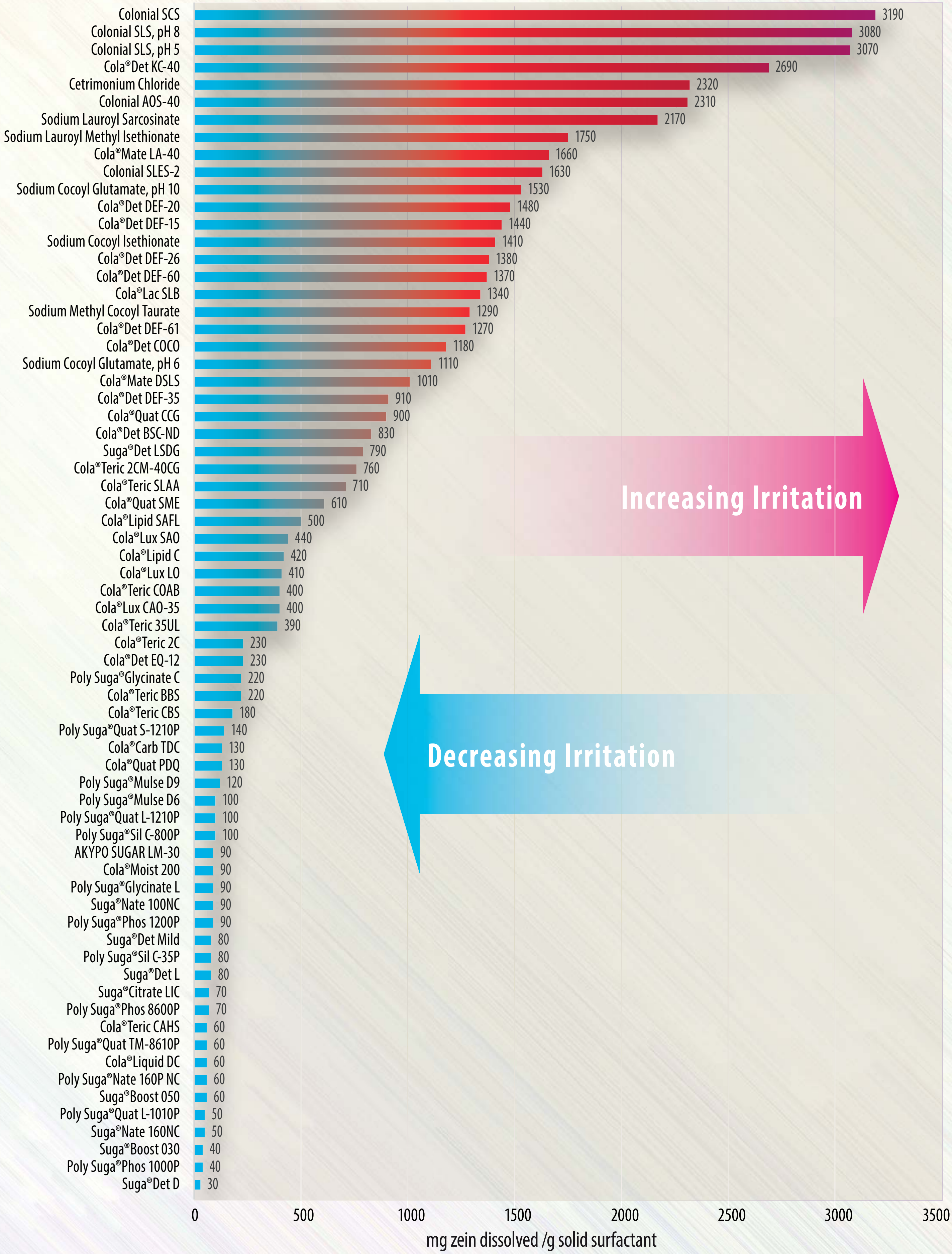
Surfactant test solutions were prepared at concentrations of 3.0% solids in deionized water. Recorded weights of zein powder were added to 50 mL of the test solutions and mixed for 60 minutes. The solutions were then poured onto filter papers (Whatman 3, 90 mm) of known weights seated inside a ceramic Büchner funnel under vacuum. After vacuum filtration, the filter papers and collected zein were dried in a convection oven at 110°C for 60 minutes. The weights of the collected, oven-dried zein were used to determine the amounts of denatured and dissolved zein in the following formula, where Z represents the initial weight of zein, IW represents the initial weight of the filter paper, and FW represents the final combined weight of the filter paper and collected zein. All results were measured in triplicate.

$$\text{Zein Dissolved (mg/g solid product)} = \frac{Z - (FW - IW)}{1.5} \times 1000$$

The amount of zein that has been denatured and dissolved is presented as "mg zein dissolved /g solid surfactant," where a lower number indicates lower potential for irritancy. This differs from the traditional "zein score", which is based on N analysis. Normalizing all data to solids allows for more ready comparisons of commercial products, where determination of true actives may be difficult.

Protein after mixing and drying using one surfactant with a high degree of denaturation/anticipated irritation (Left) and one with a low degree of denaturation (Right)

Results



Colonial SCS 3190
Colonial SLS, pH 8 3080
Colonial SLS, pH 5 3070
Cola®Det KC-40 2690
Cetrimonium Chloride 2320
Colonial AOS-40 2310
Sodium Lauroyl Sarcosinate 2170
Sodium Lauroyl Methyl Isethionate 1750
Cola®Mate LA-40 1660
Colonial SLES-2 1630
Sodium Cocoyl Glutamate, pH 10 1530
Cola®Det DEF-20 1480
Cola®Det DEF-15 1440
Sodium Cocoyl Isethionate 1410
Cola®Det DEF-26 1380
Cola®Det DEF-60 1370
Cola®Lac SLB 1340
Sodium Methyl Cocoyl Taurate 1290
Cola®Det DEF-61 1270
Cola®Det COCO 1180
Sodium Cocoyl Glutamate, pH 6 1110
Cola®Mate DSLS 1010
Cola®Det DEF-35 910
Cola®Quat CCG 900
Cola®Det BSC-ND 830
Suga®Det LSDG 790
Cola®Teric 2CM-40CG 760
Cola®Teric SLAA 710
Cola®Quat SME 610
Cola®Lipid SAFL 500
Cola®Lux SAO 440
Cola®Lipid C 420
Cola®Lux LO 410
Cola®Teric COAB 400
Cola®Lux CAO-35 400
Cola®Teric 35UL 390
Cola®Teric 2C 230
Cola®Det EQ-12 230
Poly Suga®Glycinate C 220
Cola®Teric BBS 220
Cola®Teric CBS 180
Poly Suga®Quat S-1210P 140
Cola®Carb TDC 130
Cola®Quat PDQ 130
Poly Suga®Mulse D9 120
Poly Suga®Mulse D6 100
Poly Suga®Quat L-1210P 100
Poly Suga®Sil C-800P 100
AKYPO SUGAR LM-30 90
Cola®Moist 200 90
Poly Suga®Glycinate L 90
Suga®Nate 100NC 90
Poly Suga®Phos 1200P 90
Suga®Det Mild 80
Poly Suga®Sil C-35P 80
Suga®Det L 80
Suga®Citrate LIC 70
Poly Suga®Phos 8600P 70
Cola®Teric CAHS 60
Poly Suga®Quat TM-8610P 60
Cola®Liquid DC 60
Poly Suga®Nate 160P NC 60
Suga®Boost 050 60
Poly Suga®Quat L-1010P 50
Suga®Nate 160NC 50
Suga®Boost 030 40
Poly Suga®Phos 1000P 40
Suga®Det D 30
Increasing Irritation
Decreasing Irritation
0
500
1000
1500
2000
2500
3000
3500
mg zein dissolved /g solid surfactant

4. Conclusions

Common surfactants demonstrated typical trends with regards to irritation potential in the test. Of note, Cetrimonium Chloride tested somewhat lower irritation than typical, and some nonionic surfactants scored near zero, despite demonstrating some potential for irritation in other in vitro tests or in vivo. Ammonium salt surfactants did not demonstrate the reduction in irritation that could be described as "common knowledge" among formulators. Also, true amphoteric surfactants and some amino acid surfactants have the potential to demonstrate different ionic characteristics dependent on pH. So while Sodium Lauryl Sulfate (SLS) measured at pH 5 and 8 are effectively identical scores, (Di)Sodium Cocoyl Glutamate measured at pH 6 and 10 have substantially different scores. Most products were measured at their pH as supplied. Further investigation of the true amphoteric surfactants (amphoacetates, amphopropionates) at multiple pH values is warranted. Previous investigation of true soaps has also indicated that pH is an overriding factor in irritation in those products.

There is a significant amount of system error associated with this test, such that it is difficult to differentiate between very similar scores, especially at the low end of the chart. In some tests the product adsorbed to the protein with little or no zein dissolving. This resulted in "negative" values, as the weight after drying was higher than before. This reinforces that while this is an effective screening test, further investigation is necessary to establish validated claims.

Surfactant combinations are well known to provide a synergistic reduction in irritation potential; the overall irritation tends to be lower than the predicted weighted average. By using newer generation amphoteric and nonionic surfactants (eg sultaine and alkyl glucoside), significant improvements can be realized when compared to more traditional secondary surfactants (betaine, alkanolamide). "Next generation" functionalized alkyl glucoside surfactants clearly demonstrate their favorable irritation profile relative to traditional anionic, cationic, and amphoteric surfactants.

Using an affordable and easy to use test methodology, we have quickly generated a large library of in chemico irritation data covering a wide range of frequently used surfactants. This will help formulators make better choices of specific surfactants and surfactant combinations, maximizing product performance while minimizing consumer risk. We will continue to generate data to provide the most robust body of data possible for formulators.

1. Miyazawa K, Ogawa M, Mitsui T. *The physico-chemical properties and protein denaturation potential of surfactant mixtures.* Int J Cosmet Sci., 1984. **6(1)**: p. 33-46.

2. Götte. *Skin compatibility of tensides measured by their capacity for dissolving zein protein.* In: Proc IV International Congress on Surface Active Substances, Brussels, Belgium, p 83–90 (1964).

3. Morrison Jr, B.M. and M. Paye, *A comparison of three in vitro screening tests with an in vivo clinical test to evaluate the irritation potential of.* J Soc Cosmet Chem, 1995. **46**: p. 291-299.

ACKNOWLEDGEMENTS

This poster was completed thanks to the contributions of the following:
Molly McEnery, for method development and testing, and
Alie Williams, for testing - Colonial Chemical, Inc.

Colonial Chemical
Innovative Specialty Surfactants
www.colonialchem.com