

Research Article

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Prediction of sensory textures of cosmetics using large amplitude oscillatory shear and extensional rheology

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Abstract: We propose a predictive model for various sensory textures utilizing machine learning techniques based on the largest rheology and panel-tested sensory texture database ever assembled. In addition to the conventional rheological parameters typically measured in the cosmetics field, rheological parameters obtained from the large amplitude oscillatory shear (LAOS) sequence of physical processes (SPPs) and extensional rheology analyses are employed as feature variables for the predictive model. These feature variables are chosen to mimic real flow conditions during the usage of cosmetics, such as rubbing and tapping, as they are expected to contain more information related to sensory textures. It has been demonstrated that our prediction model, based on the random forest regression algorithm, can effectively predict five sensory textures: spreadability, thickness, softness, adhesiveness, and stickiness. We investigated the rheological characteristics crucial for determining each sensory texture through permutation and feature importance analyses. The important analysis highlighted the close

correlation between rheological parameters from LAOS–SPP, extensional analyses, and sensory textures. By using this correlation, we interpret the perception of each sensory texture in the context of rheology.

Keywords: cosmetic formulations, sensory attributes, non-linear rheology, SPP analysis, machine learning

1 Introduction

Sensory texture holds a pivotal role in shaping the consumer experience and overall satisfaction with a wide array of everyday products, including cosmetics and food items [1–4]. The panel test, such as quantitative descriptive analysis (QDA) and spectrum descriptive analysis, has been the most common and direct approach used to assess the sensory texture of cosmetics [4–7]. Although panel test-based methods have traditionally been valuable for sensory texture analysis, their utility has been constrained by inherent limitations. These limitations encompass their time-consuming nature, high cost, labor-intensive requirements, and susceptibility to the influence of extraneous factors. In recent times, there has been a notable shift toward correlating the sensory texture of cosmetics with instrumental measurements, with a particular focus on rheological measurements [8–14]. This approach is favored for its economic efficiency, speed, and objectivity.

Previous studies have uncovered meaningful relationships between the sensory texture of cosmetic formulations and their rheological properties [11–14]. However, these studies have often established predictive models on the basis of the assumption of a linear, semilogarithmic, or logarithmic relationship between sensory textures and rheological properties, in accordance with the prevailing assumptions in psychophysics. Such a straightforward way of constructing a prediction model was inadequate to quantitatively capture the complicated correlation between sensory texture and rheological measurements. Therefore, the

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accurate estimation of sensory texture using rheological measures, which requires a thorough comprehension of the complex relationship between the two, has proven to be challenging. Notably, advancements in machine learning methods now allow for a deeper understanding of the complex relationship between rheology and the sensory texture of cosmetics. Our previous research has demonstrated that by combining rheological measurements with machine learning techniques, we can quantitatively predict the sensory texture of cosmetic formulations [15]. This approach effectively captures the complex nonlinear relationship between them. The successful development of a prediction model for spreadability has demonstrated the potential for achieving a quantitative understanding of various sensory textures other than spreadability through the integration of rheological measurements and machine learning techniques.

In the development of a predictive model for sensory texture in cosmetic products, the integration of rheological data with machine learning algorithms is crucial. Paramount to this process is the precise identification and selection of relevant rheological parameters that will serve as feature variables. These parameters must exhibit a robust and strong correlation with the specific sensory textures targeted by the model. A wrong choice of rheological parameters would squander time, considering the time-consuming process of establishing a database of such parameters, and diminish prediction performance. In the cosmetics industry, relatively simple rheological measurements such as steady shear viscosity and yield stress, which can be conveniently assessed using a viscometer or an affordable rheometer, have traditionally been used as feature variables. However, an effective strategy for selecting rheological parameters, as suggested by the previous study, involves utilizing rheological measurements under flow conditions that closely resemble the actual utilization process of cosmetic products. For instance, machine learning models with parameters from large amplitude oscillatory shear (LAOS), the flow conditions of which are similar to that of the cosmetics rubbing process, have been shown to be more accurate and effective in spreadability prediction than prediction models with rheological parameters that have been conventionally employed without consideration of flow condition under actual utilization process [4,16,17]. Similarly, extensional rheological parameters hold the potential to play a pivotal role in discerning the sensory textures of cosmetics, despite, to our knowledge, not having been investigated. This can be particularly relevant since the application process of cosmetics often involves tapping or other forms of manipulation that subject cosmetic formulations to extensional deformation.

The prior study, which combined rheology and machine learning techniques for sensory texture prediction, leaves

considerable room for improvement from two distinct perspectives. One crucial determinant of the accuracy and utility of the sensory texture prediction model is the size and diversity of the sample dataset. A larger and more diverse dataset encompassing rheological parameters and sensory textures from a wide range of cosmetic formulations enhances the accuracy and broadens the operational range of the sensory texture prediction model. However, establishing a dataset of rheology and sensory textures requires a substantial quantity of time and money. To the best of our knowledge, our previous work with 77 datasets of cosmetic formulations made use of the largest data [15]. Although the spreadability prediction model from the previous study demonstrated adequate performance, it is always preferable to introduce a larger dataset to improve model accuracy and operational range. In addition, the earlier research is constrained in its scope, focusing exclusively on the prediction of a single sensory texture, namely, spreadability, whereas the cosmetics industry and the psychorheology field will benefit from the prediction of multiple sensory textures.

In this work, as a continuation of our previous work, we have developed an advanced machine-learning model for predicting various sensory textures of cosmetic formulations. What sets this advanced model apart from previous prediction models is its capability to predict not only spreadability but also four additional sensory textures: thickness, softness, adhesiveness, and stickiness. The advanced prediction model uses the largest rheological measurements and panel test database of 117 samples to improve accuracy and operation range over our previous predictive model. Our advanced prediction model incorporates extensional rheological parameters of cosmetic formulations in addition to the LAOS sequence of physical process (SPP) parameters and conventional rheological parameters, which served as feature variables in the previous prediction model for spreadability. This enhancement is believed to broaden the predictive capabilities of the model, allowing it to forecast a wider range of sensory textures. To strengthen our examination of the relationship between rheological parameters and sensory textures in comparison to our previous study, we have performed feature importance analysis in addition to the permutation importance analysis. This approach has allowed us to gain a comprehensive understanding of the perception of sensory textures in cosmetic formulations in the context of rheology.

The remainder of this article is divided into three sections. The specifics of data preparation, encompassing model cosmetic formulations, sensory texture tests, and rheological measurements are presented in Section 2. Section 3 describes the machine learning algorithms used to

construct the prediction models. In Section 4, prediction performance for each sensory texture is evaluated, and the correlation between rheological parameters and sensory textures is discussed based on the results of the permutation importance and feature importance analyses. We conclude our findings and discussions at the end.

2 Measurements

2.1 Materials

In Figure 1, a schematic illustration of the data preparation processes is presented. A total of 117 cosmetics formulations were meticulously prepared. These model cosmetic

formulations consist of two categories of formulations, solubilization and emulsification types, which exhibit diverse skin sensations. As shown in Table 1, the fundamental components of all formulations are polyol, oil, silicone, thickener, emulsifier, and water. Fragrance and color ingredients were omitted from all formulations to prevent unexpected bias. However, it is important to note that these additives can significantly affect the rheological properties in reality. The preparation of these formulations was executed using standard laboratory equipment, such as an agitator and homogenizer. While it is challenging to provide an exact definition for all cosmetic formulations due to their diversity, most of them adopted the form of solutions or thick emulsions. The cosmetic samples utilized for prediction, as indicated in Table 1, are free of particulates. It can therefore be concluded that the predictive model developed in this study is applicable to nonparticulate systems.

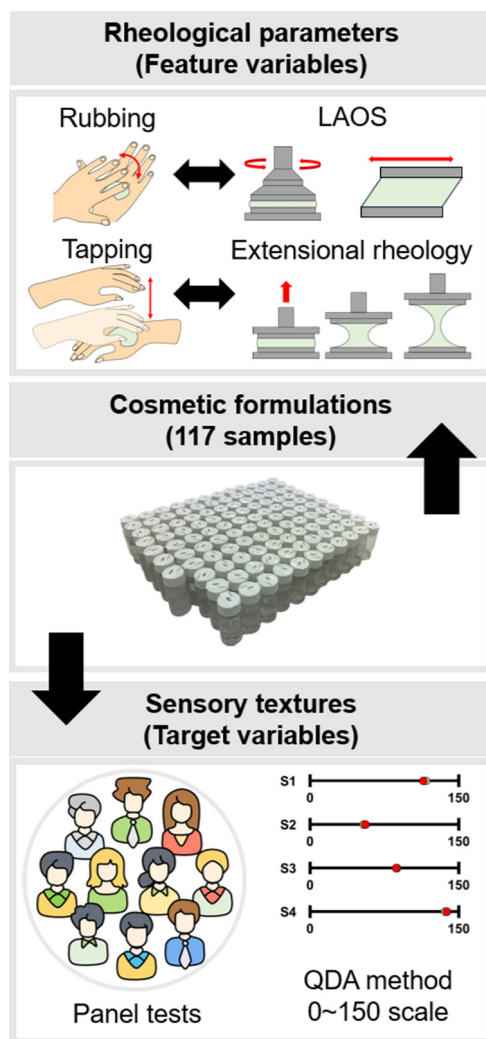


Figure 1: Schematic diagrams for the preparation processes of rheological and panel-tested sensory texture.

2.2 Sensory texture evaluation

Sensory texture evaluation was conducted with the participation of 10 well-trained panelists. In this assessment, the QDA method, commonly employed in sensory evaluations, was utilized. The evaluation was performed in a sensory evaluation room, where temperature, relative humidity, and lighting conditions were regulated in adherence to ISO guidelines (ISO 8589:2007). To eliminate potential biases such as panel and order effects, all cosmetic formulations were presented in a fully blinded fashion, concealed by random three-digit codes. Furthermore, sensory texture assessments were performed in accordance with the Latin square design sequence [18–21].

The panelists were informed of the precise definitions of each sensory texture to assure a common understanding of sensory textures. “Spreadability” is defined as the

Table 1: Ingredient information of 117 cosmetic formulations

Ingredients	Type of formulation			
	Solubilization		Emulsification	
Polyol (wt%)	~10	11–20	21~	2–37
Oil (wt%)	~1	~1	~1	~15
Silicone (wt%)	0–1	0–10	0–4	0–33
Thickener (wt%)	0–2.0	0.04–1.93	0.04–6.24	0.01–13.55
Emulsifier (wt%)	—	—	—	0–3.5
Water (wt%)	61–93	53–86	31–76	27–83
Number of samples	27	36	25	25

“perceived degree of the spread strength or the spread area within the test spot while the sample covers over the skin” according to the previous research [15]. The following definitions apply to “thickness,” “softness,” “adhesiveness,” and “stickiness.” “Thickness” is defined as “the perceived degree to which the rolled sample presented a certain height between the skin and the finger.” “Softness” is defined as “the perceived degree to which the rolled sample felt soft.” The definition of “adhesiveness” is “the perceived degree to which the sample adhered to the skin when rolled.” The definition of “stickiness” is “the perceived degree to which a finger would adhere to the product’s residue on the skin surface after using a sample.” The sensory attributes were evaluated on the inner forearm of the panelists. Each formulation was dispensed in 50- μ L quantities via a micro pipette (Gilson MICROMAN M100E, France). Panelists spread the samples within a 5 cm diameter circle at a rate of 120 BPM (beats per minute) while rolling them. Ratings were assigned on a scale from 0 to 150 (line scale) in comparison to reference samples, with these references serving as reminders of the definitions of sensory attributes.

2.3 Rheological measurements

Simple shear rheological measurements were conducted utilizing an HR-20 rheometer (TA instruments, USA) equipped with a 40-mm crosshatched geometry, which was employed to avoid wall slippage during testing. A strain-controlled rheometer is the optimal choice for LAOS testing; alternatively, due to accessibility constraints, a stress-controlled rheometer was utilized. As there can be differences between the data obtained from a stress-controlled rheometer and a strain-controlled rheometer, we closely examined the strain signal during the oscillation and discovered that it was steady sinusoidal. In addition, the rheological measurements of 10 arbitrarily chosen cosmetic formulations from HR-20 and strain-controlled rheometer ARES-G2 (TA instruments, USA) were compared and found to be nearly identical (detailed in Supplemental material, Figures S1–S3). During the rheological measurements, we maintained a temperature of 32°C, which is comparable to the skin temperature of a hand in a room with a temperature of 15–20°C [22,23]. All samples were pre-sheared with LAOS of strain amplitude $\gamma_0 = 10$ and frequency $\omega = 1$ rad/s for 300 s, followed by 300 s of equilibrium time, to assure a uniform initial state. Strain amplitude sweep tests to obtain rheological parameters that belong to the conventional rheological parameter group were performed in the strain amplitude (γ_0) range between 0.01 and 10 at a frequency $\omega = 1$ rad/s. The shear rate sweep test was conducted in the shear rate range between 0.1 and 100/s.

Extensional rheological properties were assessed using a capillary breakup extensional rheometer (CaBER, Thermo Scientific, USA). A small quantity of the sample was loaded between plates, with the initial gap set to 1 mm. Subsequently, the upper plate was elevated to a final gap of 9.3 mm using a cushioned stretching mode that imposes a constant lifting velocity of 1 mm/s followed by an exponential slowdown to mitigate issues caused by the rapid deceleration. The measurement of extensional rheological parameters was based on the change in the mid-filament diameter (D) over time, which was monitored using a laser micrometer. To determine the extensional viscosity (η_E), it was necessary to ascertain the surface tension (Γ) of each cosmetic formulation. This was accomplished through the pendant drop method using a tensiometer (SmartDrop, Femtobiomed, Republic of Korea).

2.4 Rheological parameters as feature variables in prediction model

Feature variables used for the predictive model are categorized into three groups: conventional rheological parameters, LAOS parameters, and extensional rheological parameters. First, the conventional rheological parameter group consists of six distinct rheological parameters. Among these, the elastic modulus (G'), viscous modulus (G''), $\tan(\delta)$ in linear regime, and yield strain (γ_c) measured from the strain amplitude sweep are four of them. Here, yield strain (γ_c) is defined as a strain amplitude below which the elastic modulus (G') and viscous modulus (G'') vary by less than 5% from their constant values at a small strain amplitude. These four parameters describe the basic viscoelastic properties of cosmetic formulations in the linear regime. The remaining two parameters include the shear stress at a high shear rate of 100/s (σ_{100}), and a ratio of the maximum to minimum shear stress ($R_{\sigma_{\max}/\sigma_{\min}}$) observed from the shear rate sweep. The parameters σ_{100} and $R_{\sigma_{\max}/\sigma_{\min}}$ are employed to assess the spreading stress during rapid rubbing and the relative spreading stress difference between intense and gentle cosmetic applications.

To derive LAOS parameters, we quantitatively analyze the stress response of cosmetic formulations under LAOS conditions using SPP techniques. As SPP analysis details are available in numerous prior studies [24–28], we only provide a concise explanation of SPP analysis. As shown in Figure 2, the rheological transition under oscillatory shear strain is depicted by a trajectory in a three-dimensional space composed of the strain (γ)-dimensionless strain rate ($\dot{\gamma}/\omega$)-stress (σ) axes. Hence, at any specific point in time t , the state of rheology is characterized by the point P on the trajectory, which can be expressed as a position vector

$\vec{P}(t) = (\gamma(t), \dot{\gamma}(t)/\omega, \sigma(t))$, as illustrated in Figure 2(a). At an arbitrary point P , the Frenet–Serret frame is defined as a set of vectors that consist of tangent ($\vec{T}$), normal ($\vec{N}$), and binormal vectors ($\vec{B}$):

$$\vec{T}(t) = \frac{\vec{P}'(t)}{|\vec{P}'(t)|}, \quad \vec{N}(t) = \frac{\vec{T}'(t)}{|\vec{T}'(t)|}, \quad (1)$$

$$\vec{B}(t) = \vec{T}(t) \times \vec{N}(t),$$

where time derivatives of $\vec{P}(t)$ and $\vec{T}(t)$ are denoted as $\vec{P}'(t)$ and $\vec{T}'(t)$, respectively. The span of $\vec{T}(t)$ and $\vec{N}(t)$ comprises a plane that is referred to as the osculating plane, which closely follows or coincides with the curve over the parameter interval. The osculating plane is normal to $\vec{B}$ and mathematically represented as follows:

$$\vec{B}(t^*) \cdot (\vec{P}(t) - \vec{P}(t^*)) = 0 \quad (2)$$

or

$$B_{\gamma}(t^*)(\gamma(t) - \gamma(t^*)) + B_{\dot{\gamma}/\omega}(t^*)\left(\frac{\dot{\gamma}(t)}{\omega} - \frac{\dot{\gamma}(t^*)}{\omega}\right) + B_{\sigma}(t^*)(\sigma(t) - \sigma(t^*)) = 0. \quad (3)$$

Here, B_{γ} , $B_{\dot{\gamma}/\omega}$, and B_{σ} represent the strain (γ), dimensionless strain rate ($\dot{\gamma}/\omega$), and stress (σ) components of the binormal vector $\vec{B}(t)$. Three consecutive points $\vec{P}(t^* - \Delta t)$, $\vec{P}(t^*)$, and $\vec{P}(t^* + \Delta t)$ sit within the osculating plane as $\Delta t \rightarrow 0$, and equation (2) can be written in the differential form as follows:

$$B_{\gamma}(t^*)(\gamma(t^* \pm \Delta t) - \gamma(t^*)) + B_{\dot{\gamma}/\omega}(t^*)\left(\frac{\dot{\gamma}(t^* \pm \Delta t)}{\omega} - \frac{\dot{\gamma}(t^*)}{\omega}\right) + B_{\sigma}(t^*)(\sigma(t^* \pm \Delta t) - \sigma(t^*)) = 0$$

$$= B_{\gamma}(t^*)d\gamma + B_{\dot{\gamma}/\omega}(t^*)d\left(\frac{\dot{\gamma}}{\omega}\right) + B_{\sigma}(t^*)d\sigma = 0.$$

Equation (4) can be reformulated as follows:

$$d\sigma = -\frac{B_{\gamma}(t^*)}{B_{\sigma}(t^*)}d\gamma - \frac{B_{\dot{\gamma}/\omega}(t^*)}{B_{\sigma}(t^*)}d\left(\frac{\dot{\gamma}}{\omega}\right), \quad (5)$$

and compared to the total derivative of stress $\sigma(\gamma, \dot{\gamma}/\omega)$

$$d\sigma = \frac{\partial \sigma}{\partial \gamma}d\gamma + \frac{\partial \sigma}{\partial \left(\frac{\dot{\gamma}}{\omega}\right)}d\left(\frac{\dot{\gamma}}{\omega}\right). \quad (6)$$

$-\frac{B_{\gamma}(t^*)}{B_{\sigma}(t^*)}$ and $-\frac{B_{\dot{\gamma}/\omega}(t^*)}{B_{\sigma}(t^*)}$ are equal to $\frac{\partial \sigma}{\partial \gamma}$ and $\frac{\partial \sigma}{\partial \left(\frac{\dot{\gamma}}{\omega}\right)}$ that are

defined as the transient elastic modulus $G'_t(t)$ and transient viscous modulus $G''_t(t)$, respectively. The transient moduli can be viewed as time-dependent counterparts to the dynamic moduli (G' , G''), with the exception that they provide temporally resolved information regarding the intra-cycle rheological transition. In SPP analysis, the rheological state is characterized by the transient moduli $G'_t(t)$ and $G''_t(t)$, with transitions in rheological behavior manifested as alterations in these transient moduli. In most cases, the transient Cole–Cole plot is employed to illustrate the rheological transition; the abscissa represents $G'_t(t)$ and the ordinate represents $G''_t(t)$. Figure 2 depicts (b) the elastic Lissajous curve and (c) the Cole–Cole plot of a cosmetic sample analyzed in this study. By examining the corresponding trace in the Cole–Cole plot, it is possible to comprehend the rheological transition in a region of interest.

As shown in Figure 2(d), the transient moduli at three pivotal points of the Cole–Cole plot were selected as features for the prediction model by bridging the LAOS to the cosmetic application process. Typically, the Cole–Cole plot under LAOS exhibits a deltoid configuration, predominantly as a consequence of the prevalence of the third harmonic within the Fourier spectrum [27–29]. The transient moduli at the three vertices of this deltoid shape effectively encapsulate the rheological behavior of cosmetics during the rubbing-out process, as illustrated in

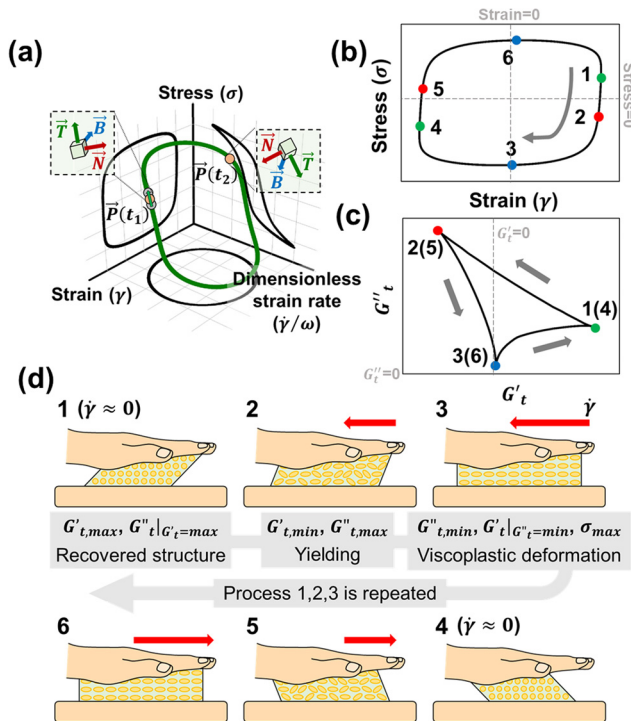


Figure 2: LAOS – SPP analysis and its analogy to rubbing out process of cosmetics. (a) Representation of the rheological behavior under oscillatory in three dimensions of strain (γ), dimensionless strain rate ($\dot{\gamma}/\omega$), stress (σ). (b) Elastic Lissajous curve. (c) Cole–Cole plot. (d) Simplified process for the application of cosmetics in comparison with LAOS, with LAOS parameters defined at each point.

Figure 2(d). Near point 1 (or 4) in Figure 2(d), the strain peaks and flow are reversed, resulting in a near-zero deformation rate, which enables cosmetic structures to relax for a longer duration. As a result, point 1 (or 4), at which the transient elastic modulus attains its maximum value ($G'_{t,\max}$), signifies the greatest degree of structural recovery during oscillation from a rheological perspective. In the context of cosmetic applications, the transient elastic modulus ($G'_{t,\max}$) and the transient viscous modulus ($G''_{t,\max}$) at point 1 (or 4) can be associated with the sensory textures perceived by the user when the application direction is modified and the cosmetics promptly restore their microstructure. Second, to describe the elastic-to-viscous transition, the minimum transient elastic modulus ($G'_{t,\min}$) and the maximum transient viscous modulus ($G''_{t,\max}$) at point 2 (or 5) were employed. During the transition from point 1 (or 4) to point 2 (or 5), where the microstructure starts to undergo deformation and rupture due to flow reversal, cosmetics experience an elastic-to-viscous transition. It can be inferred that the elastic-to-viscous transition is of particular significance at point 2 (or 5), as evidenced by the minimum transient elastic modulus ($G'_{t,\min}$) and the maximum transient viscous modulus ($G''_{t,\max}$). We included $G'_{t,\min}$ and $G''_{t,\max}$ as the feature variable to account for the elastic to viscous transition during the application of cosmetics. Following the successive processes of structural recovery and the elastic-to-viscous transition, cosmetics reach a state of minimal structure near point 3 (or 6), because the strain rate reaches its peak. At point 3 (or 6), G'_t approaches near zero, while G''_t is at its minimum, signifying a viscoplastic flow. We designated the minimum G''_t and the transient elastic modulus at the equivalent point as $G''_{t,\min}$ and $G'_t|_{G''_{t,\min}}$, respectively, and utilized these values as feature variables with the objective of elucidating the viscoplastic flow dynamics that occur during the application of cosmetics. Furthermore, the maximum stress ($\sigma_{\max}$) observed at point 3 (or 6) was chosen as a parameter for the predictive model. The selection of $\sigma_{\max}$ was informed by previous studies that have highlighted a strong correlation between shear stress and sensory textures [15]. These

LAOS parameters have shown to be closely related to spreadability of cosmetics in the previous study [15].

The extensional rheological measurements yielded four rheological parameters to be used as features in the prediction model. Figure 3 illustrates a schematic for extracting feature variables from extensional rheological tests. During the extension tests, the mid-filament diameter (D) of cosmetic samples was measured with a laser micrometer in the extensional rheometer. For the calculation of the extensional viscosity, the measured diameter was fitted with the functional form suggested by Anna and McKinley [30–34],

$$D(t) = ae^{-bt} - ct + d, \quad (7)$$

where a , b , c , and d correspond to fitting parameters. With the fitted function, the extensional viscosity is obtained with the following equation:

$$\eta_E(t) = \frac{-\Gamma}{dD/dt}. \quad (8)$$

From the extensional viscosities at different time points, we have chosen to include the maximum ($\eta_{E,\max}$) and minimum ($\eta_{E,\min}$) values as features. These parameters effectively characterize the rheological properties under the extensional deformation occurring during the cosmetics application process. In addition to these, we have also incorporated the time at which the mid-filament breaks (t_{break}) and surface tension (Γ) into our feature set. These features are expected to provide insight into the extensional breakup and their surface stability. Table 2 provides a summary of all the feature sets for the sensory texture prediction model including target sensory textures.

3 Machine learning model and variable importance analysis

Preceding studies have revealed that there exists complicated nonlinear correlation between physical properties and sensory textures [4,15,35,36]. Our prediction model is

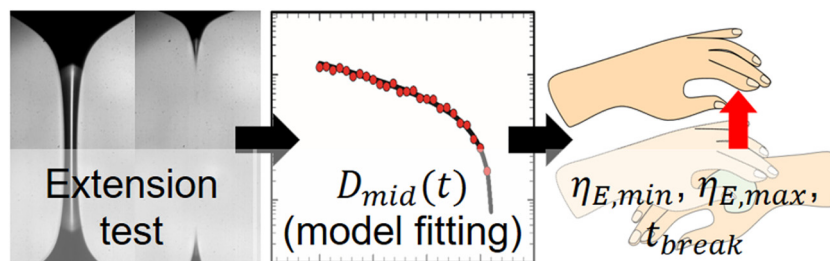


Figure 3: Extraction of feature variables ($\eta_{E,\min}$, $\eta_{E,\max}$, t_{break}) from extensional rheology tests.

Table 2: Summary of the feature selection for the prediction model

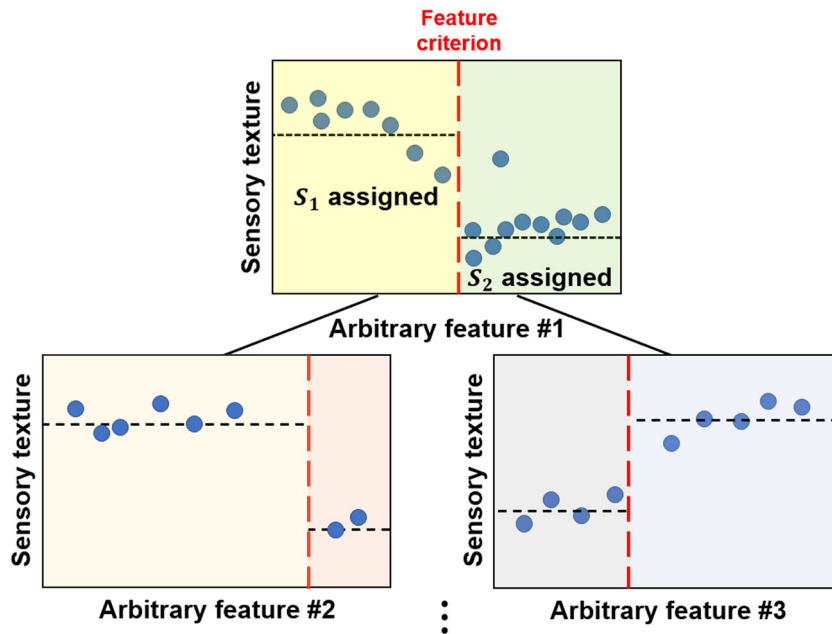
Group	Feature	Description
Conventional parameters	$G', G'', \tan(\delta), \gamma_c$	Linear rheological properties of cosmetic formulations under slight deformation
	σ_{100}	Spreading stress during rapid rubbing-out
	$R_{\sigma_{\max}/\sigma_{\min}}$	Relative difference in spreading stress between slow and rapid rubbing
LAOS-SPP	$G'_{t,\max}, G''_{t,\max} _{G'_t=\max}$	Rheological properties in a temporarily recovered state during oscillation (rubbing)
	$G'_{t,\min}, G''_{t,\max}$	Elastic-to-viscous transition during oscillation (rubbing)
	$G''_{t,\min}, G'_t _{G'_t=\min}, \sigma_{\max}$	Viscoplastic flow during oscillation (rubbing)
Extensional rheology	$\eta_{E,\max}, \eta_{E,\min}$	Rheological behavior under extensional deformation (tapping)
	t_{break}	Degree of extensional breakup tendency
	Γ	Surface stability

rooted in the random forest regression, chosen for its effectiveness in capturing this nonlinear correlation between features and target variables. Given the abundance of information available elsewhere on random forest regression [37–41], we will explain only its fundamental principles here. The random forest regression model comprises numerous decision trees that exhibit a structure akin to actual trees, as depicted in Figures 4 and 5. A decision tree initiates at the root node, iteratively branching on the basis of the outcome variables until it eventually reaches a leaf node and assigns the predicted value. In a more detailed explanation, consider the root node of Figure 4, where the sensory texture and a selected feature domain are divided into two subdomains based on a specific feature criterion,

represented by a long-dashed red line. Individual data points are assigned prediction values, denoted as S_1 and S_2 with black short-dashed lines, within each subdomain. In this instance, the feature criterion and designated values are selected so as to minimize the loss function, in this case, the root-mean-squared error (RMSE). RMSE is calculated using the following formula:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n \{y(i) - \hat{y}(i)\}^2}, \quad (9)$$

where $y(i)$ and $\hat{y}(i)$ indicate the actual and predicted sensory texture of the i th sample, respectively. The subdomains are then subdivided into the next internal nodes, which exhibit analogous characteristics, and the final

**Figure 4:** Principle of decision tree operation. The root node is divided into two internal nodes (leaves). The black short-dashed line and red long-dashed represent an assigned value in subdomains and a feature criterion, respectively.

prediction values are attributed when the subdomains attain the terminal of leaf nodes. In this study, for example, the prediction of a specific cosmetic formulation's sensory texture is determined by the pathway taken from the root node to the leaf node, guided by the rheological parameters.

The random forest regression model, as the name suggests, employs a technique of ensemble machine learning to derive a final prediction value by averaging the output produced by each decision tree. While the random forest regression model is sophisticated and resource-intensive, with an order of magnitude of $O(v \times n \log n)$, where v represents the number of training data and n denotes the number of features, it exhibits robustness against outliers and effectively catches the nonlinear correlations between features and the target variable without overfitting issue [42–44]. In this study, the *RandomForestRegressor* module of the *scikit-learn* library was used to establish the random forest regression model. *GridSearchCV* module is used to optimize the detailed hyperparameters, while the number of decision trees (estimators) is fixed to 1,000 for calculation efficiency. Given the constraints of a limited dataset, we employed a fivefold cross-validation technique to both resample and assess our machine learning models,

optimizing the utility of the available data [45–48]. The chosen evaluation metric was the RMSE, as delineated in equation (9). Our machine-learning pipeline is illustrated in Figure 5, which provides a representative example of the predictive algorithm for sensory texture, specifically focusing on thickness.

To elucidate the significance of rheological parameters in predicting various sensory textures, two distinct feature analysis approaches were utilized. Feature importance that is measured by the average decrease in evaluation metric across all trees in the forest due to each feature was utilized as a first tool to quantify relevance between rheological parameters and sensory texture. Specifically, when a particular feature is used in a tree, the improvement in the evaluation metric, here RMSE, is calculated. The more the feature decreases the evaluation metric, the more relevant it is [49,50]. Permutation importance assesses the impact on the model's prediction accuracy by randomly shuffling the values of each feature across samples, thereby disrupting the relationship between the feature and the target. For each feature, its values are shuffled among all observations, and the change in the model's error is observed. A significant increase in the error upon shuffling is indicative of a high

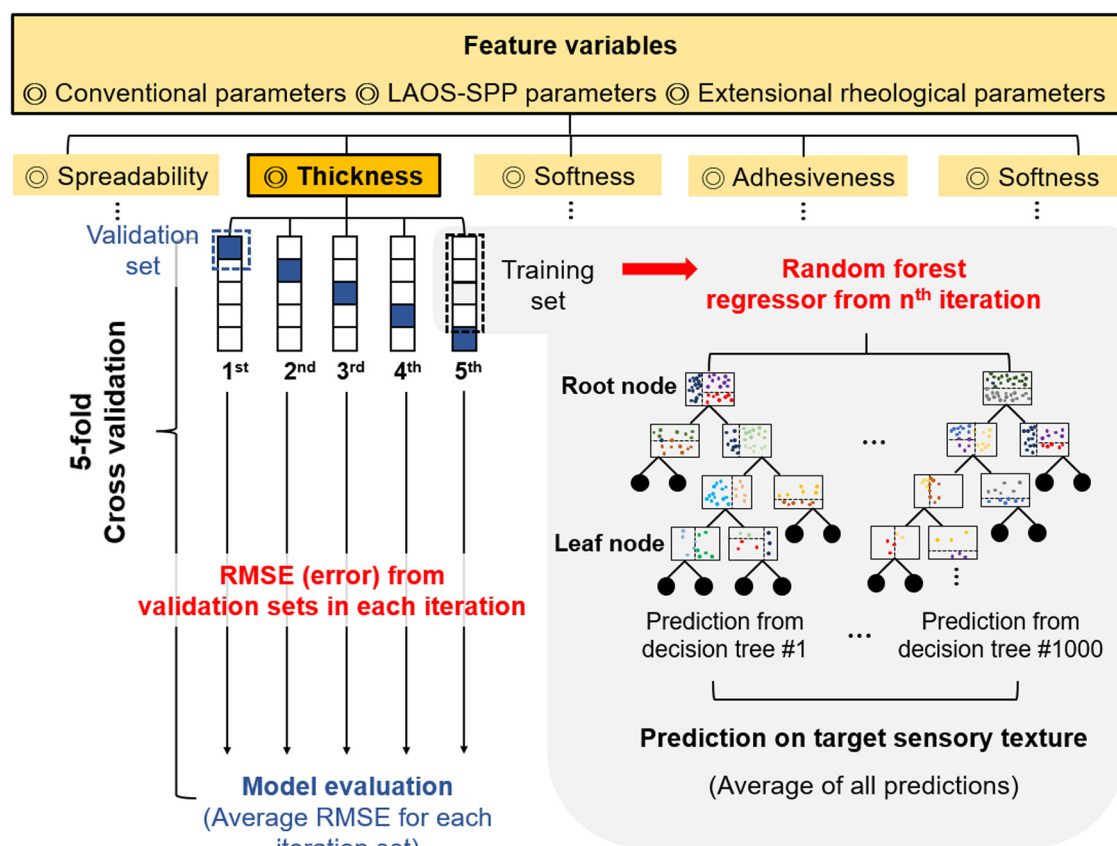


Figure 5: Schematic of the random forest regression algorithm used for predicting sensory texture.

importance of that feature [51,52]. Utilizing two different analyses offers a more balanced and accurate interpretation of the relationship between rheological measurements and sensory textures by mitigating potential issues inherent in each approach, such as the bias problem associated with feature importance.

4 Results and discussion

4.1 Spreadability prediction

In Figure 6, the performance of the spreadability prediction model is displayed, along with an analysis of its feature

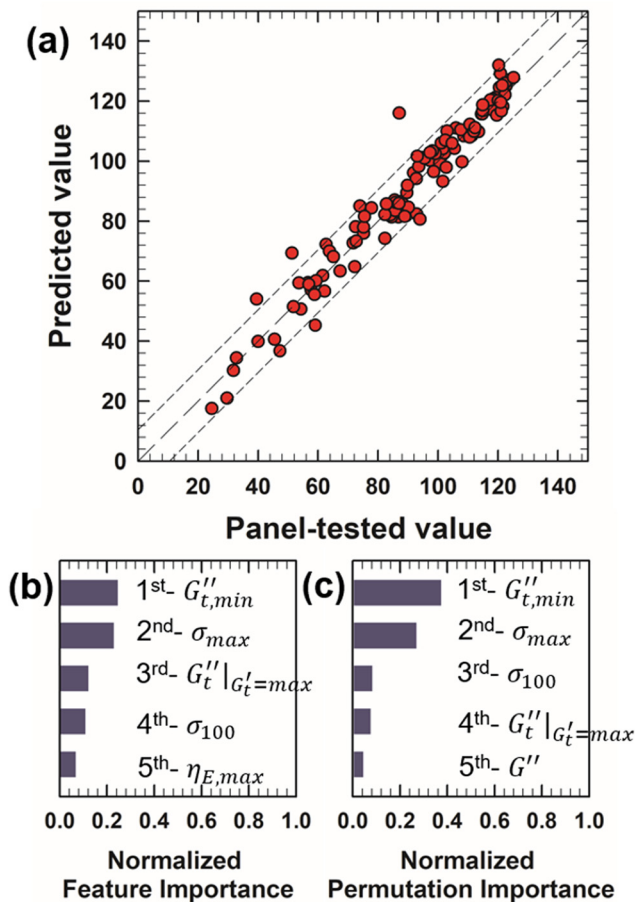


Figure 6: Performance of the spreadability prediction model and analysis of feature importance. (a) Comparison of predicted (machine learning model) vs actual (panel test) values of 117 samples. The range of RMSE deviation (10.47) from the accurate prediction line (model prediction = panel-tested value, long dashed line) is indicated by short-dashed lines. (b) Top five features from feature importance analysis. (c) Top five features from permutation importance analysis.

importance results. The spreadability prediction model demonstrates an RMSE of 10.47, suggesting that the spreadability of any given cosmetic formulation can be effectively predicted within an error range of 10.47 on the 150-score scale. Although the specific pipelines of the prediction model vary, its performance is comparable to the previously developed spreadability prediction model, which was based on a smaller dataset from 77 cosmetic formulations [15]. Given that this work utilizes a larger dataset (117 samples) that encompasses a broader range of formulations with broader ingredient compositions and rheological properties, the satisfactory performance in predicting spreadability suggests that the current strategy for developing a prediction model is robust. When exposed to new cosmetic formulations, it is expected that our prediction model will make effective and accurate predictions. In addition, it is noteworthy that the spreadability values of most formulations are predicted with remarkable precision. This accuracy is evidenced by the points closely clustered around the line of perfect prediction ($y = x$) in Figure 6.

To identify which rheological metrics are critical for determining the spreadability of cosmetic formulations, feature importance and permutation importance analyses were conducted. The results are displayed in Figure 6(b) and (c). In both importance analyses, $G''_{t,min}$ and σ_{max} were revealed to be the two dominantly important features. Both $G''_{t,min}$ and σ_{max} are associated with the visco-plastic deformation process during LAOS, where cosmetic formulations undergo strong flow at high shear rates with G'_t of nearly zero. In terms of the cosmetics application process, the visco-plastic deformation process corresponds to the right middle of rubbing process that is marked as point 3 and 6 in Figure 2 where cosmetics formulation is applied fastest and most fluidized. The significant role of σ_{max} highlights that the magnitude of stress experienced during the rapid application of cosmetic formulations under large shear rates is crucial for determining spreadability. In the same vein, σ_{100} , which is analogous to σ_{max} , ranks as the fourth and third most important feature in the feature importance and permutation importance analyses, respectively. Given that G''_t is defined as the partial derivative of

stress with respect to shear rate $\left(\frac{\partial \sigma}{\partial \left(\frac{\dot{\gamma}}{\omega} \right)} \right)$, the pronounced importance of $G''_{t,min}$ indicates that both the magnitude of shear stress and its variations in response to shear rate changes during the rapid application of fluidized cosmetic formulations are key factors in the perception of spreadability.

$G''_t |_{G'_t=max}$ is identified as third and fourth important features in both feature importance and permutation

importance analyses. Under LAOS, the point at which G'_t is at its maximum corresponds to the moment when the cosmetic formulation has largely recovered its microstructure, due to the small shear rate near the maximum or minimum strain ($\gamma = \pm\gamma_0$). Therefore, the significance of $G''_t|_{G'_t=\max}$ indicates that the perception of spreadability is influenced by the extent to which the viscous properties of cosmetic formulation can recover during the rubbing process.

4.2 Thickness prediction

The predictive performance and feature importance analysis results of our model for thickness are illustrated in

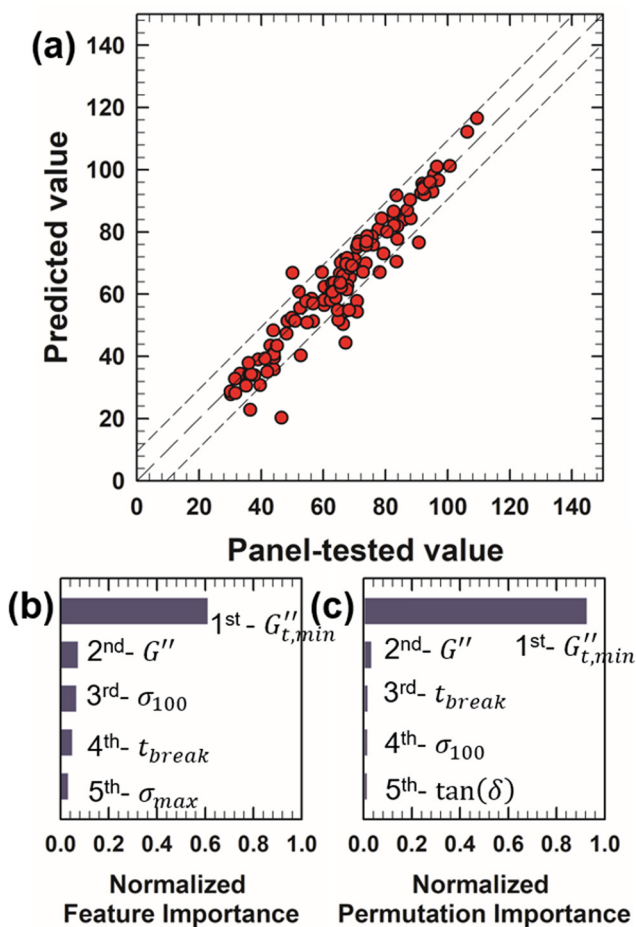


Figure 7: Performance of the thickness prediction model and analysis of feature importance. (a) Comparison of predicted (machine learning model) vs actual (panel test) values of 117 samples. The range of RMSE deviation (9.45) from the accurate prediction line (model prediction = panel-tested value, long dashed line) is indicated by short-dashed lines. (b) Top five features from feature importance analysis. (c) Top five features from permutation importance analysis.

Figure 7. The RMSE for thickness prediction stands at 9.45, representing the best performance among the five sensory attributes investigated in this study. Points in Figure 7(a) are most closely clustered around the line of perfect prediction ($y = x$), showing minimal deviations. The analyses of feature importance and permutation importance, as depicted in Figure 7(b) and (c), demonstrate that $G''_{t,\min}$ is the predominant feature influencing the perceived thickness of cosmetic formulations. This indicates that transient viscous behavior (shear stress in response to changes in shear rate) during a high-shear rubbing process is the most critical factor, akin to those affecting perceptions of spreadability, yet it carries even more weight. It is noteworthy that, unlike in the perception of spreadability where the magnitude of shear stress ($\sigma_{\max}$ or σ_{100}) is a decisive factor, its role is substantially less significant in determining the perception of thickness.

Traditionally, shear stress and the work of shear (shear dissipation) have been the principal rheological properties linked to the sensory texture of cosmetic formulations [4,15,22,53,54], with thickeners primarily used to adjust viscosity or the intensity of shear stress [55,56]. However, our findings suggest that transient rheological behavior, represented by the transient elastic modulus G'_t or the viscous transient modulus G''_t – defined as the variations in shear stress in response to strain or shear rate changes – may be equally or more influential in defining sensory textures. This underscores the necessity for a multifaceted approach in the design and selection of cosmetic thickeners, taking into account various rheological properties, including transient metrics like $G''_{t,\min}$.

4.3 Softness prediction

Figure 8 displays the predictive performance and feature importance analysis of our softness prediction model. The prediction model demonstrates satisfactory performance with an RMSE of 13.69, although it exhibits a comparatively lower level of performance when contrasted with the spreadability, thickness, or adhesiveness prediction models that will be introduced later. In Figure 8(a), while the data points representing the predicted value versus panel-tested value for most cosmetic formulations are closely clustered near the line of perfect prediction ($y = x$), some data points exhibit a significant disparity between predicted and panel-tested values. The higher RMSE observed in the softness prediction model can be attributed to the substantial deviations noted in the predictions of certain cosmetic formulations.

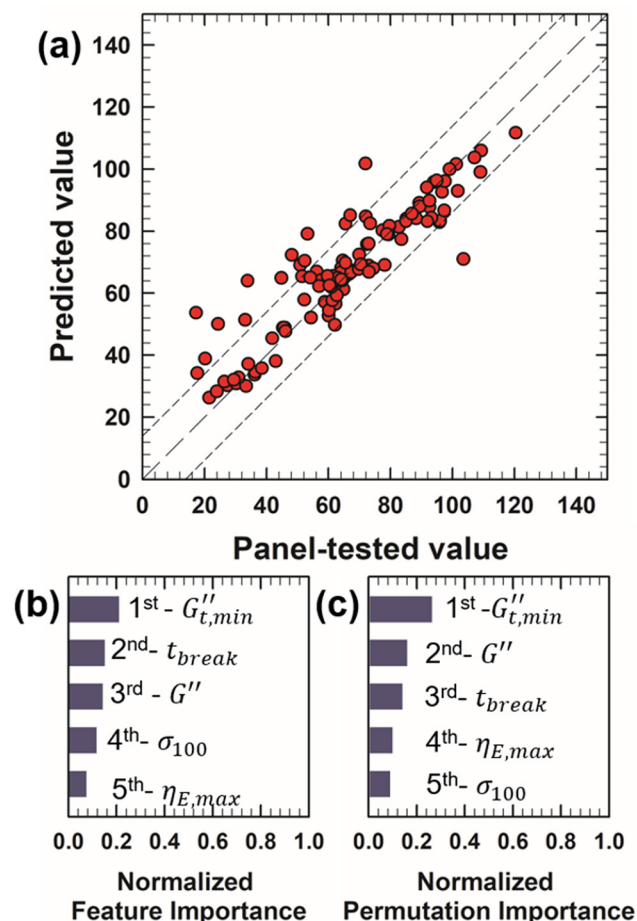


Figure 8: Performance of the softness prediction model and analysis of feature importance. (a) Comparison of predicted (machine learning model) vs actual (panel test) values of 117 samples. The range of RMSE deviation (13.69) from the accurate prediction line (model prediction = panel-tested value, long dashed line) is indicated by short-dashed lines. (b) Top five features from feature importance analysis. (c) Top five features from permutation importance analysis.

Feature importance and permutation importance analyses indicate that many rheological parameters play similarly important roles in determining softness. The top five features from both analyses show comparable importance, with no single feature exhibiting a dominantly high value. This contrasts with the cases of spreadability and thickness, where one or two rheological parameters demonstrate significantly greater importance. Similar to the cases of spreadability and thickness, $G''_{t,min}$ is shown to be the most influential feature in determining softness. In terms of the cosmetics application process, this indicates that the transient viscous properties exhibited during a viscoplastic flow under a high-shear rubbing process are primarily responsible for softness.

G'' and $\eta_{E,max}$ are ranked third and fifth in the feature importance analysis and second and fourth in the permutation

importance analysis, respectively. Since both metrics represent the shear and extensional viscous properties of cosmetic formulations in their fully structured or minimally disturbed state, the viscous properties of a cosmetic formulation at the initial usage stage – where imposed deformation is minimal – appear to significantly impact the perception of softness. t_{break} from the extensional rheological measurements is ranked second and third in importance analyses, the importance of which suggests that perception of softness is influenced by the tendency to breakup during the elongational deformation. The magnitude of shear stress at high shear rates, as indicated by σ_{100} , is found to be another critical rheological metric, similar to its significance in determining spreadability.

4.4 Adhesiveness prediction

As shown in Figure 9, our prediction model exhibits good performance in predicting adhesiveness, with an RMSE of 11.13. Remarkably, no cosmetic formulation displays significant prediction error, as evidenced by Figure 9(a), where most of the points are closely aligned with the line of perfect prediction ($y = x$). Similar to the perception of softness, both feature importance and permutation importance analyses in Figure 9(b) and (c) reveal that numerous rheological parameters play similarly important roles in determining adhesiveness. No single feature emerges as predominant, although σ_{100} shows relatively high importance. Adhesiveness is distinguished from the previously mentioned sensory textures in that the most important feature for determining it is σ_{100} rather than $G''_{t,min}$. The close correlation between adhesiveness and shear stress at a high shear rate (100 s^{-1}) implies that perception of adhesiveness is strongly influenced by the shear stress experienced during the rapid rubbing out process of cosmetic formulation. The importance of the fourth-ranked feature, σ_{max} , can be understood in the same vein. While adhesion is defined by the International Union of Pure and Applied Chemistry as “the process of attachment of a substance to the surface of another substance” and is scientifically distinct from shear stress (or viscosity) [57], it is intriguing that the psychological perception of adhesiveness is highly correlated with shear stress.

In both feature importance and permutation importance analyses, G'' and $G''_{t,min}$ are identified as significant, ranking second and fifth in feature importance, and third and fifth in permutation importance, respectively. As previously discussed in the spreadability section, these results suggest that the viscous properties in the structured state, such as during the initial usage stage with minimal deformation or the transient viscous properties observed

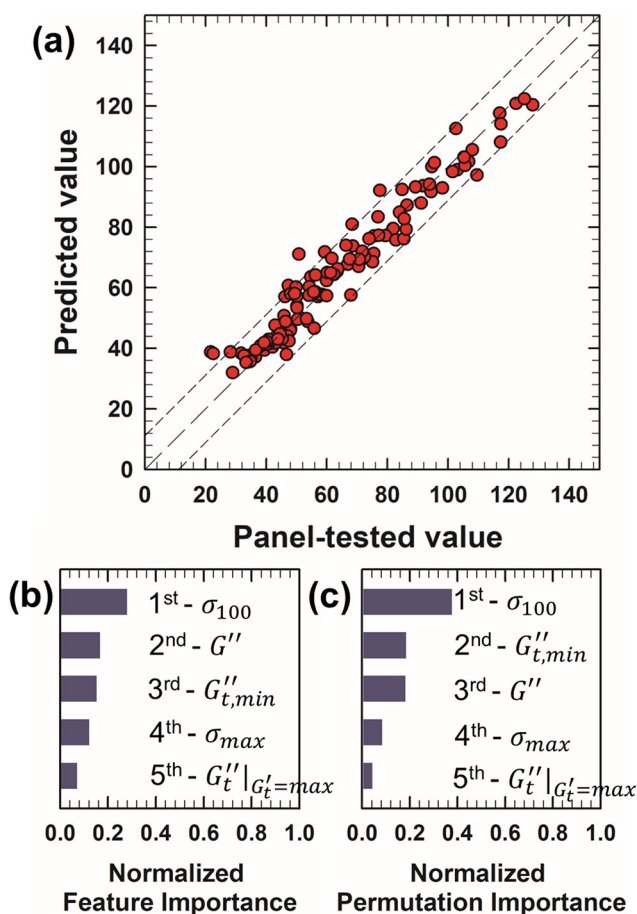


Figure 9: Performance of the adhesiveness prediction model and analysis of feature importance. (a) Comparison of predicted (machine learning model) vs actual (panel test) values of 117 samples. The range of RMSE deviation (11.13) from the accurate prediction line (model prediction = panel-tested value, long dashed line) is indicated by short-dashed lines. (b) Top five features from feature importance analysis. (c) Top five features from permutation importance analysis.

in the most structured state during LAOS (point 1 and 4 in Figure 2), significantly impact the perception of adhesiveness.

4.5 Stickiness prediction

In Figure 10(a), which compares predicted and panel-tested stickiness values of cosmetic formulations, multiple data points are situated far from the line of perfect prediction ($y = x$). This deviation is relatively greater compared to the results for other previously discussed sensory textures. Consequently, stickiness proves to be the most challenging sensory texture to predict, as demonstrated by the lowest prediction performance, with an RMSE of 22.15. It is noteworthy that all the top five feature importance values from the feature importance analysis in Figure 10(b) and the

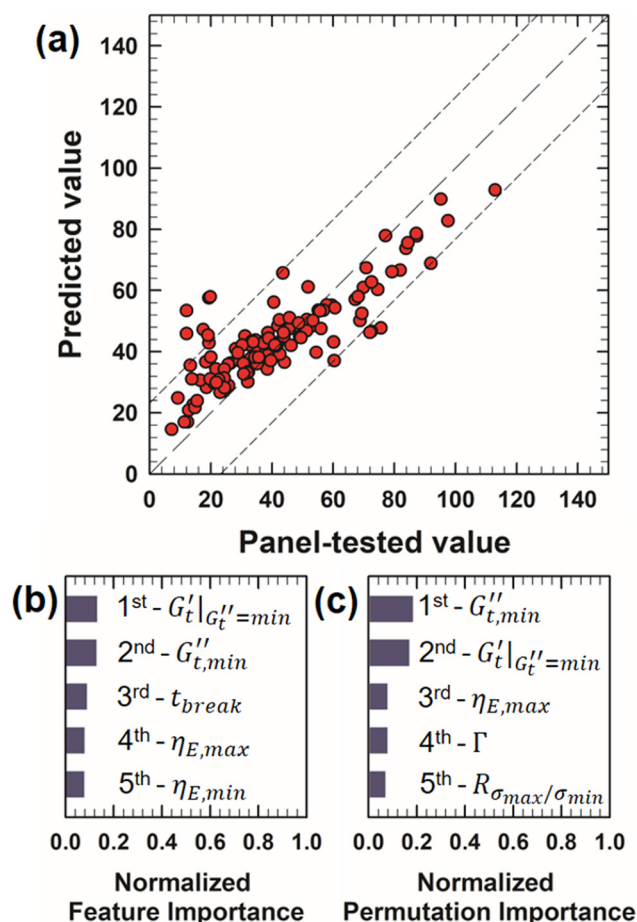


Figure 10: Performance of the stickiness prediction model and analysis of feature importance. (a) Comparison of predicted (machine learning model) vs actual (panel test) values of 117 samples. The range of RMSE deviation (22.15) from the accurate prediction line (model prediction = panel-tested value, long dashed line) is indicated by short-dashed lines. (b) Top five features from feature importance analysis. (c) Top five features from permutation importance analysis.

permutation importance analysis in Figure 10(c) are relatively small compared to those for other sensory textures, with no dominant feature emerging. In addition, only three rheological properties ($G''_t|_{G'_t=max}$, $G''_{t,min}$, $\eta_{E,max}$) out of the top five features are common in the permutation importance analysis. These results suggest an evenly distributed influence among all rheological properties beyond the top five, indicating a more complex relationship between rheological properties and stickiness compared to other sensory textures.

The feature importance analysis results in Figure 10(b) and (c) reveal that properties associated with extensional deformation are influential in determining stickiness. This is reasonable, considering that the perception of stickiness is likely linked to the tapping process, during which the cosmetic formulation undergoes extensional deformation.

$\eta_{E,\max}$ observed near the initial small deformation condition where the microstructure is minimally disturbed, ranks within the top five in both the feature importance and permutation importance analyses. This underscores the significance of extensional viscous properties at the initial stage of cosmetic application in the perception of stickiness. The high ranking of the features t_{break} and $\eta_{E,\min}$ indicates that both the ease with which a cosmetic formulation disconnects and extensional viscous properties at that moment also play important roles in determining the sensory texture of stickiness. Surface tension (Γ) has been identified as an important metric in the permutation importance analysis, which is linked to the increase in the surface area between air and cosmetic formulation caused by the tapping, a process involving extensional deformation.

The highest ranked rheological metrics are $G'_t|_{G''=\min}$ and $G''_{t,\min}$. Both metrics characterize the transient elastic and viscous properties of cosmetic formulation under viscoplastic deformation during the rapid rubbing process, which is marked as point 3 (or 6) in Figure 2. Therefore, we can conclude that the transient elastic and viscous properties during viscoplastic deformation under high shear conditions in cosmetic applications are the most influential factors in determining the perception of stickiness. In addition, $R_{\sigma_{\max}/\sigma_{\min}}$ is identified as the fifth most important metric in the permutation importance analysis. Intriguingly, metrics from simple shear rheology rank the highest despite the perception of stickiness likely being more closely associated with rheological properties obtained from extensional measurements that is analogous to the tapping of cosmetic formulations. These results offer two possible interpretations of the relationship between rheological metrics and stickiness. First, the metrics derived from simple shear tests, including LAOS, genuinely determine the perception of stickiness. Second, these simple shear-based test metrics effectively represent the extensional rheological properties, which are relatively difficult to measure and analyze.

5 Conclusion

A predictive model for five sensory textures of cosmetics formulations – spreadability, thickness, softness, adhesiveness, and stickiness – has been developed by integrating rheological analysis and machine learning techniques. This model expands upon previous work that established a prediction model for the limited texture of spreadability using a relatively small database. In this advanced model, rheological measurements including LAOS and extensional rheological analyses served as feature variables. These were

selected considering their analogical resemblance to the flow conditions experienced during the actual cosmetics application process, such as rubbing and tapping. For the target sensory texture values, panel-tested results from 10 highly trained panels were employed. The random forest regression technique reveals complex correlations between the rheological measurements and the sensory textures. In addition, important features that play a crucial role in determining each sensory texture are investigated using feature importance and permutation importance analyses.

The prediction model exhibited highly reliable performance in predicting sensory textures, achieving reasonable RMSE values, except for the stickiness, where the prediction performance relatively lagged behind those of other sensory textures. On the basis of the results of the importance analysis, we identified key rheological metrics that are crucial in determining each sensory texture and correlated them with the actual cosmetics application process. Intriguingly, many rheological metrics from the LAOS-SPP analysis proved to be key factors in all cases of sensory texture, indicating that feature selection, which considers the analogous flow conditions of rubbing and LAOS, is effective. Particularly, $G''_{t,\min}$ has consistently emerged as either the first or second most decisive feature in all sensory texture cases, underscoring the importance of the transient viscous property manifested during the viscoplastic deformation process at high shear rates in the rubbing of cosmetics formulations. In the stickiness analysis, distinguished from other sensory textures, rheological metrics from extensional rheological analysis are highly ranked in importance analysis. Such results can be attributed to the analogous flow conditions between extensional deformation and the tapping process of cosmetics application, during which stickiness is primarily perceived.

In conclusion, we emphasize the significance of our study from several distinct viewpoints. First, our established predictive model for various sensory texture of cosmetic formulations enables rapid and convenient sensory texture assessments replacing the time-consuming and costly panel tests. In terms of psychorheology, our study offers insights into how individuals perceive the sensory textures of materials, identifying the key rheological features that play a major role in this determination. Furthermore, our results are expected to be particularly useful in designing and controlling the formulations of various consumer products including cosmetics and food. From a broader perspective, our findings demonstrate how rheological analysis can be effectively combined with machine learning approaches to quantitatively examine physical phenomena that are subtly and ambiguously linked to rheological behaviors. It is interesting and encouraging that advanced rheological analyses,

such as LAOS-SPP, which naturally encompasses diverse flow conditions, can effectively capture the rheological behavior of materials under actual flow conditions encountered in consumer usage or manufacturing, thereby facilitating such approaches.

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Ethical approval: The conducted research is not related to either human or animal use.

Data availability statement: The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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