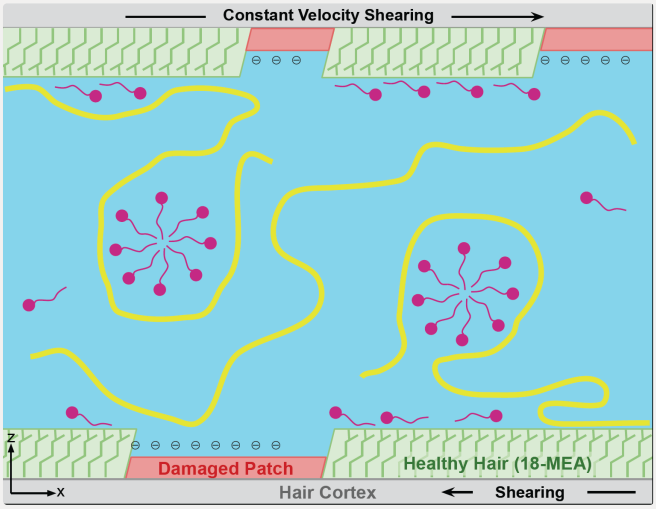
CASE STUDY

Molecular dynamics and coarse-grained simulations facilitate the design of new eco-friendly cosmetic formulations

L'Oreal and Schrödinger scientists gain a deeper understanding of the shearing behavior differences between synthetic and polysaccharide polymers on biomimetic surfaces

Executive Summary

- **Gained novel insights** into the aggregation behavior of shampoo formulations with a model hair surface
- **Demonstrated the impact of polymer topology** and related the observed polymer interactions to experimental observables
- **Established a framework for studying complex formulations** in contact with biomimetic surfaces using molecular dynamics simulations
- **Accelerated rational design** of eco-friendly cosmetic formulations



A simplified representation of a typical molecular model system for shampoo interacting with hair surfaces studied in this work.[1]

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Challenges

Changes in consumer behaviors are driving increased demand for green and eco-friendly products in the cosmetic industry. Substitution of natural, bio-based polymers for petrochemical-derived ingredients in consumer formulations has become an active area of research. However, the complexity of these formulations, typically mixtures of surfactants, salt and polymers, makes it non-trivial to replace an ingredient and anticipate its effect on product properties.

Effective and efficient reformulation that maintains comparable performance to existing products requires a deep understanding of the differences in behavior between polymers, which can be time and resource intensive using the traditional experimental approach.

Approach

Scientists from L'Oreal and Schrödinger explored the behavioral differences of synthetic polymers and eco-friendly polymers in hair formulations by building realistic models of complex formulation and hair surfaces. All models and simulations were performed using the Schrödinger Materials Science Suite and Desmond for molecular dynamics (MD) according to the following procedure:

Build, parameterize and equilibrate coarse-grained experiment-inspired bulk formulations at dilute and concentrated conditions

Introduce a model hair surface (healthy, extremely damaged and partially damaged) in contact with the formulation and run simulations

Apply shear to the model hair surfaces and investigate the response of the formulations to these drag forces

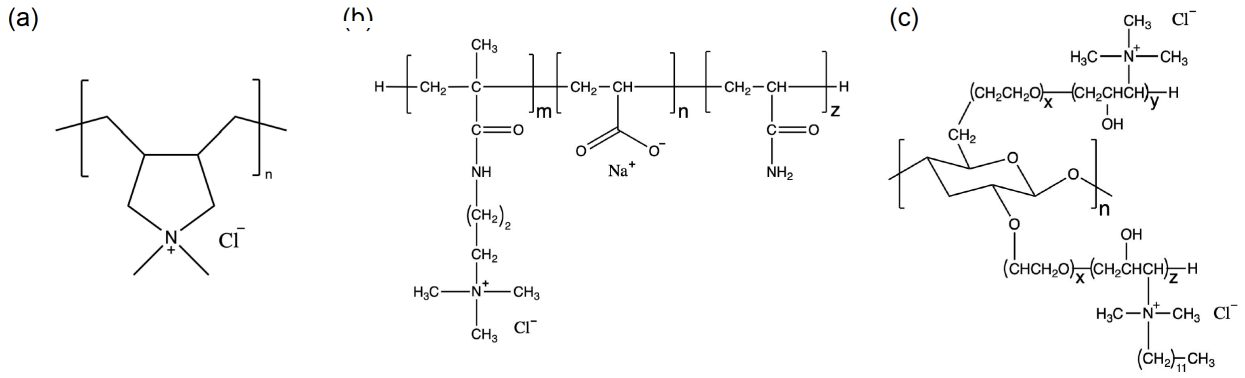

Figure 1. Structures of polymers used in this work: (a) Merquat M100™, (b) Merquat M2003™ and (c) a polysaccharide, PS.[1]

Results

This work demonstrates an approach for studying the interaction of complex polymer/surfactant formulations with biological substrates via MD simulations. Detailed, experiment-inspired all-atom molecular models were used in order to parameterize coarse-grained simulations capable of portraying aggregation and adsorption behavior. Continued progress in this area will establish particle-based simulation as a viable technique for designing new eco-friendly formulations.

Summary

- Distinct behaviors are observed among polymers (M100, M2003 and PS) as a result of their chemical architecture. The quaternary ammonium groups common to all three polymers play an important role in bulk aggregation, as well as in interactions with surfactant-coated healthy hair surfaces
- In M2003, the hydrophilic block does not incorporate into aggregates, but it does adhere to the damaged surface, a quality not shown by the other polymers
- In PS, the highly branched carbohydrate backbone offers a favorable environment for surfactants, and may help increase surfactant solubility. The 12-carbon alkane chains branching off each monomer makes it the only polymer that comes in direct contact with the healthy hair surface
- The data suggests that the length of the polymer chain can play a role in lubrication properties

What's next

The exploratory measurements in this study demonstrate that it is possible to quantify frictional coefficients of hair against complex formulations. Large scale, systematic studies that allow for more detailed comparisons between polymers of interest are a clear next step in advancing this area of study. In future work, we intend to examine friction as a function of variations to formulation compositions, polymer chain lengths, model hair surface topology, shear rate as well as distance between hair surfaces.

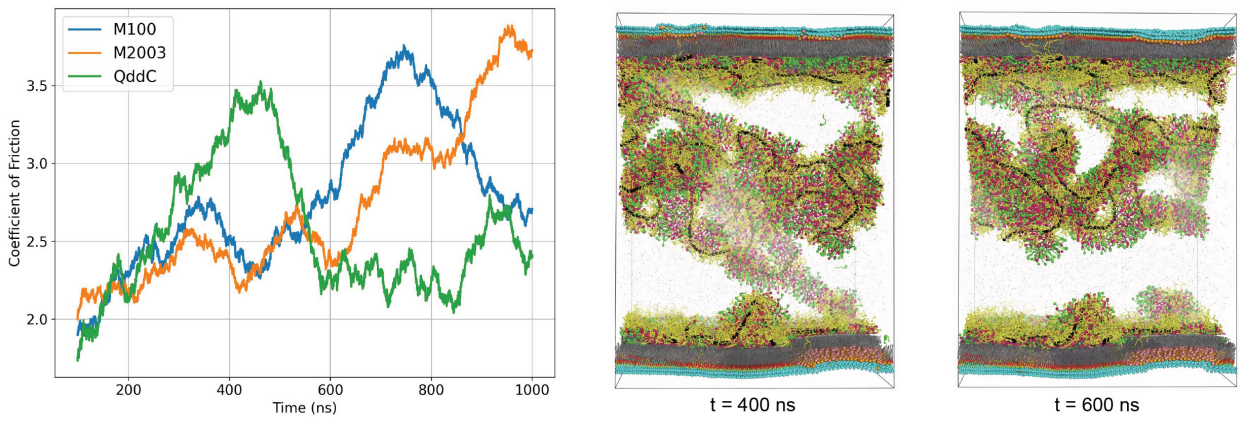

Figure 2. 100 ns moving averages of coefficient of friction, μ_k, versus time for systems undergoing shear. After about 400 ns of simulation, the measured drag force in the PS system drops significantly. We can understand this visually by observing the detachment of a large aggregate from the bottom layer.[1]

References

1. Shearing Friction Behaviour of Synthetic Polymers Compared to a Functionalized Polysaccharide on Biomimetic Surfaces: Models for the Prediction of Performance of Eco-designed Formulations

   Benjamin J. Coscia, John C. Shelley, Andrea R. Browning, Jeffrey M. Sanders, Robin Chaudret, Roger Rozot, Fabien Léonforte, Mathew D. Halls, and Gustavo S. Luengo, *Phys. Chem. Chem. Phys*., 2023, Advance Article, doi.org/10.1039/D2CP05465E

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