CHEMICAL ENGINEERING TRANSACTIONS
VOL. 68, 2018
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Selena Sironi, Laura Capelli

ISBN 978-88-95608-65-5; **ISSN** 2283-9216
DOI: 10.3303/CET1868063

Odor Intensity Detection and Evaluation Method Considering Odor Prediction Model

Gaixia Chen

Hebi Automotive Engineering Professional College, Hebi 458030, China
123434535@qq.com

Volatile organic pollutants produced during people's living and production are the main source of stink pollution. The rapid and efficient detection and evaluation of odors in gas through effective methods is a key step for improving the level of supervision and ensuring people's living health. Because the chemical composition of the stink and odor gas is complex, the single odor intensity detection and evaluation method can hardly meet the requirement. Therefore, based on the odor research of domestic and foreign scholars, a multi-component odor mixture prediction model is established in this paper. The prediction model comprehensively considers and analyzes the interaction between odor and volatile organic compounds (VOCs), and the relationship between the concentration of chemical components and the intensity of odor; basing on the linear equation between the odor intensity and the logarithm of the activity to modify the U model and the vector model can better achieve detection and evaluation of the total odor intensity of the mixture gas, and can improve the prediction accuracy of the odor intensity prediction model. The research has important guiding significance for improving domestic evaluation and detection level of gas odor.

1. Introduction

Stink pollution is one of the main components of environmental pollution, it causes great harm to people's health and ecological environment (Pettarin et al., 2015; Zheng et al., 2018). How to improve the detection and evaluation level of stinks and other odorous gases, and thus improve the monitoring and control of sudden pollution events and stink pollution is the main content of gas odor research (Iranpour et al., 2010). Odor sensory evaluation method, odor intensity prediction model, electronic nose (e-nose) and other odor detection devices are the main methods for gas odor evaluation and detection, and they played a key role in gas odor detection. Among them, the prediction of gas odor intensity can effectively avoid limitations of odor test and environment, and it is a hot spot for domestic and foreign research.

Some scholars have conducted fixed-point monitoring studies on stink pollution in landfills, sewage treatment plants and other places, and they have analyzed the stink source and chemical components of the VOCs (De et al., 2006); some scholars have established an odor prediction model for single organic compound and studied the evaluation of odors for single component compound (Sakai et al., 2006). At present, the research on the evaluation of stink and odor has enriched the research content of the field to a certain extent and laid a solid foundation for the evaluation of odor research. However, in the current odor evaluation method, the accuracy and repeatability of odor intensity evaluation results are poor. There is a lack of prediction methods for odor intensity based on chemical concentrations of VOCs, meanwhile there are few studies considering the interaction law between odorous substances. It is important to accurately predict the odor intensity of odor gas mixtures based on the above factors (Mussio et al., 2001).

Aiming at the problems existing in the evaluation of gas odor, this paper first establishes an odor prediction model for multi-component chemical mixtures; in order to derive the mapping relationship between the chemical component concentration and the odor intensity of the odor gas, the paper adopts the modified U model and the modified vector model to correct the prediction model; and then it demonstrates the prediction results of the modified prediction model by experimental methods, and the results show that the modified vector model is suitable for the prediction of odor intensity of multi-component chemical odor gas, and it has good prediction accuracy (Soares ei al., 2018).

Please cite this article as: Chen G., 2018, Odor intensity detection and evaluation method considering odor prediction model, Chemical Engineering Transactions, 68, 373-378 DOI: 10.3303/CET1868063

2. Gas odor intensity prediction model

Generally, odorous gas is not composed of a single chemical component, but includes organic sulfides, carbon oxides, benzenes, phenols, benzene aromatic hydrocarbons, etc., where complex interactions exist between chemical components (Hansen et al., 2016). The evaluation of odor intensity is not a simple addition of the intensity of each odor, but a comprehensive result of complex reactions of various chemical components. This chapter introduces a multi-component odor gas prediction model based on the introduction of single component gas prediction model (Sironi et al., 2006).

2.1 Single component gas prediction model

The prediction models for predicting chemical component concentration and odor intensity are mainly three models: The Weber-Fechner Law, the Power Law Model and the Linear Model.

2.1.1 Weber-Fechner Law

Weber-Fechner Law is a law that expresses the relationship between perceived quantities and physical quantities. Its formula is shown as Formula 1:

$$\mathrm{OI} = \mathrm{k} \cdot \log \mathrm{C} \tag{1}$$

Where, OI represents the intensity of the odor, C represents the chemical concentration, and k is the empirical value obtained by experimental accumulation.

2.1.2 Power Law Model

$$\mathrm{OI} = \mathrm{k} \cdot \mathrm{C}^{n} \tag{2}$$

The Power Law constant n is a real number in the range of [0.2, 0.8], OI represents the intensity of the odor, and C represents the chemical concentration (Schauberger et al., 2006).

2.1.3 Linear Model

Through chemical experiments on aldehydes, scholars have found that when the chemical concentration of aldehydes is divided by the odor threshold, the odor activity value (OAV) can be obtained, after the OAV is logarithmically processed, there is a linear relationship between its value and the odor intensity value. Based on this, for other chemical components of same functional group or similar structure, after its concentration is divided by the odor threshold and logarithmically processed, we can get linear relationships as shown in the following Table (Piringer et al., 2015).

Table 1: Relationship between odor activity value and odor intensity of several odorous substances

Substance type	Linear formula	R^2
Alcohols	OI=0.0546lnOAV+0.994	0.88
Aldehyde	OI=0.681lnOAV+1.143	0.85
Ketones	OI=0.630lnOAV+0.998	0.91
Ester	OI=1.325lnOAV+0.548	0.89
Alkane	OI=0.598lnOAV+1.001	0.92
Aromatic hydrocarbon	OI=0.589lnOAV+0.710	0.85

2.2 Multi-component gas prediction model

The prediction model of a single component is relatively simple, while for multi-component odor chemicals, there are fusion, synergy, inhibition and other interactions. $OI_{ab} = OI_a + OI_b$ (fusion), $OI_{ab} > OI_a + OI_b$ (synergy), $OI_{ab} < OI_a + OI_b$ (inhibition). Based on the relationship between odorous substances, the prediction models of odor gas intensity such as ERM model, vector model, U model and UPL2 model are proposed. Although these models can reflect the independent relationship between intensity and each component, it is difficult to achieve prediction of the total intensity of odor gases (Capelli et al., 2009). The multi-component gas mixture prediction model can better predict the concentration and total intensity of the mixture.

2.2.1 Extended U model

The model calculation formula is shown as Formula 3:

$$OI_{(p)} = \frac{1}{p}\left(\sum_1^p OI_{(p-1)} + OI_p\right) + \frac{2cos\alpha(p)}{p}\sum_1^p \sqrt{OI_{(p-1)}OI_1} \tag{3}$$

P represents the odor type of the mixture, and the calculated value of cosα is shown as Formula 4:

$$\cos\alpha(\mathrm{p}) = \frac{\sum_{BIN=1}^{p(p-1)/2} cos\alpha_{BIN} \cdot OI_{BIN}}{\sum_{BIN=1}^{p(p-1)/2} OI_{BIN}} \quad (4)$$

Where OI_{BIN} is the odor intensity after the fusion, synergy and inhibition of two compounds (Piringer et al., 2007).

2.2.2 Maximum intensity component model

The maximum intensity component model is an idealized model that equates the overall odor intensity of the mixture to the maximum intensity value of the odor when the component exists alone (Teixeira et al., 2013). As shown in Formula 5:

$$\mathrm{OI} = \max(OI_i), \forall i = 1, \ldots, N \quad (5)$$

2.2.3 Comparison of multi-component prediction models

In addition to the models in 2.2.1 and 2.2.2, there are extended vector model, cumulative model, and EA model. The experimental comparison shows that the prediction accuracy of each model of the two components is higher. For the multi-component chemical mixture, different models have different prediction effects with different degrees of complexity, but the overall prediction effect of vector model and EA model is poor, and the prediction result of the extended U model is more stable and has higher prediction accuracy (Teixeira, MA et al., 2003).

3. Gas odor intensity prediction model correction methods

To promote the application of gas odor intensity model in the detection and evaluation of odor gas, improving the accuracy and application range of the prediction model is the focus of this paper. For mixture with determined chemical component concentration, perform quantitative analysis on the relationship between overall odor intensity and single odor intensity, so as to achieve prediction of the total odor intensity of the gas according to its chemical components (Ruth & O'Connor, 2001).

3.1 Modified U model

The extended U model has higher prediction accuracy, so it has important reference significance for the modification of the U model. According to the linear relationship between the average odor intensity and the overall odor intensity of the two aromatic hydrocarbon components, use the linear relationship of OI-lnOAV of the single component aromatic hydrocarbon to replace the lnOAV value of the OI of each component, so as to construct a gas odor intensity prediction model for lnOAV of each component.

3.1.1 Experimental reagents and instruments

The experimental reagents include: benzene, propyl benzene, o-xylene, styrene; the experimental instruments include: odorless gas sample bags, dynamic dilution olfactometer, gas chromatography, microsyringe; besides, three male and three female scent identifiers were arranged.

3.1.2 Experimental methods

First, according to the $OI_{Mea} - OI_{Pre}$ linear relationship and the U model calculation formula, the cosα term is simplified to establish the gas odor intensity prediction model; then, according to the odor intensity measurement value OI_{mea} which is identified by the scent identifier group, modify the overall odor intensity $OI_{pre}$of the prediction model.

3.1.3 Discussion of experimental results

Formula 6 shows the calculated value of cosα when the two components have equal intensity.

$$\cos\alpha_{ab} = \frac{OI_{ab} - OI_a - OI_b}{2\sqrt{OI_{aOI_b}}} \quad (6)$$

Since the relationship between the lnOAV value of each component and the chemical concentration can be calculated, the overall predicted intensity of the aromatic hydrocarbon is shown in Table 2.

Table 2: Comparison of odor intensity and predicted value of two aromatic porphyrin compounds

Compound	$\mathbf{lnOAV}_a$	$\mathbf{lnOAV}_b$	OI_{Mea}	OI_{Pre}	OI_{Pre}/OI_{Mea}
Benzene(a)+ Toluene(b)	1.48	1.57	1.7	2.1	1.24
	2.13	2.87	3.2	3.6	1.13
	3.05	2.85	4.1	4.2	1.02
Benzene(a)+Ethylbenzene(b)	4.28	4.83	6.4	6.4	1.00
	3.82	2.45	4.1	4.6	1.12
	3.47	2.41	4.5	4.2	0.93
Toluene(a)+Ethylbenzene(b)	3.93	4.83	7.1	6.3	0.89
	3.23	4.18	4.3	5.6	1.30
	2.32	2.41	3.1	3.5	1.13

To view the predicted results more clearly, the odor intensity measured value is the abscissa, the U model total predicted value is the ordinate, the fitting curve is set, and the prediction precision of the two-component mixture is analyzed, as shown in Figure 1.

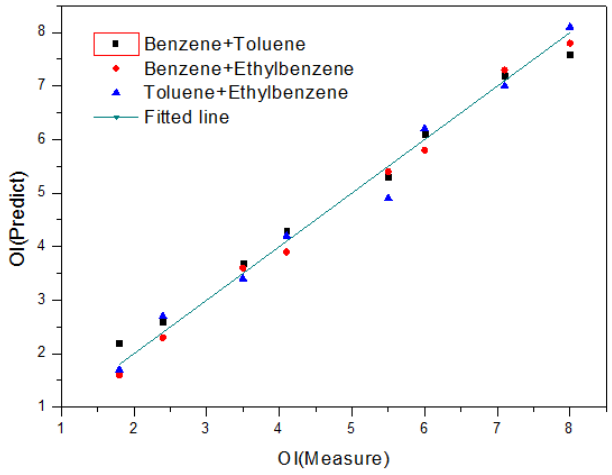

Figure 1: Modified U model predicts odor intensity fitting curve

Since the U model itself considers the interaction between the odor chemical gas substances, and then considers the cosα value modification, the odor intensity prediction accuracy shown in Figure 1 has achieved good results. The predicted values of benzene, toluene and ethylbenzene are not significantly different from the measured values, which proves that the modified U model is suitable for the prediction of odor intensity of benzene mixtures.

3.2 Modified vector model

The vector model has similar calculation methods and prediction effects with the U model. In order to enrich the vector model for the prediction of gas odor intensity of multi-component mixtures, we also modify the vector model and apply it to the prediction of odor intensity of multi-component odor mixture.

3.2.1 Experimental reagents and instruments

The experimental reagents and instruments are the same as section 3.1.1.

3.2.2 Experimental methods

First, the vector model is modified, then the benzene multi-component odor mixture sample is configured, the lnOAV value of each sample is determined, and the total odor intensity of the mixture is predicted by the modified vector model. Finally, analyze the effect of the modified vector method on the prediction of the odor intensity of the multi-component mixture through comparison of the measured value OI_{mea} and the predicted value OI_{pre}.

3.2.3 Experimental results and discussion

According to the data in the literature we can see that, for the prediction of two-component mixture, the prediction accuracy of the vector model is poorer than the U model. The two-component cosα value of the vector model is -0.142, according to the modification method to correct the vector model of the three-component and four-component mixture, concentration prediction calculation models can be obtained as Formula (7) and (8).

$$OI_{abc} = 1.082\sqrt{lnOAV_a^2 + lnOAV_b^2 + lnOAV_c^2 - 0.284 \times (lnOAV_a lnOAV_b + lnOAV_a lnOAV_c) + lnOAV_b lnOAV_c} \quad (7)$$

$$OI_{abcd} = 1.082\sqrt{\begin{matrix} lnOAV_a^2 + lnOAV_b^2 + lnOAV_c^2 + lnOAV_d^2 - 0.284 \times [(lnOAV_a lnOAV_b + lnOAV_a lnOAV_c) + \\ (lnOAV_a lnOAV_c + lnOAV_b lnOAV_c + lnOAV_b lnOAV_d + lnOAV_c lnOAV_d)] \end{matrix}} \quad (8)$$

Table 3 shows the results of the odor intensity predicted values and measured values of the multi-component aromatic hydrocarbon mixture.

Table 3: Comparison of odor intensity and predicted value of multicomponent aromatic porphyrin compound

Compound	$\mathbf{lnOAV}_a$	$\mathbf{lnOAV}_b$	$\mathbf{lnOAV}_c$	$\mathbf{lnOAV}_d$	OI_{Mea}	OI_{Pre}
Toluene(a)+Ethylbenzene(b)+ O-xylene(c)	2.32	3.52	2.7	-	3.7	4.7
	2.32	2.45	3.48	-	5.1	4.5
	1.64	1.77	2.14	-	3.5	3.0
Ethylbenzene(a)+ Phenylpropane(b)+ Styrene(c)	3.52	2.21	3.82	-	6.4	6.4
	4.22	2.21	4.52	-	4.1	4.6
	2.81	2.19	2.63	-	4.5	4.2
Toluene(a)+Ethylbenzene(b)+ O-xylene(c)+ Styrene(d)	4.21	2.19	3.82	2.14	4.8	5.5
	2.19	3.17	2.20	2.14	4.4	4.1
	1.84	1.76	2.19	2.14	3.4	3.3

Figure 2 shows the predicted results of the multi-component odor mixture by the modified vector model.

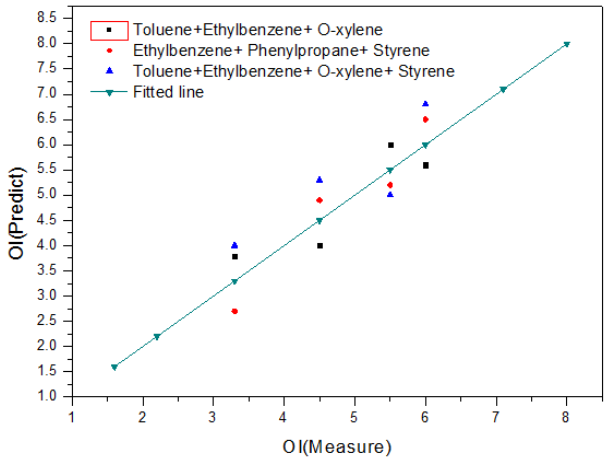

Figure 2: Modified vector model predicts odor intensity fitting curve

It can be seen from Table 3 and Figure 2 that the modified vector model is suitable for odor intensity prediction of multi-component mixtures, and the prediction accuracy is also high.

4. Conclusion

Stink gas has caused great trouble to the living of residents, meanwhile it has potential harms to the life and health. The detection and prediction of odor intensity in stink gas has become the focus of environmental protection work and academic research. This paper analyzed the problems existing in the detection and research of odor at present, and studied the intensity prediction of multi-component odor mixture gas. By constructing the prediction models and modification methods for the prediction models, this study improved

the accuracy of odor gas intensity prediction, through experiment, the measured values and the model predicted values were obtained, and the corresponding experimental results were concluded. The main research results of this paper are as follows:

(1) The intensity prediction model of multi-component odor mixture considers the interaction relationship between the components of the mixture, its predicted results had higher precision, this paper demonstrated the accuracy of the predicted values by the fitting results of the measured values.

(2) The modified U model and the modified vector model have higher accuracy among the odor prediction models and can be applied to the prediction of multi-component odor gas mixtures.

References

Capelli L., Sironi S., Rosso R.D., Céntola P., 2009, Predicting odour emissions from wastewater treatment plants by means of odour emission factors, Water Research, 43(7), 1977-1985, DOI: 10.1016/j.watres.2009.01.022

De M.L.H., Guillot J.M., Fanlo J.L., Le C.P., 2006, Dispersion of odorous gases in the atmosphere - part i: modeling approaches to the phenomenon, Science of the Total Environment, 361(1–3), 220-228, DOI: 10.1016/j.scitotenv.2005.05.010

Hansen M.J., Jonassen K.E.N., Løkke M.M., Adamsen A.P.S., Feilberg A., 2016, Multivariate prediction of odor from pig production based on in-situ measurement of odorants, Atmospheric Environment, 135, 50-58, DOI: 10.1016/j.atmosenv.2016.03.060

Iranpour R., Cox H.H.J., Deshusses M.A., Schroeder E.D., 2010, Literature review of air pollution control biofilters and biotrickling filters for odor and volatile organic compound removal, Environmental Progress & Sustainable Energy, 24(3), 254-267, DOI: 10.1002/ep.10077

Mussio P., Gnyp A.W., Henshaw P.F., 2001, A fluctuating plume dispersion model for the prediction of odour-impact frequencies from continuous stationary sources, Atmospheric Environment, 35(16), 2955-2962, DOI: 10.1016/s1352-2310(00)00419-2

Pettarin N., Campolo M., Soldati A., 2015, Urban air pollution by odor sources: short time prediction, Atmospheric Environment, 122, 74-82, DOI: 10.1016/j.atmosenv.2015.09.037

Piringer M., Knauder W., Petz E., Schauberger G., 2015, A comparison of separation distances against odour annoyance calculated with two models, Atmospheric Environment, 116, 22-35, DOI: 10.1016/j.atmosenv.2015.06.006

Piringer M., Petz E., Groehn I., Schauberger G., 2007, A sensitivity study of separation distances calculated with the austrian odour dispersion model (aodm), Atmospheric Environment, 41(8), 1725-1735, DOI: 10.1016/j.atmosenv.2006.10.028

Ruth S.M.V., O'Connor C.H., 2001, Evaluation of three gas chromatography-olfactometry methods: comparison of odour intensity-concentration relationships of eight volatile compounds with sensory headspace data, Food Chemistry, 74(3), 341-347, DOI: 10.1016/s0308-8146(01)00142-x

Sakai S., Hiraoka K., Yamashita R., Matsumoto Y., 2006, Effect of tio2 photocatalyst on odorous gases using glass fiber filter for repeatable use, Japanese Journal of Applied Physics, 45(8), DOI: 10.1143/jjap.45.l343

Schauberger G., Piringer M., Petz E., 2006, Odour episodes in the vicinity of livestock buildings: a qualitative comparison of odour complaint statistics with model calculations, Agriculture Ecosystems & Environment, 114(2), 185-194, DOI: 10.1016/j.agee.2005.10.007

Sironi S., Capelli L., Céntola P., Rosso R.D., Grande M.I., 2006, Odour emission factors for the prediction of odour emissions from plants for the mechanical and biological treatment of msw, Atmospheric Environment, 40(39), 7632-7643, DOI: 10.1016/j.atmosenv.2006.06.052

Soares C.E.D.S., Weber A., Moecke E.S., Reiter M.G., Scussel V.M., Krebs De Souza C., 2018, Use of ozone gas as a green control alternative to beetles (alphitobius diaperinus) infestation in avian bed utilized in poultry industry, Chemical Engineering Transactions, 64, 589-594, DOI: 10.3303/CET1864099

Teixeira M.A., Rodríguez O., Mota F.L., Macedo E.A., Rodrigues A.E., 2003, Evaluation of group-contribution methods to predict vle and odor intensity of fragrances, Industrial & Engineering Chemistry Research, 50(15), 9390-9402, DOI: 10.1021/ie200290r

Teixeira M.A., Rodríguez O., Rodrigues A.E., Selway R.L., Riveroll M., Chieffi A., 2013, Prediction model for the odor intensity of fragrance mixtures: a valuable tool for perfumed product design, Industrial & Engineering Chemistry Research, 52(2), 963-971, DOI: 10.1021/ie302538c

Zheng W., Wang J., Zhang S., 2018, Analysis on carbon emission decoupling effect and driving factors of environmental pollution in china's transportation industry, Chemical Engineering Transactions, 66, 637-642, DOI:10.3303/CET1866107