A Mathematical Model for Odors Applied to Binary Odor Mixtures

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This expanded mathematical model is a modification of Berglund's model (1973).[1] The modification explains the elimination of one odor by another, the synergy of odors of low intensity and the existence of odorless substances, which have deodorant properties.

To begin, we shall distinguish the"odor" attached to any substance, even if it is not detectable, from the "perceived odor" of a substance resulting from the composition of the "odor" of said substance and the "odor" of the environment in which it is immersed (generally air), which we suppose even though it may be odorless.

In the following, we represent the odor of a substance with the vector of a fixed origin *O*, and we represent the odor of the environment with the vector of origin *O* supported by the axis $\overrightarrow{Ox}$. Let $\overrightarrow{OA}$ be the vector that represents the odor of substance *A*, and $\overrightarrow{OU}$ the vector that represents that of the surrounding environment. The perceived odor of substance *A* will be represented with the vector $\overrightarrow{OA'} = \overrightarrow{OA} + \overrightarrow{OU}$. The intensity of the perceived odor of *A* will be noted down ψ_A = length of vector $\overrightarrow{OA'}$. All of the perceived odors of *A*, whatever their intensities, will be represented with vectors $\overrightarrow{OA'}$, whose extremity *A′* is on half-line passing through *O* such that $(\overrightarrow{OU}, \overrightarrow{OA'}) = \lambda$. If another substance *B* exists in the same environment, the perceived odor resulting from the presence of *A* and *B* will be represented with a vector $\overrightarrow{OC'} = \overrightarrow{OA} + \overrightarrow{OB} + \overrightarrow{OU}$ (**1**).

It may be observed that $\overrightarrow{OC'} \neq \overrightarrow{OA'} + \overrightarrow{OB'}$; that is, it is the vectors representing the odors that are actually added, and not those representing the perceived odors (in Berglund's model the vectors representing the perceived odors were added).

We have noted down in Figure 1:

$\alpha = (\overrightarrow{OU}, \overrightarrow{OA})$, $\beta = (\overrightarrow{OU}, \overrightarrow{OB})$, $\lambda = (\overrightarrow{OU}, \overrightarrow{OA'})$, $\mu = (\overrightarrow{OU}, \overrightarrow{OB'})$,

Ψ_A = length of $\overrightarrow{OA'}$, Ψ_B = length of $\overrightarrow{OB'}$,

Ψ_C = length of $\overrightarrow{OC'}$ and u = length of $\overrightarrow{OU}$.

Figure 1. The notations used for the composition of odors A and B

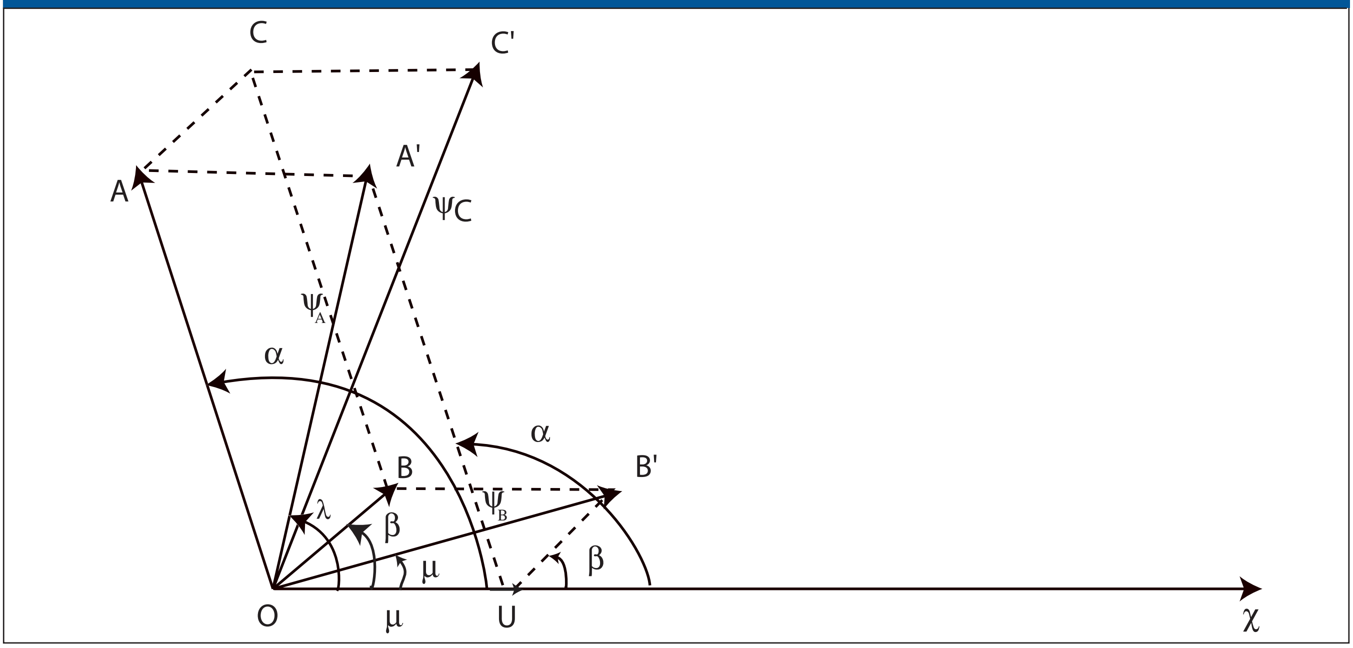

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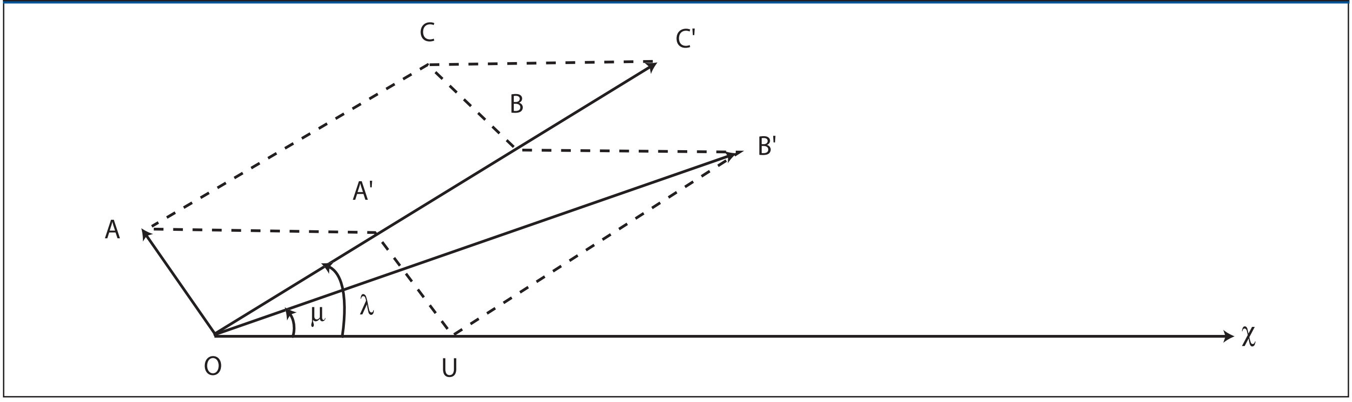
Figure 2. *A* eliminates the odor of *B*



Intensity and Quality of Odor Resulting from the Mixture of Substances *A* and *B*

Ψ_A, Ψ_B, and Ψ_C, respectively, represent the intensities of the perceived odors of *A*, *B* and *C*. λ and μ, respectively, represent the qualities of the perceived odors of *A* and *B*. The quality of the perceived odor of *C* will be represented by $(\overrightarrow{OU}, \overrightarrow{OC'})$.

We infer from **1**:

$$\Psi_C = [\Psi_A^2 + \Psi_B^2 + 2\Psi_A\Psi_B\cos(\mu - \lambda) + u^2 - 2u\Psi_A\cos\lambda - 2u\Psi_B\cos\mu]^{1/2} \quad (\mathbf{2})$$

which, in the case of high-intensity odors, may be approximately:

$$\frac{\Psi_C^2 - \Psi_A^2 - \Psi_B^2}{2\Psi_A\Psi_B} \approx \cos(\mu - \lambda) \ (\mathbf{3}).$$

$(\overrightarrow{Ox}, \overrightarrow{OC'})$, which gives us the quality of the perceived odor of the mixture of *A* and *B*. is determined with:

$$\tan(\overrightarrow{Ox}, \overrightarrow{OC'}) = \frac{\Psi_A\sin\lambda + \Psi_B\sin\mu}{\Psi_A\cos\lambda + \Psi_B\cos\mu - u} \quad (\mathbf{4}).$$

Elimination of the Odor of a Substance by that of Another Substance

In the following, we shall suppose $\sin l > 0$ and $\sin\mu > 0$. The odor of *A* will eliminate that of *B* if and only if the vectors $\overrightarrow{OC'}$ and $\overrightarrow{OA'}$ are co-linear; that is, if $\tan(\overrightarrow{Ox}, \overrightarrow{OC'}) = \tan(\overrightarrow{Ox}, \overrightarrow{OA'})$ and then, by applying formula (4), if:

$$\frac{\Psi_A\sin\lambda + \Psi_B\sin\mu}{\Psi_A\cos\lambda + \Psi_B\cos\mu - u} = \frac{\sin\lambda}{\cos\lambda}$$

The resolution of the above equation gives us

$$\Psi_B = \frac{u\sin\lambda}{\sin(\lambda - \mu)}$$, which is only possible if $\sin(\lambda - \mu) > 0$.

In this way, the odor of *B* will eliminate the odor of *A* — if

$$\Psi_A = \frac{u\sin\mu}{\sin(\mu - \lambda)}$$, which is only possible if $\sin(\mu - \lambda) > 0$.

Thus, we can see that if the odor of *A* is capable of eliminating the odor of *B*, the odor of *B* cannot possibly eliminate that of *A*, and vice-versa. This reveals a dissymmetry in the mathematical model we have just explained, a dissymmetry that did not appear in the preceding models.[4] It also leads to the notion of predominating odor: the odor of *A* predominates the odor of *B* if and only if $\sin(\lambda - \mu) > 0$, that is if $0 < \lambda - \mu < \pi$.

Figure 2 shows us how *A* (whose perceived odor is of lower intensity than the perceived odor of *B*) eliminates the odor of *B*.

Synergy of Some Low-Intensity Odors

If, in formula **2**, we assume Ψ_A and Ψ_B to be very small with respect to u, and more particularly $2(\Psi_A + \Psi_B)$ to be small with respect to u, we have:

$\Psi_C^{2a} \approx u^2 - 2u\Psi_A\cos\lambda - 2u\Psi_B\cos\mu$

$\Psi_C^2 \approx u(u - 2\Psi_A\cos\lambda - 2\Psi_B\cos\mu)$

with $|2\Psi_A\cos\lambda + 2\Psi_B\cos\mu| \le 2(\Psi_A + \Psi_B) << u$,

and thus $u - 2\Psi_A\cos\lambda - 2\Psi_B\cos\mu \approx u$, and finally, $\Psi_C \approx u$, which we assumed to be greater than Ψ_A and Ψ_B.

We are then able to get, by combining two low-intensity odors, an odor of much greater intensity than each of the intensities of the singular odors. One can realize this phenomenon in Figure 3, in which the odors in question are such that α and β are not very different from π. In fact, $\sin(\pi - \alpha) \le \frac{\Psi_A}{u}$; and then, when $\frac{\Psi_A}{u}$ is small, $\pi - \alpha$ is also very small. In the same manner, when $\frac{\Psi_B}{u}$ is small, $\pi - \beta$ is also very small.

Existence of Odorless Substances with Deodorant Properties

In our mathematical model, we assume the existence of the odor of the environment in which odorant substances are immersed. It is thus reasonable to suppose, in our representation, that there exists a zone *Z* that has the

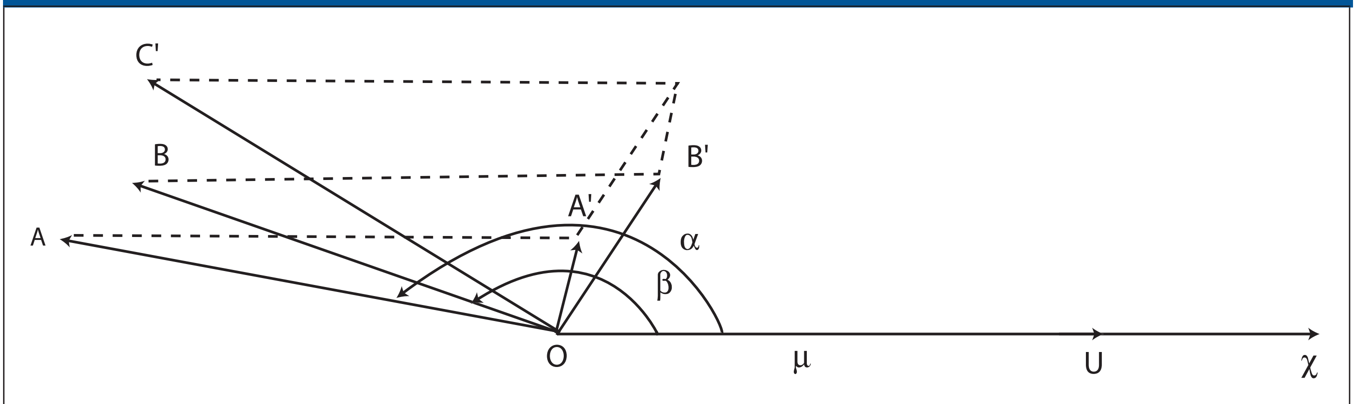
Table 1. Validation of the author's model (part a)

Mixture	Experimental magnitude			$y_1 = \dfrac{\Psi^2_{AB_1} - \Psi^2_A - \Psi^2_{B_1}}{2\Psi_A\Psi_{B_1}}$
A = propanol	Ψ_{AB_1}	Ψ_A	Ψ_{B_1}	
B_1 = amyl butyrate				
0.09 mg/l	6.1	4.2	4.4	0.01
	7.7	7.6	4.4	-0.27
	12.9	14.4	4.4	-0.48
	25.3	28.1	4.4	-0.68

Table 2. Validation of the author's model (part b)

Mixture	Experimental magnitude			$y_1 = \dfrac{\Psi^2_{AB_2} - \Psi^2_A - \Psi^2_{B_2}}{2\Psi_A\Psi_{B_2}}$
A = propanol	Ψ_{AB_2}	Ψ_A	Ψ_{B_2}	
B_2 = amyl butyrate	5.9	4.6	9	-0.81
3.0 mg/l	7.8	8.8	9	-0.62
	15	17.1	9	-0.48
	30	33	9	-0.45

Figure 3. The odors in question are such that α and β are not very different from π



following property: any vector $\overrightarrow{OA}$ belonging to *Z* represents the "perceived odor" of an odorless substance *A*. Of course, $\overrightarrow{OU}$ belongs to *Z*. Let $\overrightarrow{O\Gamma}$ be such that $(\overrightarrow{Ox},\overrightarrow{O\Gamma}) = \gamma$ and $\overrightarrow{O\Gamma}'$, such that $(\overrightarrow{Ox},\overrightarrow{O\Gamma}') = -\gamma$. We suppose *Z* defined by the *A'*, such that $-\gamma \le (\overrightarrow{Ox},\overrightarrow{OA'}) \le -\gamma$ or $\pi - \gamma \le (\overrightarrow{Ox},\overrightarrow{OA'}) \le \pi + \gamma$.

Let $\overrightarrow{OD}$ be such that $(\overrightarrow{Ox},\overrightarrow{OD}) = \gamma + \frac{\pi}{2}$ and $\overrightarrow{OD}'$, such that $(\overrightarrow{Ox},\overrightarrow{OD}) = -\gamma + \frac{\pi}{2}$. Of course, we suppose γ is small, so that $\cos\gamma \ge 0$. We suppose that $A' \in Z$. (i.e. *A* is an odorless substance) and we try to find the *B'* points such that $C' \in Z$. The condition for that is:

$- \tan\delta \le \tan(\overrightarrow{Ox},\overrightarrow{OC'}) \le \tan\gamma$ or

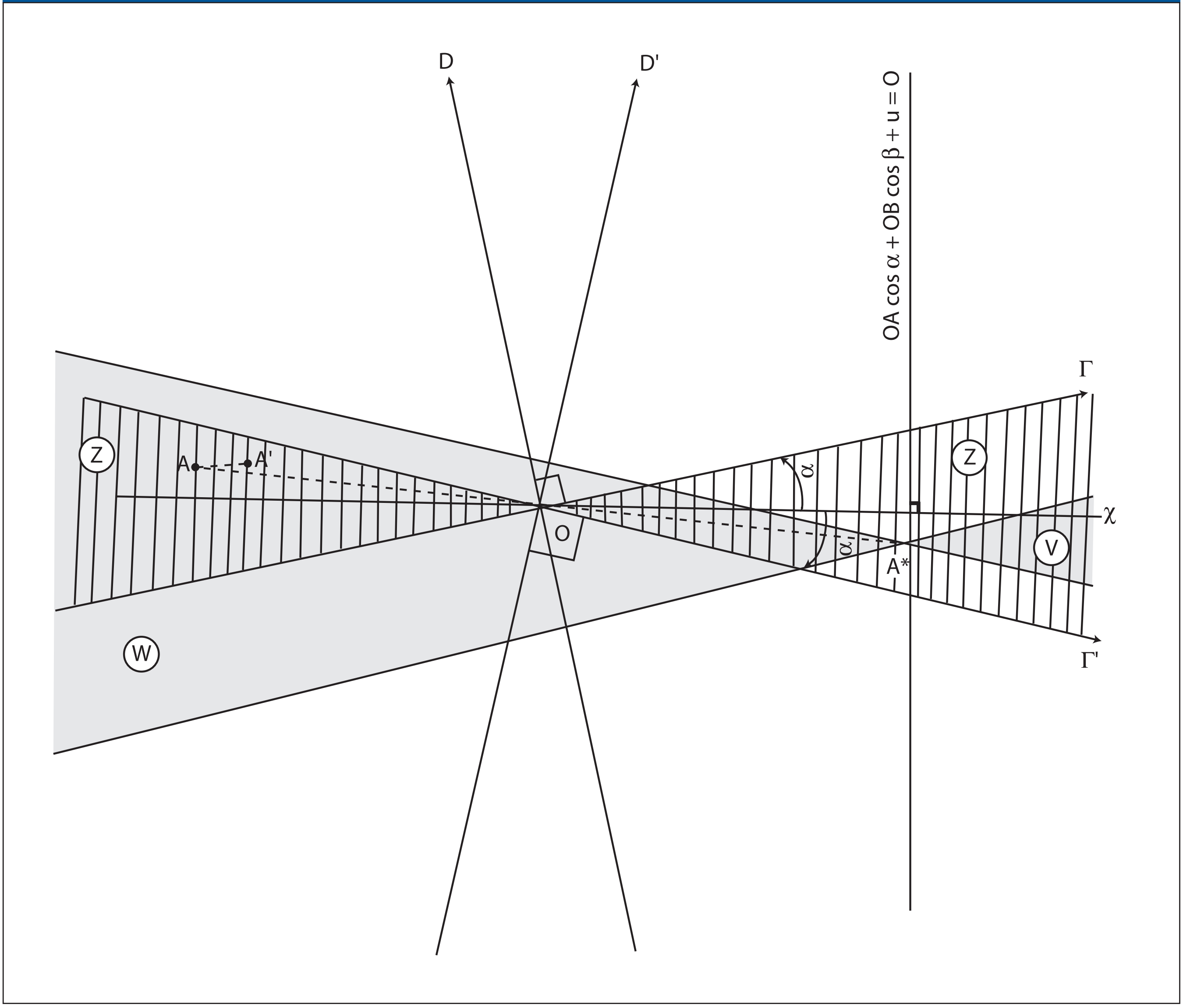
$$- \sin\delta \le \frac{OA \sin\alpha \cos\gamma + OB \sin\beta \cos\gamma}{OA \cos\alpha + OB \cos\beta + u} \le \sin\gamma.$$

Case 1: $OA \cos\alpha + OB \cos\beta + u \ge 0$ or $\mathrm{Proj}_{\overrightarrow{Ox}} \overrightarrow{OB'} \le \mathrm{Proj}_{\overrightarrow{Ox}} \overrightarrow{OA}^*$, where A^* is the symetric of *A* with respect to *O*. We then obtain the two conditions:

$$\begin{cases} \mathrm{Proj}_{\overrightarrow{OD'}} \overrightarrow{OB'} \le \mathrm{Proj}_{\overrightarrow{OD'}} \overrightarrow{OA} \\ \mathrm{Proj}_{\overrightarrow{OD}} \overrightarrow{OB'} \ge \mathrm{Proj}_{\overrightarrow{OD}} \overrightarrow{OA} \end{cases}$$

and *B'* must belong to zone *V* (see Figure 4).

Figure 4. Zones V and W to which B' must belong in order for C' to belong to zone Z



Case 2: $OA\cos\alpha + OB\cos\beta + u \le 0$ or $\mathrm{Proj}_{\overrightarrow{Ox}}\overrightarrow{OB'} \le \mathrm{Proj}_{\overrightarrow{Ox}}\overrightarrow{OA}$. We then obtain the two conditions:

$$\begin{cases} \mathrm{Proj}_{\overrightarrow{OD}}\overrightarrow{OB'} \le \mathrm{Proj}_{\overrightarrow{OD}}\overrightarrow{OA} \\ \mathrm{Proj}_{\overrightarrow{OD'}}\overrightarrow{OB'} \ge \mathrm{Proj}_{\overrightarrow{OD'}}\overrightarrow{OA} \end{cases}$$

And *B'* must belong to zone *W*. We have darkened zones *V* and *W* on Figure 4 and cross-hatched zone *Z*. Thus, we can see in Figure 4 that an odorless substance *A* has deodorant properties for an infinite number of substances *B*.

Conclusion

We now refer to data of W.S. Cain and we look for the validity of our model.[2] The data are given in Table I and Table II with:

Table 1: *A* = propanol and we notice $(\overrightarrow{Ox}, \overrightarrow{OA'}) = \lambda$; B_1 = amyl butyrate 0.09 mg/l and notice $(\overrightarrow{Ox}, \overrightarrow{OB_1'}) = \mu_1$.

Table 2: *A* = propanol and we notice $(\overrightarrow{Ox}, \overrightarrow{OA'}) = \lambda$; B_2 = amyl butyrate 3.0 mg/l and we notice $(\overrightarrow{Ox}, \overrightarrow{OB_2'}) = \mu_2$.

First, we notice that the odors of B_1 and B_2 cannot be considered the same odor because $y_1 \searrow$ when $\Psi_A \nearrow$ and $y_2 \nearrow$ when $\Psi_A \nearrow$. Secondly, in Berglund's model, $y_1 = \dfrac{\Psi^2_{AB_1} - \Psi^2_A - \Psi^2_{B_1}}{2\Psi_A \Psi_{B_1}}$ must be a constant value. However, we obtain the mean value y_{1M} of y_1: $y_{1M} = -03.55$ with $\dfrac{\sum_{i=1}^{4} |y_{1i} - y_{1M}|}{4} = 0.220$, which is very great with respect to -0.355, and thus y_1 cannot be reasonably considered a constant value. In the same manner, y_2 cannot be reasonably considered a constant value for y_{2M} = –0.59 with $\frac{\sum_{i=1}^{4} |y_{2i} - y_{2M}|}{4} = 0.125$, which is great with respect to -0.59. Third, it might be imagined that y_1 is a linear function of Ψ_A, and adjusting y_1 by the mean of the least squares method we obtain from Table I: $y_1^* = -0.261\ \Psi_A - 0.0005$ and $\frac{\sum_{i=1}^{4} |y_{1i} - y^*_{1M}|}{4} = 0.087$, which is less than 0.220, but still great with respect to the mean value -0.355. In the same manner, $y_2^* = 0.011\ \Psi_A - 0.766$ and $\frac{\sum_{i=1}^{4} |y_{2i} - y^*_{2M}|}{4} = 0.072$, which is less than 0.125, but still great with respect to the mean value -0.59. Finally, according to our mathematical model, we adjust by the mean of the least squares method $y^* = \alpha \frac{1}{\Psi_A} + \beta$, and thus obtain $y_1^* = 3.29 \frac{1}{\Psi_A} - 0.744$, which gives us

$$\frac{\sum_{i=1}^{4} |y_{1i} - y^*_{1M}|}{4} = 0.040$$, which is far less than 0.220 (Berglund's model) and 0.087 (the linear model). In the same manner, $y_2^* = -2.65 \frac{1}{\Psi_A} - 0.300$, which gives us $\frac{\sum_{i=1}^{4} |y_{2i} - y^*_{2M}|}{4} = 0.051$, which is far less than 0.125 (Berglund's model) and less than 0.072 (the linear model). Then, we are able to find λ, μ_1, μ_2 and u by resolving the following system of equations:

$$\cos(\mu_1 - \lambda) - \frac{u\cos\lambda}{4.4} = -0.744$$

$$\frac{u^2}{8.8} - u\cos\mu_1 = 3.29$$

$$\cos(\mu_2 - \lambda) - \frac{u\cos\lambda}{9} = -0.300$$

$$\frac{u_2}{18} - u\cos\mu_2 = -2.65$$

The resolution of the above system gives: λ = 25º5, μ_1 = 69º5, μ_2 = –40º5 and u = 7.15, which demonstrates that Berglund's model is not effective because, according to this model, u may be very near to O, which validates our hypothesis: the existence of the odor of the surrounding environment.

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References:

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