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MODELING ODOR OPTIMIZATION OF VEHICLES BASED ON DATA-DRIVEN GOAL PROGRAMMING

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ABSTRACT

In recent years, there is an increase in customer requirement on the comfort of vehicles. As a result, reducing the odor inside the vehicles has become an important and elusive task. Extensive experimental results show that the odor inside vehicles mainly comes from VOC (volatile organic compounds) emitted by the interior ornaments and parts. Given there are many VOC components affecting the odor, determining which VOC components are essential to the odor becomes a main difficulty in optimizing the odor in vehicles. In this paper, we proposed a new approach to optimize the odor of VOC in vehicles based on data-driven modeling and goal programming. To this end, we first collected mass spectrograms of vehicle parts and their odor ratings, where the mass spectrograms are obtained by mass spectrometer and ratings are scored by olfactory engineers. Then we used these data to build a data-driven model based on Weber-Fechner Law. The data-driven model is solved using lasso regression. Based on the data-driven model, we found out the contributions of the VOC components to the odor rating, which enables us to focus on certain specific VOC components that contribute much to the odor ratings. By strategically reducing those specific VOC components using goal programming, we finally obtained an optimized design with a better odor rating. To be specific, when performing the optimization, instead of minimizing the VOC odor rating, we set an ideal odor rating as the goal and formulated the optimization as a goal programming problem. To validate our approach, we collected 179 VOC mass spectrograms to train and test our data-driven model. The average accuracy of predicting odor ratings from mass spectrograms can reach 85% $\sim$ 90%. This data-driven model implies the contributions of VOC components on different mass weights to the odor rating, and the selected high-contribution mass weights can give reasonable optimization scheme to reduce the VOC gas odor.

NOMENCLATURE

m	Index of mass weights
n	Index of experimental samples
y_n	True odor rating of the n-th sample
$\hat{y_n}$	Prediction of odor rating, calculated from model
$z_{n,m}$	Mass spectrogram cps signal of n-th sample on m-th mass weight
β_m	Model parameter on m-th mass weight
s_m	Sensitivity coefficient on m-th mass weight
t_m	Odor detection threshold on m-th mass weight
$\beta_0^{'}$	Constant effect of systematic bias, sensitivity coefficient and odor detection threshold on odor rating
γ	Importance factor of regulation term in Lasso regression
C_m	Contribution of cps signal on m-th mass weight to the odor rating
I	Set of selected mass weight used in optimization

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w_i Weight factor reflecting the tractability of adjusting cps signal on i-th selected mass weight
d_i^+ Positive deviation of log-scale cps signal on i-th mass weight to the goal
d_i^- Negative deviation of log-scale cps signal to the goal
$l_{i,+}$ Lower bound of positive deviation
$l_{i,-}$ Lower bound of negative deviation
$u_{i,+}$ Upper bound of positive deviation
$u_{i,-}$ Upper bound of negative deviation

INTRODUCTION

VOC (Volatile Organic Compounds) is a class of organic compounds with boiling point in the range of 50-250 degrees Celsius and exist in gas phase in the air under room temperature. Many VOC components have unpleasant odors and some are even toxic, which will do harm to human health if exposed to such environment for a long time. In vehicle production, the ornaments and parts inside vehicles are usually made of plastic composite materials, and the emitted VOC gases from these materials become the main cause of the odor pollution inside vehicles. Considering user's comfort and health, analyzing and optimizing the VOC gas odor inside the vehicle tend to be more and more important in actual production.

Since a large amount of different organic compounds belong to the category of VOC gases, this causes much complexity and uncertainty in analyzing the detailed composition of VOC and determining which specific VOC component is the source of the odor and should be reduced for improvement. Current researches have already analyzed VOC components using sampling method together with analysis method. Sampling method is used to extract VOC samples from various substances, while analysis method is used to analyze the properties of VOC samples. For example, Solid Phase Micro Extraction (SPME) method is a kind of sampling method that can be used in evaluating and locating the presence of VOC . By using SPME fiber to extract samples from solid or liquid media, the analyte is separated for following analysis [1]. Another example of sample preparation is Needle Trap Micro Extraction (NTME), which uses needle trap devices as new tools to collect samples and requires very small sample volume without undermining sensitivity [2]. After sampling preparation, analysis of samples is needed to get more details on molecules and concentrations. A commonly used approach to analyze VOC composition is called the Gas Chromatography-Mass Spectrometry (GC-MS) method, which estimates and separates VOC components according to their different mass weights and adsorption abilities [3]. Besides, sensor technology is also introduced into chemistry field. Chemical sensors are integrated as an array to form an electronic nose which can detect and recognize special features of each VOC component [4]. Reference [5] gives a comparison between the above two methods, and the results show that both methods perform well in distinguishing among different VOC components and quantifying their concentrations. Proton transfer reaction mass spectrometry (PTR-MS) is also an analyze method. This method determines the detailed VOC composition by recognizing the mass-resolved fingerprints of different VOC components [6, 7].

The above studies relate much to laboratories and experiments, as the sampling and chromatography require delicate chemical operations. However, applying such complex sampling and analyzing steps in vehicle production is not very practical, since simple and fast detection is required during the production process. With this thought, we decided to collect the VOC gases emitted by vehicle parts directly and passed these gases through mass spectrometer to generate mass spectrograms. This whole process is rather simple for industrial operation [8]. Concerning the main propose of our research is to find a fast way of determining the odor of a given VOC gas and trying to optimize the odor, instead of analyzing the detailed molecule composition of the VOC gas, we focus on a macro level to build a data-driven model reflecting the relationship between mass spectrograms of VOC gases and the odor ratings of gases. By constructing such a model, we can get rid of all the chemical and experimental analysis on VOC components, and only a mathematical model is solved and tested to describe and predict the odor rating according to given mass spectrogram. From the resulted model, we can quantify the contributions of VOC components with different mass weights to the odor rating of the gas, and then we are able to select proper VOC components according to their contributions to conduct odor optimization.

Overall, our main contributions in this paper are: 1) build a model describing the relation between VOC gas mass spectrogram and odor rating for the interior ornaments and parts in vehicles; 2) find the contributions of VOC components to odor ratings and select proper ones to optimize the odor rating to a target rating.

DATA-DRIVEN MODELING

To analyze the odor of VOC gas, instead of using complex experiments such as Gas Chromatography to determine all gas components and find the smelly ones, our approach is to build a mathematical model which can predict the odor rating of VOC gas according to its spectrogram data, and can also help us analyze which mass weights contribute more to the bad odor, so we can figure out specific smelly VOC components according to these mass weights. To acquire such a model, we first derived a mathematical model with unknown parameters according to Weber-Fechner law, and then we plugged large amount of data into the equation and applied Lasso regression to solve the model parameters.

Original Data Used in Modeling

At the beginning of this part, we will first introduce all the data used to build the model. The original data contain the following two parts: 1) mass spectrograms of the VOC gases emitted by vehicle part samples and 2) the odor ratings of the VOC gases. Here we display a part of the whole dataset in Table 1.

TABLE 1. ORIGINAL DATASET

	Sample 1	Sample 2	⋯
Mass weight [amu]	signal [cps]	signal [cps]	⋯
10	14	150	
11	24	44	⋯
⋮	⋮	⋮	
Odor Rating	3	3.5	⋯

As shown in Table 1, the mass spectrogram of a sample gives the molecule signal intensities on a range of mass weights (for example, from 10amu to 500amu, related to the full scan range of mass spectrometer), and the intensity unit 'cps' (counts per second) represents how many molecules with a certain mass weight are counted per second by the mass spectrometer detector. The odor ratings are scored by odor engineers to describe the comfort level for people to smell the odor. Our odor rating levels are based on the definition of olfactory intensity scales in [9], and the detailed descriptions are listed in Table 2:

TABLE 2. DEFINITION OF ODOR RATINGS

Odor rating	Description of comfort level
1	Unperceivable smell
2	Slightly perceivable but does not cause discomfort
3	Obvious smell but does not cause discomfort
4	Strong smell, cause discomfort
5	Very strong smell, cause much discomfort
6	Unbearable smell

*0.5-scale for odor comfort levels between integer odor ratings

Data Modeling Based on Weber-Fechner Law

According to our data, mass spectrograms are physical measurements of the VOC odor, while odor ratings are human senses of the odor. To link human senses with physical measurements, we referred to the Weber-Fechner Law, which proposes a mathematical approach to quantify the relationships between physical measurements and human perceptions such as feelings on touch, sound, light, odor and so on [10].It is widely used in the detection and classification of pollutant odor intensity and other environmentally related fields [11, 12]. One mathematical model based on this law describing the relation between gas concentration and human sensation is proposed in [13] as follows:

$$P = k \log \frac{C}{C_{OT}} + d, \tag{1}$$

where P represents the human perceived magnitude of the odor, C represents the gas concentration with unit $mg \cdot m^{-3}$, C_{OT} is the odor threshold concentration with unit $mg \cdot m^{-3}$, k is a constant factor related to the effect of stimulus on human sensation, and d is a systematic intercept of the Weber-Fechner law.

In our data, the perceived magnitude is the odor rating given by engineers, and the physical measurements are the cps signals obtained from mass spectrometer. For a fixed type of mass spectrometer apparatus, we can use a standard sample with known concentration for each mass weight to calibrate the relation between cps signal intensity and concentration, which can provide us with a conversion coefficient for this mass weight [14]. By doing such conversion, we can obtain concentration data from cps signals and apply Eq. (1) for each mass weight. Note that different mass weights correspond to different gas components with different odors, so we sum their effects together to obtain the final odor rating of the VOC mixture. Our model is formulated as Eq. (2):

$$\hat{y}_n = \sum_{m=1}^{M} \beta_m \log\left(\frac{z_{n,m}}{s_m \cdot t_m}\right) + \beta_0 \tag{2}$$

where $\hat{y_n}$ is the odor rating of the n-th vehicle part calculated by this model, $z_{n,m}$ is the cps signal value of the n-th vehicle part sample on the m-th mass weight, s_m is the conversion coefficient describing the relation between cps signal and chemical concentration on the m-th mass weight, and t_m is the odor detection threshold of the corresponding chemical component on the m-th mass weight [15]. The original data give full-range mass spectrograms with hundreds of mass weights, but part of them are irrelevant to VOC components. Therefore, to simplify our model from excessive information, we add practical consideration and choose M mass weights according to the possible gas composition in vehicles. Referring to Eq. (1), we define β_m as the constant factor on the m-th mass weight, as the role of k in Eq. (1)

to link the log-scale concentration to the odor rating. Finally, we combine all the systematic bias together and introduce a constant unknown parameter β_0 to describe this bias in our model.

Till now, there is still a difficulty that the odor detection thresholds t_m and conversion coefficients s_m of some gases are unknown because of the lack of experimental data for all mass weights. However, a solid truth is that all these unknown coefficients must be constant values under fixed condition with the same apparatus. Therefore, we apply some mathematical transformations to merge these constants into β_0 and form a new term $\beta_0^{'}$. Now Eq.(2) is converted as follows:

$$\begin{aligned}\hat{y}_n &= \sum_{m=1}^{M} \beta_m \log(\frac{z_{n,m}}{s_m \cdot t_m}) + \beta_0 \\ &= \sum_{m=1}^{M} \beta_m \log z_{n,m} + (-\sum_{m=1}^{M} \beta_m \log(s_m \cdot t_m) + \beta_0) \\ &= \sum_{m=1}^{M} \beta_m \log z_{n,m} + \beta_0^{'}\end{aligned} \tag{3}$$

Eq.(3) is the final form of the mass spectrogram-odor rating prediction model. Given the cps signals on M mass weights of a sample, the odor rating of this sample can be calculated once all the model parameters $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_M, \beta_0']$ are determined. Among these parameters, β_0' represents a constant effect on odor rating caused by systematic bias together with unknown constant odor detection thresholds and sensitivity coefficients; $\beta_m \log z_{n,m}$ depicts how the log-scale of cps signal on m-th mass weight contributes to the odor rating. Recall that one important goal of our model is to figure out those VOC components that contribute much to the bad odor, and now the contribution term $C_m = \beta_m \log z_{n,m}$ provides an approach to quantitatively estimate the odor rating contribution of m-th mass weight. Therefore, our model can not only predict the odor rating according to mass spectrogram, but also help us find principal odorous VOC components for the following optimization.

So far, all the model parameters $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_M, \beta_0']$ are still undetermined in this model. They will be solved by plugging in large amount of original data and minimizing the loss function, as the following section shows.

Model Parameter Determination Based on Lasso Regression

In the experiment, the engineers score the odor rating for N vehicle part samples as $y_1, y_2, \cdots, y_N$. With mass spectrogram data and our model, we can calculate N predictions of odor ratings as $\hat{y}_1, \hat{y}_2, \cdots, \hat{y}_N$. The optimal model should minimize the difference between the predictions and the true values, which is depicted using a loss function. In this paper, the optimal parameters are determined by minimizing the loss function formulated as follows:

$$\boldsymbol{\beta}^*_{opt} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} (y_n - \hat{y_n})^2 + \gamma \|\boldsymbol{\beta}\|_1 \tag{4}$$

Here y_n is true odor rating, $\hat{y_n}$ is the predicted odor rating obtained from Eq. (3), and our aim is to minimize the summation of squared residue $(y_n - \hat{y_n})^2$ to obtain optimal $\boldsymbol{\beta}$. Besides the residue between true and predicted odor ratings, an extra L_1-norm regulation term $\|\boldsymbol{\beta}\|_1$ with a constant γ is added to the loss function. This term comes from Lasso regression, and is used to avoid overfitting, especially when we have many unknown model parameters to be determined [16, 17]. In our case, there are $M+1$ model parameters $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_M, \beta_0']$ waited to be solved, which can be a large number due to the variety of organic compounds. The penalty parameter γ controls the influence of regulation term in the loss function.

Till now, we can obtain optimal model parameters $\boldsymbol{\beta}^*_{opt}$ by minimizing the above loss function, and then the model will be completely defined. From Eq. (4), the optimization problem is obviously a convex problem, and we directly use the `cvx solver`[1] to solve for the best model parameters.

ODOR OPTIMIZATION BASED ON GOAL PROGRAMMING

In our model, mass spectrogram provides the information of all mass weights, which is too much for optimization. In reality, although VOC gas consists lots of organic compounds, the main sources of bad odor only come from a few components. Therefore, before we start optimization, we should first figure out which mass weights have large contribution to the bad odor, and this can be done by calculating the 'contribution' factors $C_m = \beta_m \log z_{n,m}$ of all M mass weights and make comparison. Now our optimization problem can be formulated based on the following considerations:

1. Select important mass weights. It's not realistic to consider all VOC components in optimization, so we only consider those components that are more important to the main source of bad odor. According to our model, mass weights with large contribution C_m will be selected, and we collect these mass weights into a set I. The optimization only performs on mass weights with index $i \in I$.
2. Choose goal programming technique. Instead of minimizing the odor rating to its best possible result, we set our aim as improving the odor rating to reach a better target odor rating. Therefore, what we did is to find a scheme to adjust cps signals on selected mass weights so that the new odor rating

[1] `http://cvxr.com/cvx/`

equals to the goal. Such formulation is in the form of goal programming [18, 19].

3. Define optimization objectives. The sense of optimality comes from two considerations: 1) The adjustments on cps signals should be as small as possible to save the cost of optimization 2) The operations to adjust cps signals in actual production should be simple and tractable. Therefore, the objective function in optimization is to find the minimum cps deviations needed to reach the goal. In addition to minimizing deviations, we further consider the tractability of realizing these deviations on the selected mass weights, so we assign different weighting factors w_i to mass weights based on the easiness of adjusting the concentrations of their corresponding VOC components. In this way, the finalized optimization design is of much practical significance.
4. Satisfy more practical constraints. The inequality constraints are given by the lower and upper bounds l_i u_i of deviations, since we cannot adjust the cps signals arbitrarily. For example, we cannot reduce the cps signal to zero on some mass weight, which means that there is absolutely no gas molecules on this mass weight and is impossible to achieve. Therefore, upper bounds and lower bounds exist in actual operations.

With the above considerations, the whole goal programming problem is completely formulated with objective function, goal and boundary constraints. The system is shown in Eq. (5):

$$\begin{aligned} &\text{minimize} \sum_{i\in I} w_i(d_i^+ + d_i^-) \\ &\text{s.t.} \quad y_{goal} = \sum_{m=1,m\notin I}^{M} \beta_m \log z_m + \sum_{i\in I} \beta_i(\log z_i - d_i^+ + d_i^-) + \beta_0' \\ &\qquad l_{i,+} \le d_i^+ \le u_{i,+} \\ &\qquad l_{i,-} \le d_i^- \le u_{i,-} \end{aligned} \tag{5}$$

Here the set I contains selected mass weights indices. Assume that to improve the current odor rating to the goal rating y_{goal}, we want to change the signal on mass weights with significant contributions, which have indices $i \in I$, then we have d_i^+ and d_i^- being the positive and negative deviations from the goal. According to the model given in Eq. (3), the model parameters in $\boldsymbol{\beta}$ are related to the logarithm of cps signals, therefore our deviations are also defined as log scale of cps signals to keep consistency. Now we obtain the goal function of the goal programming formulation, and it acts as an equality constraint in optimization. By assigning larger weighting factors w_i to the mass weights that are more difficult to operate, the deviations on these mass weights will tend to be smaller in order to minimize the objective function, which satisfies our requirement that we try to avoid difficult operations in actual production. The u_i and l_i terms are upper and lower bounds for positive and negative deviations.

According to Eq. (5), to optimize the odor of a certain VOC gas, we will change the cps signals on selected mass weights by deviations d_i^+ and d_i^- within their lower and upper bounds to reach the target odor rating, and the optimal solution gives minimum deviations as well as considers the difficulty of adjusting cps signals on these mass weights.

The whole methodology from data-driven modeling to goal programming is summarized in the following flow chart:

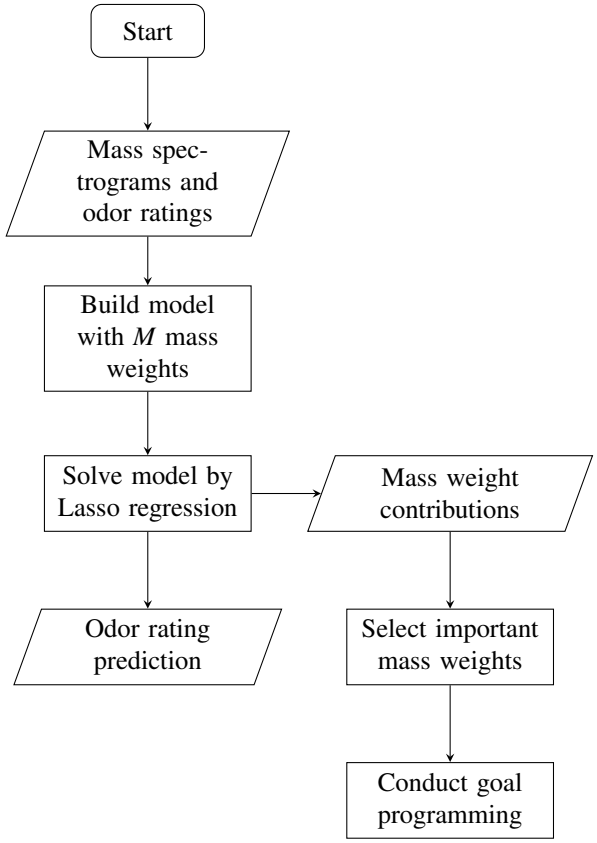

FIGURE 1. FLOW CHART OF WHOLE METHODOLOGY

RESULTS AND DISCUSSION

Model Performance and Contribution Analysis

We collected 179 sets of VOC mass spectrogram data with full-range mass weights from 10amu to 500amu, and we chose 64 mass weights which may exist in vehicle VOC gases to build the model. Then we collected the true odor ratings of these samples from odor engineers. The true odor rating distribution of the 179 samples is shown in Fig. 2. We can see that the distribution of odor rating is uneven, and is mainly clustered around 3,3.5 and 4.

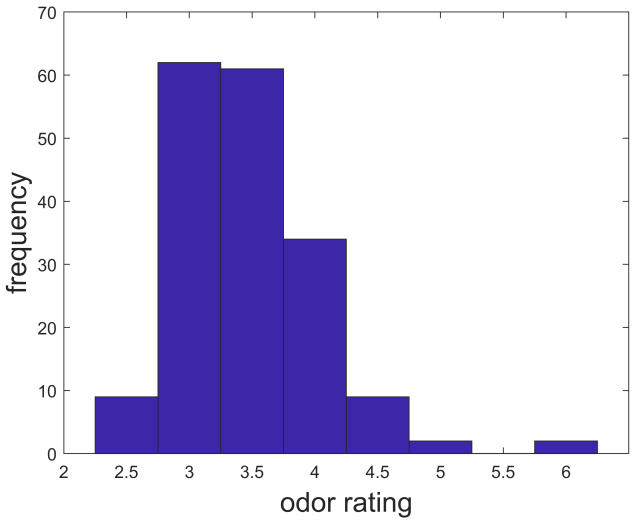

FIGURE 2. ODOR RATING DISTRIBUTION OF 179 SAMPLES

In Lasso regression process, we need to divide all the original data into training data and testing data. The training data are used to solve for the optimal model parameters and then we test the model performance using the testing data. We chose 149 sets of data for solving the model and the remaining 30 sets of data for testing, and we set the γ factor in the loss function to be 0.6. The performance of odor rating prediction on 30 test samples is shown in Fig. 3.

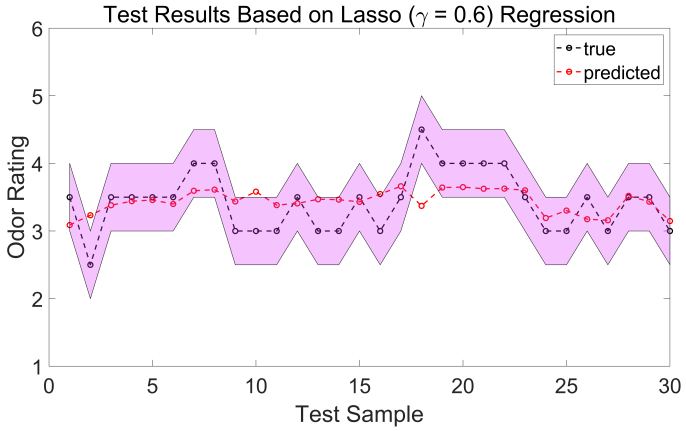

FIGURE 3. THE PREDICTION RESULTS OF 30 TEST SAMPLES

In above Fig. 3, the black dots are true values of odor ratings and the red dots are predicted values of odor ratings. Since the true odor ratings are discrete values 1,1.5,2,2.5,$\cdots$,6 while the predicted odor ratings by model are continuous values, we defined that if the predicted odor rating lies within the ± 0.5 region of the true odor rating (shown as the purple shadow region in Fig. 3), then the predicted result is considered as accurate. We observed that in Fig. 3, there are 4 test samples don't obtain accurate predictions, so the model accuracy is about 87%. These 4 inaccurate predictions have original odor ratings 2.5, 3.5, 3.5 and 4.5 ,respectively. Combining with the distribution of sample odor ratings in Fig. 2, it's reasonable to conclude that the lack of samples in odor rating 2.5 and 4.5 causes a lack of features in our model and therefore the prediction error on these odor ratings is relatively large.

After analyzing the prediction performance of our model, now we will show how this model can visualize the odor contribution of each mass weight. We know that $\beta_0^{'}$ reflects the systematic bias and the effect of unknown constant coefficients which will always be a fixed value, while $\beta_1, \beta_2, \cdots, \beta_{64}$ describe how the cps signals contribute to the odor rating. Therefore, we plugged a set of cps signal data z_m for a certain sample into the model and calculate the contribution $C_m = \beta_m \log z_m$ on m-th mass weight ($m = 1, 2, \cdots, 64$). The resulting mass weight-contribution plot is given in Fig. 4.

FIGURE 4. THE MASS WEIGHT-CONTRIBUTION PLOT OF A SAMPLE

Since all the cps signals obtained from mass spectrometer are nonnegative integers (the signal cannot have negative counts), and we converted zero cps signals to 1 while preprocessing the data to avoid error in logarithm calculation, then the values of $\log z_m$ will always be nonnegative. Therefore, in Fig. 4, the positive peaks relate to positive β_ms and the negative peaks relate to negative β_ms. Furthermore, if the cps signal on mass weight increases, positive β_ms will cause the odor rating to be higher (higher odor rating means more discomfort to people according

to Table 2), and negative β_ms will lead to a more comfortable odor. In reality, the odor optimization process is usually to decrease the concentration of bad odor gases rather than increase the concentration of good odor gases, so we only focus on the mass weights with positive peaks, and we can select important mass weights to be optimized according to the height of positive peaks.

Optimization Performance

In this part, we chose a VOC gas sample with original odor rating 4.0 to be optimized to a target odor rating 3.0. Based on the previous discussion, we need to select important mass weights first. We plugged in the cps signal data of this sample into the model, then we obtained the mass weight-contribution plot and selected the first 5 mass weights with highest positive contribution peaks. Denote these 5 mass weights as #1,#2,#3,#4,#5, and then we conducted our odor optimization on these five important mass weights.

To validate the effect of weighting factors w_i, we considered two different scenarios. In one scenario we didn't consider the tractability of practical operation, so we assigned equal weighting factors to all the selected mass weight. In the other scenario we assigned inequal w_is to describe the difficulty of reducing the cps signals on selected mass weights, and we compared these two optimization schemes. The detailed weight assignment is listed in Table 3.

TABLE 3. EQUAL & INEQUAL-WEIGHT SCENARIOS FOR GOAL PROGRAMMING

Massweight No.	#1	#2	#3	#4	#5
Equal-weight w_i	1	1	1	1	1
Inequal-weight w_i	4	1	2	1.3	1.5

In Table 3, we defined the weighting factors to lie within 1 to 5. If the weight factor is close to 1, the actual operation to reduce the signal on this mass weight will be easier; and if the weight factor is close to 5, this indicates a more complex operation in real production. The weight value 4 means that the first selected mass weight is difficult to operation, and we hope to avoid or reduce the operation on this mass weight. Besides the weighting factors, the lower and upper bounds of adjusting the cps signal also need to be defined. Since the values of cps signals vary with different VOC gas samples, the limitation is given in the percentage form. For example, the lower bound of the deviation for mass weight #1 is 5% of the original level, which means that the cps signal on mass weight #1 will be decreased at least 5% of the original signal once it should be decreased. In our case, we set the lower bound of signal adjustment to be 5% for all selected mass weights, while the upper bound varies with mass weights and the exact values we used are listed in the following Table 4.

TABLE 4. UPPER & LOWER BOUNDS FOR 5 MASS WEIGHTS

Massweight No.	#1	#2	#3	#4	#5
Lower bound	5%	5%	5%	5%	5%
Upper bound	20%	14%	30%	26%	22%

After determining all these conditions, we referred to Eq. (5) and solve the goal programming system. Table 5 summarizes the optimization schemes to reach the goal odor rating under equal and inequal cases.

TABLE 5. OPTIMIZATION RESULTS OF TWO SCENARIOS

Original odor rating 4.0 to Goal odor rating 3.0		
Massweight No.	Equal-weight case	Inequal-weight case
#1	8%	5%
#2	5%	10%
#3	0	0
#4	0	0
#5	0	0
	reach the goal	reach the goal

Each column of Table 5 is a complete optimization scheme, and can be explained as follows: For equal-weight case, if we want to optimize the sample with original odor rating 4.0 to reach the goal odor rating 3.0, we need to reduce the cps signal on mass weight #1 by 8%, reduce the cps signal on mass weight #2 by 5%, let the other cps signals remain unchanged, and we can achieve this goal. For inequal-weight case, the weight of mass weight #1 is 4, representing that this mass weight is difficult to operate in actual production though it has high contribution to the odor rating. Therefore, we can see that compared with equal-weight case, the inequal-weight case reduces more percentage of cps signal on mass weight #2 with the consideration of both

contribution and the tractability of operation, which gives a more practical optimization scheme. Overall, our optimization formulation can deal with practical considerations well enough.

CONCLUSION

In this paper, we proposed a mathematical model describing the relationship between mass spectrogram cps signal of a VOC gas sample and the odor rating of the VOC gas. Using this model, we can achieve two tasks, one is to predict the odor rating given the mass spectrogram of a sample, the other is to select important mass weights with large contributions to the bad odor and therefore find out odorous VOC components. This model helps us to get rid of the complex chemical component analysis of the VOC gas, and we use a concise math equation to predict the odor and find the components in need of optimization. The models can generally achieve 85% to 90% accuracy, which is a reliable range, and we also believe that the accuracy can be further improved if we can provide more samples with extreme odor ratings so that the model can collect enough features for different odor ratings. With the contribution analysis, we are able to select mass weights with large contribution to bad odor and conduct goal programming accordingly to improve the odor to a given target odor rating. Our optimization formulation considers both the odor contribution and the operation difficulty of each mass weight, which can generate very practical optimization schemes for vehicle production.

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