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The Trail of Perfumes

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A methodology is proposed for modeling the diffusion of fragrances released from a moving source. First, we started with a one-dimensional model considering molecular diffusion of α-pinene in air as the only mass transport mechanism. The validation was performed in a diffusion tube, and a system was developed to move the scented source along the axial direction. Results showed that experimental data fitted well with the numerical simulation, suggesting this model as a valid tool to describe the trail of a fragrance released from a moving source for low Re of the order of 10. In the case of a person walking at the speed of 1.34 m/s in a room or corridor inside a building, three-dimensional models are required and mass transport of the perfume to the surrounding air will be dominated by turbulent diffusion or eddy diffusion D_t which is two orders of magnitude higher than molecular diffusion. © 2018 American Institute of Chemical Engineers AIChE J, 64: 2890–2897, 2018
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Introduction

Perfumes are complex homogeneous liquid mixtures, composed of fragrant ingredients and solvents, that humans perceive through their olfactory system.[1] Fragrant components are classified in top, middle, and base notes, depending on their volatility.[2] Top notes, the most volatile molecules, represent 15–25% of the perfume composition and are the first that a consumer perceives, lasting no longer than a few minutes.[3] As the evaporation takes place and the top notes fade away, the middle notes (20–40% of the perfume composition) start to be noticed. Finally, after several hours of a perfume application, appear the base notes (45–55% of the perfume composition) which have the lowest volatility lasting in the air more than 8 h or even days. Base notes play a key role in the perfume performance acting as fixatives, once they influence molecular interactions with the purpose of changing evaporation rates of the top and middle notes.[3]

People, generally, love perfumes. But why do we choose a particular perfume over another? Probably, most of us will answer that we appreciate a particular smell because it brings us childhood memories, increases our confidence, or simply because it last longer on our skin. The truth is that perfumes have the incredible power to tell a story and reveal, until a certain extent, the identity of its wearer. According to Byrne-Quinn,[4] when a woman wears a perfume she is very concerned with the message sent about herself. In fact, fragrances are used by people to build their self-image and self-esteem, or to create a favorable impression on other people: it is expected that a person who smells good induces a positive response from others.[5] Perfumes have the potential to leave an impression on anyone who catches a passing scent, being the reason why people are so interested on choosing a perfume with a noticeable scented trail or *sillage*.[6] *Sillage*, in French, is the technical word to describe the scented trail left by the fragrance wearer. It is not about how long a fragrance lasts on the skin, but how far it travels away and diffuses around from the wearer. The bigger the distance where the fragrance is perceived the stronger *sillage* is.[6] So, it is important to study, and ultimately predict, the diffusion of fragrances when a scented source is moving. As far as we know, all methodologies available in the literature to predict the diffusion of fragrances in the air are based on static fragrance sources. Therefore, this study presents, for the first time, a study on fragrance release and diffusion from a moving source, with the objective of predicting the trail of a fragrance left by a person. Thus, a theoretical model (considering one-dimensional [1-D] and three-dimensional [3-D] diffusion) for predicting the diffusion of a perfume model from a moving source is proposed based on the extension of a solution for a stationary impulse source replacing the source position by the moving path of the source as a function of time.[7] First, we started with a 1-D model considering molecular diffusion of α-pinene (as scented source or perfume model) in air as the only mass transport mechanism. The 1-D diffusion model was experimentally validated using a diffusion tube and a system moving along the *z*-direction is designed and built to simulate a scented source with *Re* of the order of 10. Experimental gas concentrations collected in the sampling ports (SPs) of the diffusion tube were quantified through gas chromatography with flame ionization detector (GC-FID) and compared with those predicted by the proposed theoretical model. In the case of a person walking at the speed of 1.34 m/s in a room or corridor inside a building, mass transport of the perfume to the surrounding air will be dominated by turbulent diffusion or eddy diffusion D_t which is two orders of magnitude higher than molecular diffusion[8] and 3-D models

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are required. Simulation of 3-D diffusion models allow the study of turbulent diffusion by changing D by one and two orders of magnitude, and analyzing its influence on the diffusion profiles, as a function of distance and time.

Theory

The diffusion equation (Eq. 1) can be used to describe the dispersion of chemical species from regions of high concentration to regions of lower concentration due to its random motion

$$\frac{\partial C_i}{\partial t} = D_i \left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2} \right) \quad (1)$$

where C_i is the concentration in gas phase at a space position (x,y,z), t is the time variable, and D_i is the molecular diffusion coefficient of the fragrance species in air.

The solution of Eq. 1 is the product of the solutions of the three single spatial-variable problems (Eq. 2), according to Carslaw and Jaeger[9]

$$C_i(\boldsymbol{r},t) = C_i(x,t) \; C_i(y,t) \; C_i(z,t) \quad (2)$$

where $\boldsymbol{r}$ is 3-D position vector.

For 1-D diffusion problem in the z-direction (Eq. 3)

$$\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial z^2} \quad (3)$$

and considering a homogeneous semi-infinite medium, that is, impermeable boundary condition at $z = 0$, and a Dirac impulse source of a unit mass stationary at $z = z_0$, that is, the initial condition is $C_i(z,t) = \delta(z - z_0)\,\delta(t - t_{\mathrm{I}})$, the solution of Eq. 3 is

$$C_i(z,t) = \frac{1}{2\sqrt{\pi D_i(t - t_{\mathrm{I}})}} \left\{ \exp\left[-\frac{(z - z_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \right.$$
$$\left. + \exp\left[-\frac{(z + z_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \right\} \quad (4)$$

Thus, combining the solutions of the three space variables (Eq. 2) and considering that the impermeable boundary condition exists only in the z-direction, it is possible to obtain the concentration distribution of a fragrance for a 3-D case (Eq. 5), where x_0, y_0, z_0 represent the Cartesian coordinates of the source

$$C_i(\boldsymbol{r},t) = \frac{1}{8\,[\pi D_i(t - t_{\mathrm{I}})]^{3/2}} \left\{ \exp\left[-\frac{(x - x_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \right.$$
$$\exp\left[-\frac{(y - y_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \left(\exp\left[-\frac{(z - z_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \right.$$
$$\left. \left. + \exp\left[-\frac{(z + z_0)^2}{4\,D_i(t - t_{\mathrm{I}})} \right] \right) \right\} \quad (5)$$

1-D diffusion from a moving source

The gas concentration profiles of the perfume model continuously released from a moving source were predicted based on the methodology proposed by Zhao and Nehorai[7] to solve equations involving a moving source. Basically, it consists on the extension of the solution for a stationary impulse source replacing the fixed source position by the moving path of the source as a function of time. When a source is moving, the fragrance gas concentration at the current time is affected by all past values of source position and release rate. Thus, the time-

Table 1. Typical Values for Molecular Diffusivity (D) and Film Thickness (δ) for Gases and Liquids

	Gas	Liquid
D (m²/s)[a]	(10^{-4} to 10^{-6}) $\sim 10^{-5}$	(10^{-8} to 10^{-10}) $\sim 10^{-8}$
δ (m)[b]	10^{-3} to 10^{-4}	10^{-4} to 10^{-5c}

[a]From Perry and Green[11] and Bird et al.[12]
[b]From Taylor and Krishna[13]
[c]E. L. Cussler in "*Diffusion: Mass transfer in fluid systems*"[14] recommends a value of $\delta = 10^{-4}$ for liquids.

cumulative effects on the fragrance gas concentrations need to be considered in order to obtain the solution of the fragrance diffusion model, which is represented by the following integral:

$$C_i(\boldsymbol{r},t) = \int_{t_i}^{t} \mu_i^{\mathrm{mass}}(\tau) \; C_{\mathrm{Green}}(\boldsymbol{r} - \boldsymbol{r}_0(\tau), \, t - \tau) \; d\tau \quad (6)$$

where μ_i^{mass} is the releasing rate (mass) of component i and C_{Green} is the Green function given by Eq. 4 in the case of 1-D diffusion.

Considering an impermeable boundary condition and assuming that the substance is released at a constant rate ($\mu_i^{\mathrm{mass}}(t) = \mu_i^{\mathrm{mass}}$), using the 1-D solution (Eq. 4) as the Green's function of the stationary source case, the gas concentration of a fragrance in a semi-infinite medium is described by Eq. 7

$$C_i(z,t) = \mu_i^{\mathrm{mass}} \int_{t_i}^{t} \frac{1}{2[\pi \, D_i \, (t - \tau)]^{\frac{1}{2}}}$$
$$\left\{ \exp\left[-\frac{(z - z_0(\tau))^2}{4\,D_i(t - \tau)} \right] + \exp\left[-\frac{(z + z_0(\tau))^2}{4\,D_i(t - \tau)} \right] \right\} \; d\tau \quad (7)$$

where the moving source path is represented by z_0, and it is defined as $z_0(t) = z_i + v_s t$, with z_i as the initial position of the source (m) and v_s the velocity of the moving source (m/s). The molar evaporation rate of the liquid, μ_i^{molar} [mol/(m² s)] can be expressed by Eq. 8[10]

$$\mu_i^{\mathrm{molar}} = k_i \left(C_i^{\mathrm{gas}} - C_i^{\infty} \right) \quad (8)$$

where k_i is the mass-transfer coefficient (m/s), C_i^{gas} is the gas concentration of odorant i in equilibrium with the liquid (mol/m³). Considering that the concentration of the fragrance species in the air far from the liquid/gas interface (C_i^{∞}) can be neglected,[10] and expressing Eq. 8 in mass units [g/(m² s)], the evaporation rate (μ_i^{mass}) can be defined as

$$\mu_i^{\mathrm{mass}} = k_i \; M_i \; C_i^{\mathrm{gas}} \quad (9)$$

where M_i is the molecular weight of fragrance component i. The mass-transfer coefficient is defined as $k_i = D/\delta$, where δ is the film thickness, which depends on the Reynolds number, Re. Typical values for these parameters are presented in Table 1.

The mass-transfer coefficients are then calculated in the gas and liquid phases, and their values are $k_g = 10^{-1}$ to 10^{-2} (m/s) and $k_l = 10^{-4}$ to 10^{-5} (m/s), respectively.

The overall mass-transfer coefficient, assuming a linear model for the description of the vapor-liquid equilibrium, can be determined by the following equation[15]

$$\frac{1}{k_i} = \frac{1}{k_g} + \frac{1}{k_l} \frac{C_{\mathrm{T}}^{\mathrm{g}}}{C_{\mathrm{T}}^{\mathrm{l}}} \; K_i \quad (10)$$

where k_i is the overall mass-transfer coefficient, $C_{\mathrm{T}}^{\mathrm{g}}$ and $C_{\mathrm{T}}^{\mathrm{l}}$ are the total concentrations in gas and liquid phases, respectively, and K_i is the equilibrium ratio ($y_i = K_i x_i$).

Table 2. Properties of the Studied Fragrance Component Used in This Work: Molecular Formula, Molecular Weight (M_i), Vapor Pressure (P_i^{sat}), Density (ρ_i), and Diffusion Coefficient (D_i)

Fragrance Component	Molecular Formula[a]	M_i (g/mol)[a]	P_i^{sat} (Pa)[b,c]	ρ_i (g/mL)[a,c]	D_i (m²/s)[d]
α-Pinene	$C_{10}H_{16}$	136.2	513.4	0.879	6.04×10^{-6}

[a]From Chemspider Database.[16]
[b]Vapor pressures at 296.15 K.
[c]From Teixeira et al.[15]
[d]Estimated from Fuller et al.[17]
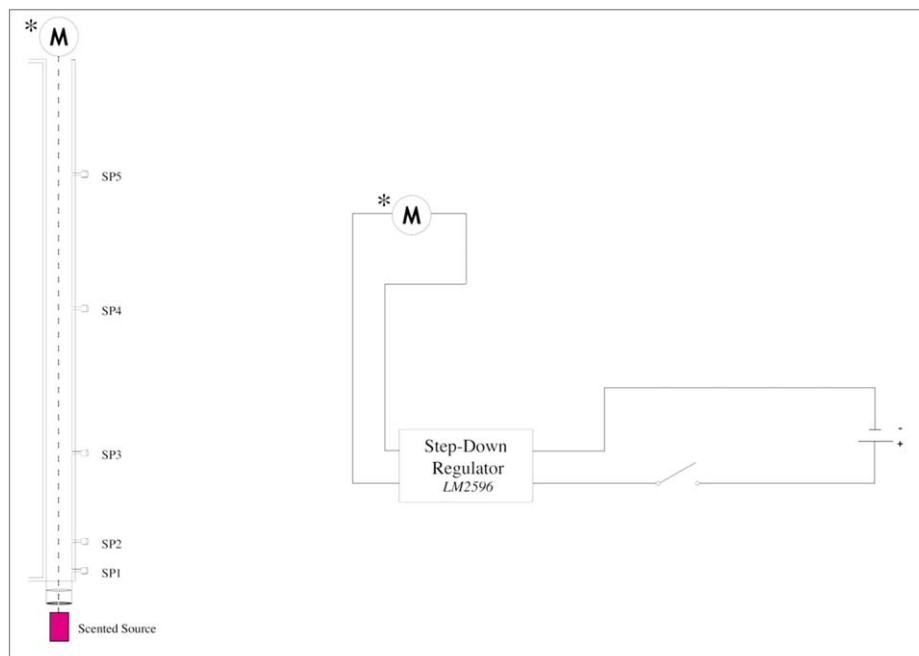
Figure 1. Mechanical (left) and electrical (right) schemes of the moving system constructed in the lab.

[Color figure can be viewed at wileyonlinelibrary.com]
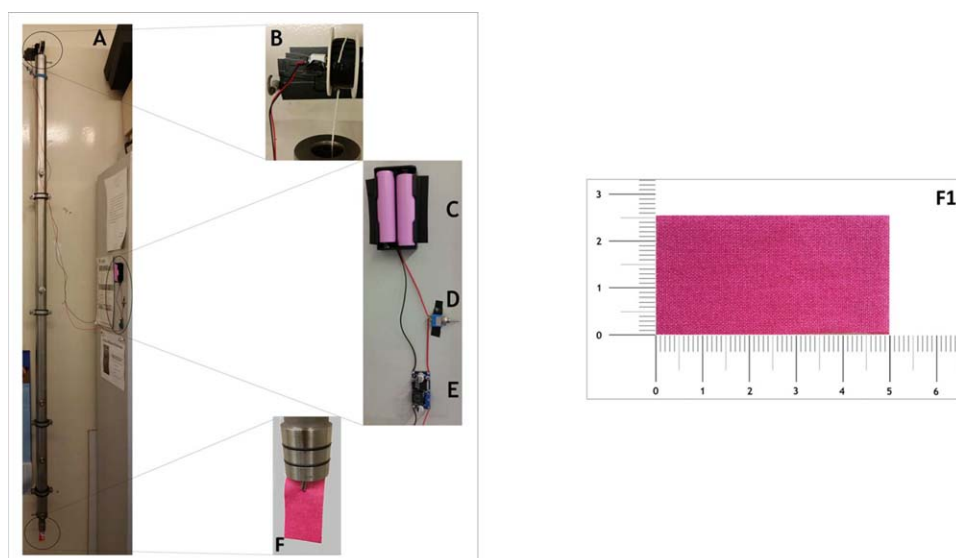
Figure 2. System developed in the laboratory; F1, zoom of the textile used as the source, and the respective dimensions; A, complete system; B, motor; C, battery; D, switch; E, step-down regulator; and F, scented fabric.

[Color figure can be viewed at wileyonlinelibrary.com]

Table 3. Electrical Components and Respective Manufacturers

Electrical Component	Manufacturer
Battery Li-Ion MR18650	GP Batteries International
Micro-motor with reducer 35 rpm	Shenzhen Kinmore Motor Co., Ltd
Step-down voltage regulator	Texas Instruments
Switch on-off	Not identified

Table 4. Parameters Used in the 1-D Numerical Simulation: Diffusion Coefficient ($D_{\alpha\text{-pinene}}$), Time (t), Evaporation Rate ($\mu_{\alpha\text{-pinene}}$), and Source Velocity ($v_s$)

$D_{\alpha\text{-pinene}}$ [a] (m^2/s)	t [b] (s)	$\mu_{\alpha\text{-pinene}}$ [c] [g/(m^2 s)]	v_s [b] (m/s)
6.04×10^{-6}	100	2.75×10^{-1}	1.34×10^{-2}

[a]From Fuller et al.[17]
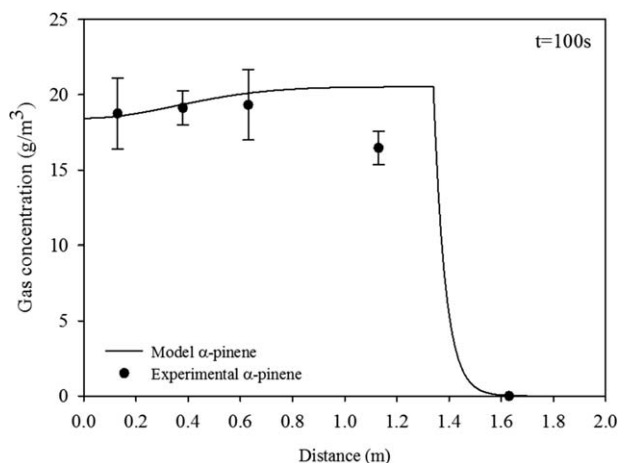[b]Arbitrary value.
[c]From Eq. 8.

Figure 3. Theoretical and experimental gas concentration profiles of α-pinene over distance, at a fixed time of 100 s, of a source moving at 1.34×10^{-2} m/s, and $D_{\alpha\text{-pin}} = 6.04 \times 10^{-6}$ m^2/s.
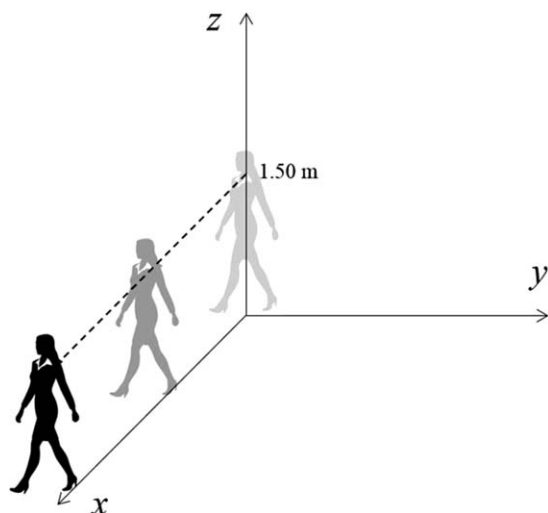

Figure 4. Three-dimensional moving source path.

[Color figure can be viewed at wileyonlinelibrary.com]

Table 5. Parameters Used in the 3-D Numerical Simulation: Evaporation Rate ($\mu_{\alpha\text{-pinene}}$), Source Velocity ($v_s$), and Diffusion Coefficient Values ($D_{\alpha\text{-pinene}}$)

$\mu_{\alpha\text{-pinene}}$ (g/(m^2 s))	v_s (m/s)	$D_{\alpha\text{-pinene}}$ (m^2/s)		
2.75×10^{-1}	1.34	6.04×10^{-6}	6.04×10^{-4}	6.04×10^{-5}

3-D diffusion from a moving source

With the purpose of reproducing a more realistic scenario, a 3-D diffusion model (Eq. 11) for a moving source was developed, also based on the work of Zhao and Nehorai.[7] This methodology takes into account the same conditions described above leading to

$$
C_i(\boldsymbol{r}, t) = \mu_i^{mass} \int_{t_i}^{t} \frac{1}{8[\pi \ D_i \ (t-\tau)]^{\frac{3}{2}}}
$$
$$
\left\{ \exp\left[-\frac{|\boldsymbol{r} - \boldsymbol{r}_0(\tau)|^2}{4 \ D_i(t-\tau)} \right] + \exp\left[-\frac{|\boldsymbol{r} - \boldsymbol{r}_1(\tau)|^2}{4 \ D_i(t-\tau)} \right] \right\} \ d\tau \tag{11}
$$

where $\boldsymbol{r}_0(t) = [x_0(t), y_0(t), z_0(t)]^T$ represents the source path and $\boldsymbol{r}_1(t) = [x_0(t), y_0(t), -z_0(t)]^T$. It is also assumed that the releasing rate is constant ($\mu_i^{mass}(t) = \mu_i^{mass}$) and it is determined by Eq. 9.

Here, it should be noted that for the case of a person walking at 1.34 m/s indoor, turbulent diffusion or eddy diffusion D_t must be added to molecular diffusion D_i and becomes dominant.

Experimental

The perfume model tested in the present study was composed of (-) α-pinene (CAS No. 7785-26-4, purity $\geq 98\%$), which was obtained from Fluka and it was used as received, without further purification. Table 2 shows some relevant physicochemical properties of this fragrance component.

The experimental validation of the 1-D model was performed in a diffusion tube (already available in our laboratory for diffusion studies) and a new system designed and built to move the scented source along the *z*-direction. The 2-m long tube of stainless steel and a nominal diameter of 1 in. has five SPs positioned at different heights. The SPs are placed at distances of 0.13, 0.38, 0.63, 1.13, and 1.63 m from the bottom of the tube, and it consist of perforated parts of the tube properly
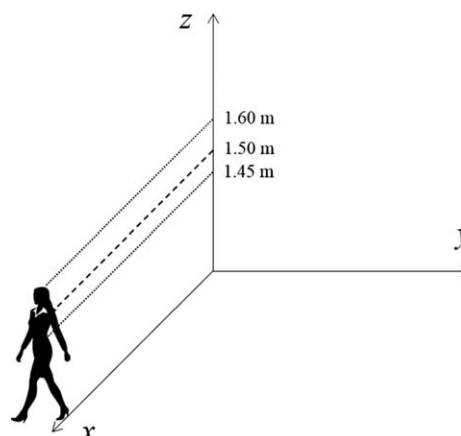

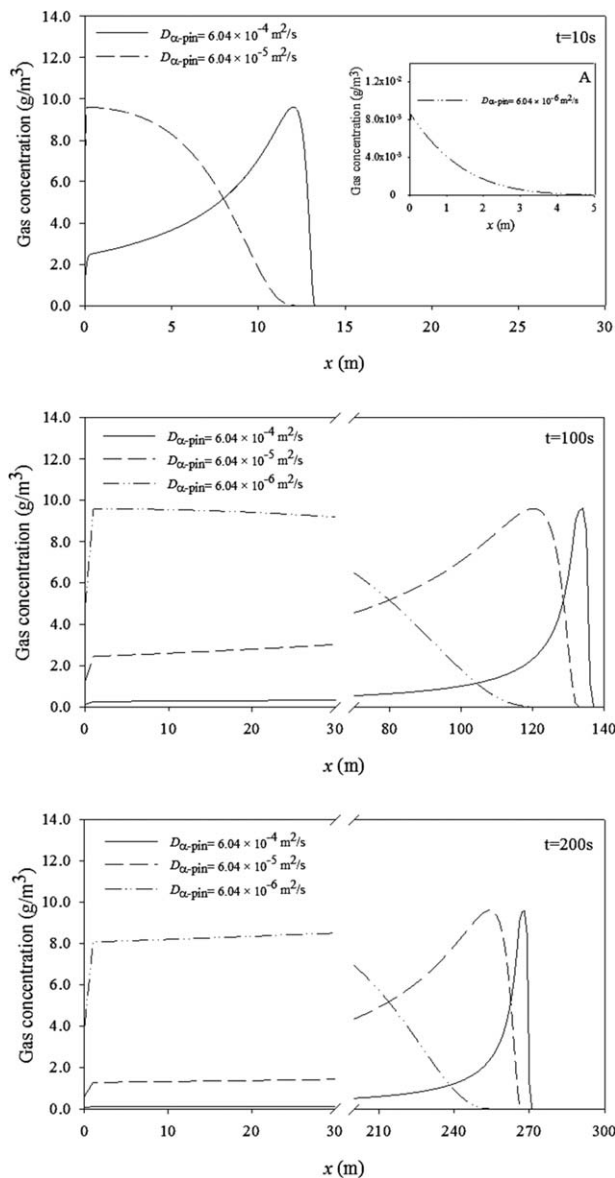**Figure 5.** Heights where the gas concentrations were evaluated (1.45 and 1.60 m).

Figure 6. Gas concentration profiles of a scented source moving along *x* axis (at a velocity of 1.34 m/s), assessed at a height of 1.45 m, for times of 10, 100, and 200 s; A, zoom of the gas concentration profile for $D_{\alpha\text{-pin}} = 6.04 \times 10^{-6}$ m^2/s.

sealed with a silicone septum, which allows the measurement of the odorant concentration in the headspace. The system containing the scented moving source was constructed according to the mechanical and electrical schemes of this system displayed in Figure 1. The system, represented by letter A in Figure 2, is composed of motor, battery, switch, step-down regulator, and the scented fabric (identified with the letters B, C, D, E, and F, respectively, in Figure 2, and the respective manufacturers are presented in Table 3). This allowed moving the textile (source), with dimensions of 2.5 cm × 5 cm (Figure 2-F1), scented with the desired odorant component, at a constant velocity.

As a preliminary experiment, 1 mL of pure α-pinene (perfume model) was pipetted in the textile, and the source was immediately moved at a constant velocity of 1.34×10^{-2} m/s; this value of velocity is the minimum rpm of the motor. After

100 s, gas samples with a volume of 0.4 mL were collected from the SPs of the diffusion tube, using a gas-tight syringe (Hamilton). The experiments occurred at a controlled room temperature of $(23 \pm 1)°C$. It is important to note that, right after the source started to move, the bottom side of the tube was capped with parafilm, in order to reproduce the impermeable boundary condition. Then, the samples were injected in a GC Varian CP-3800 with a split/splitless injector and a Rxi®-5Sil MS column (30 m × 0.25 mm, 0.25 μm film thickness) with a FID. The oven temperature was set at 100°C, and the injector and FID detector temperatures were programed at 240 and 250°C, respectively. The carrier gas was helium (He N60) with a constant flow rate of 1.2 mL/min. It was used a split ratio of 1:20, and the quantification of α-pinene was achieved using the respective calibration curve.
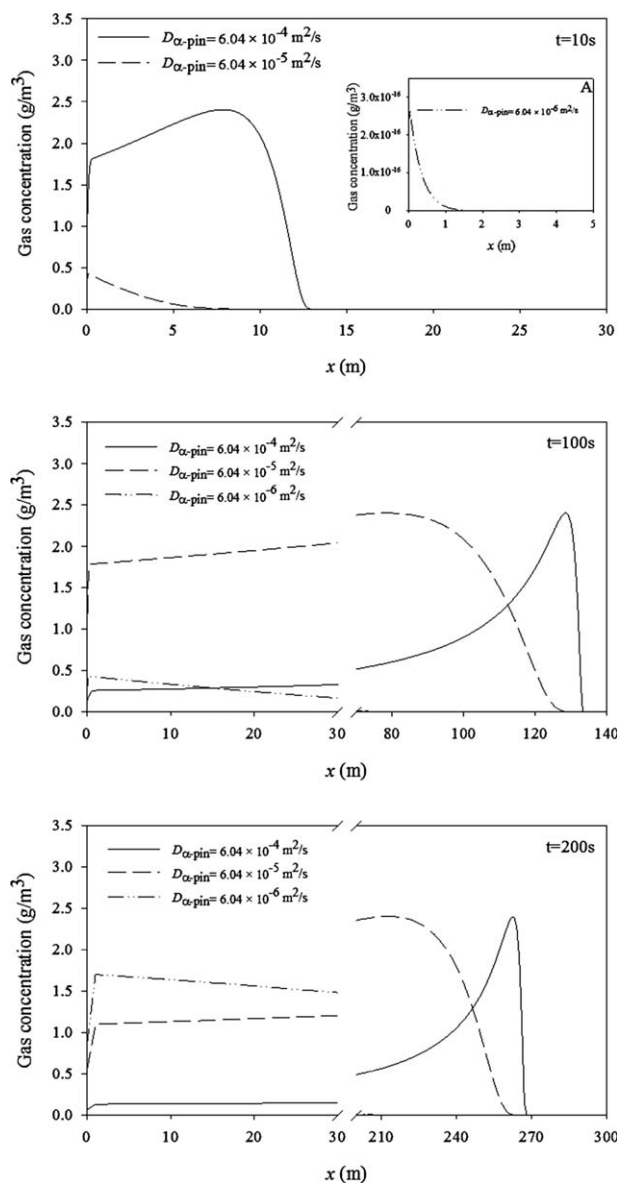

Figure 7. Gas concentration profiles of a scented source moving along *x* axis (at a velocity of 1.34 m/s), assessed at a height of 1.60 m, for times of 10, 100, and 200 s; A, zoom of the gas concentration profile for $D_{\alpha\text{-pin}} = 6.04 \times 10^{-6}$ m^2/s.

Results and Discussion

1-D diffusion from a moving source: Numerical solution and experimental validation

The numerical solution of Eq. 7 allowed obtaining the gas concentration profiles of the perfume model α-pinene released from a source moving along the z-direction. The software MATLAB® was used for numerical integration, in particular the *integral* package, which numerically integrates the function from t_i to t using global adaptive quadrature, and a relative and absolute tolerances equal to 10^{-15}. The parameters used in the numerical simulation are specified in Table 4.

After numerically solving Eq. 7, the gas concentration profiles of α-pinene over distance were obtained for a fixed time of 100 s and the results are displayed in Figure 3. Here, we can also find the experimental data measured in the diffusion tube with the scented source moving along z-direction. It is important to mention that the experimental data represented in Figure 3 were all obtained at 100 s from the average of three consecutive assays for each SP.

Inspecting Figure 3, it is possible to see that 100 s after the scented source starts to move it already traveled 1.34 m. In addition, results indicate that the theoretical model for the 1-D fragrance diffusion fits well with the experimental data, meaning that the diffusion of the perfume model α-pinene can be well described by the proposed model when a scented source is moving.

3-D diffusion from a moving source: Numerical solution

The numerical solution of Eq. 11 was performed in the software MATLAB® using the *integral* package. In the present study, it was considered a scented source moving through a straight-line parallel to x axis at a height of 1.50 m—assumed as the average height where a person applies a perfume—and a constant velocity of $v = 1.34$ m/s (Figure 4). The initial position of the moving source is at the point $r_0 = (0, 0, 1.50)$ m.

α-Pinene was also used as perfume model and the parameters used in the numerical simulation are specified in Table 5.

The trail left by a fragrance when it is applied in a moving source will be affected by the diffusion coefficient value. In fact, the diffusion coefficient is not only the molecular diffusion D_i but it should be replaced by $D_i + D_t$, where D_t is the turbulent or eddy diffusion arising from the movement of the fragrant source such as a person walking in a room or corridor indoor. It was decided to investigate the influence of this parameter on the gas concentration profiles, considering three values: the molecular diffusion coefficient determined by Fuller et al.[17] (6.04 × 10^{-6} m²/s) and two arbitrary values, namely, 10 and 100 times higher than molecular diffusion coefficient (6.04 × 10^{-5} and 6.04 × 10^{-4} m²/s). One can note that an estimate of turbulent diffusion indicates that D_t is two orders of magnitude higher than molecular diffusion.[8] Despite the source is moving at a constant height of 1.50 m, the gas concentrations were evaluated at two different heights: 1.45 and 1.60 m in order to assess the odor space near the scented source (Figure 5).
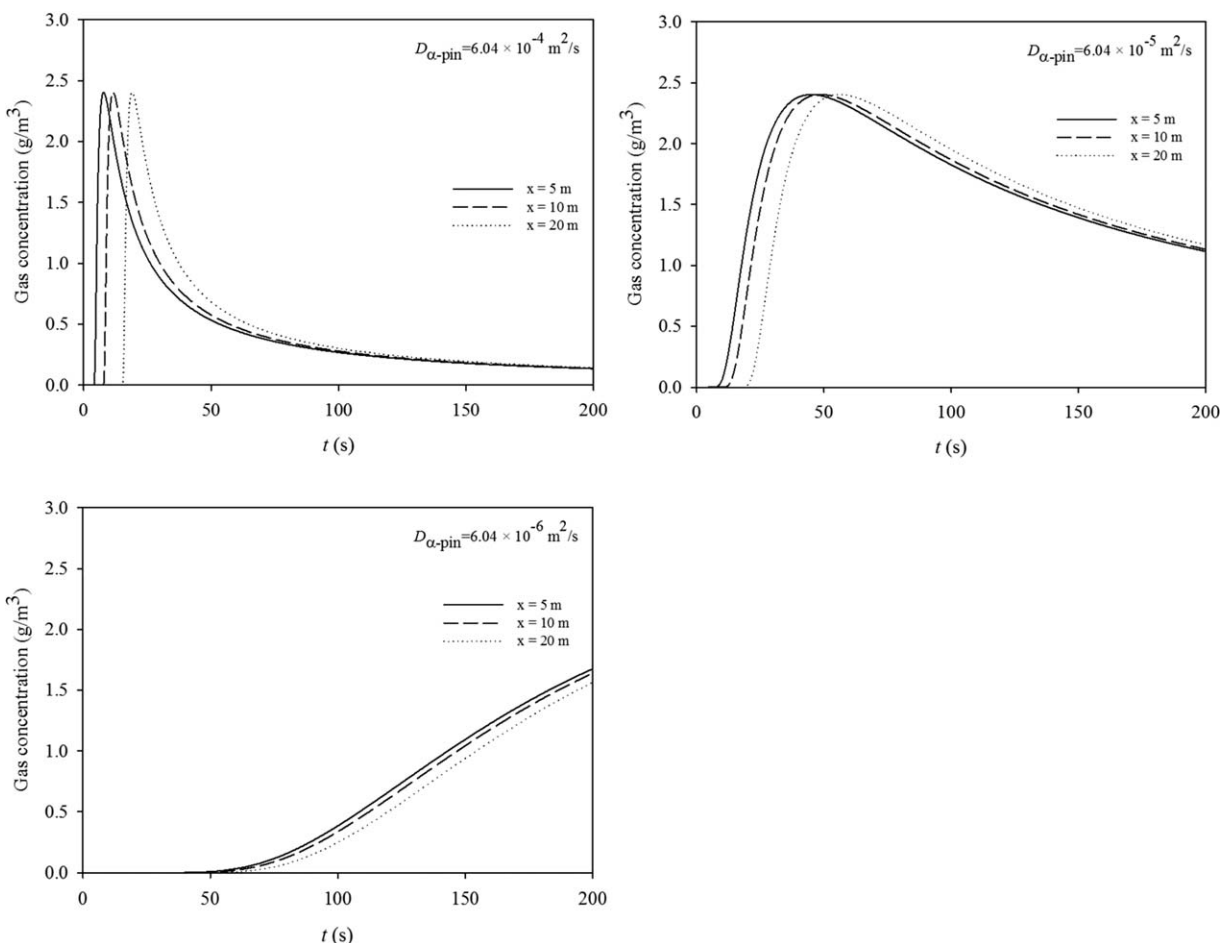

Figure 8. Gas concentration profiles as a function of time of a scented source moving at 1.34 m/s, evaluated at a height of 1.60 m and three fixed distances (5, 10, and 20 m) using three diffusion coefficient values: $D_{\alpha\text{-pin}} = 6.04 \times 10^{-4}$ m²/s, $D_{\alpha\text{-pin}} = 6.04 \times 10^{-5}$ m²/s, and $D_{\alpha\text{-pin}} = 6.04 \times 10^{-6}$ m²/s.

Diffusion Profiles from a Moving Source as a Function of Distance. The gas concentration profiles of the perfume model α-pinene continuously released from a moving source were evaluated at two different heights, 1.45 and 1.60 m, along the *x* axis (Figures 6 and 7). The simulation was performed for 10, 100, and 200 s after the scented source starts to move, and for three diffusion coefficient values, in order to study their influence on the gas concentration profiles. From Figure 6, we observe that after 10 s the source has already traveled a distance of 13.4 m, once it moves at a velocity of 1.34 m/s. The maximum gas concentration corresponds to approximately 10 g/m^3 and, depending on the diffusion coefficient value, the distance corresponding to this maximum is different. As expected, the lower the value of this parameter, the longer it takes for the perfume model α-pinene travel the same distance. The same is observed for 100 and 200 s after the source starts to move. The behavior of the perfume model α-pinene described by the proposed methodology over heights and for the same time is in accordance with expected as the fragrance component takes longer to travel long distances. For instance, closer to the source (1.45 m; Figure 6) the trail of the perfume model α-pinene is more intense as compared to a height of 1.60 m (Figure 7), reaching a maximum gas concentration of 2.5 g/m^3. Finally, we confirmed that the value of the diffusion coefficient has a great impact on the diffusion profiles, for both heights of 1.45 and 1.60 m.

Diffusion Profiles from a Moving Source as a Function of Time. Figure 8 presents the gas concentrations as a function of time of the perfume model α-pinene, evaluated at a height of 1.60 m and for three fixed distances—5, 10, and 20 m— away from the initial position of the scented source. Also, three diffusion coefficient values of α-pinene were studied: 6.04×10^{-6}, 6.04×10^{-5}, and 6.04×10^{-4} m^2/s. From here, we concluded that the maximum value of the gas concentration is reached earlier for a higher diffusion coefficient (6.04×10^{-4} m^2/s) and for a distance closer to the initial position of the source (5 m).

Future work should concern the trail of fragrances from a walking person in open space. This problem is much more complicated by consideration of convection and wind effects. One can learn from atmospheric dispersion models (Gaussian plume models, Gaussian Puff models, Lagrangian/Eulerian models, Particle-in-Cell models)[18–20] but the scale of application (meso-scale 20–200 km) is very different from what is of interest in the study of *sillage*.

Conclusions

In this study, a theoretical 1-D diffusion model is proposed for predicting the trail of perfumes. This methodology takes into account a scented source moving through space and a continuous fragrance release from the moving source. The trail of a perfume model α-pinene was simulated, and the 1-D experimental data showed good agreement with the numerical simulation, which allows concluding that the presented model is suitable for modeling the diffusion of fragrances when applied in a moving source. Regarding the 3-D diffusion model, where the same perfume model α-pinene was used, we studied the effect of turbulent diffusion to account for the movement of the scented source—a person walking in a room or corridor indoor at 1.34 m/s; the influence of the diffusion coefficient values on the gas concentration profiles (trail), as a function of time and distance. As expected, the results were very different depending on the diffusion coefficient value: the

lower this value, the longer it takes for α-pinene to cover the same distance. The simulation results confirmed the impact of turbulent diffusion on the trail of perfumes by increasing *D* by one and two orders of magnitude. Comparing the profiles at different heights for a fixed time, it was observed that for a height closer to the source the gas concentrations are higher than for a longer distance from the source. Based on the obtained results, we proposed our methodology as a valid tool for predicting the trail of fragrances. We consider this model as a huge advance for the fragrance industry in what concerns the opportunity to achieve the desired trail of fragrance more quickly and efficiently.

Notation

C_i = gas concentration of component i, g/m^3
C_i^∞ = gas concentration of component i far from the gas/liquid interface, g/m^3
C_{Green} = Green function
C_T^g = total concentration in the gas phase, g/m^3
C_T^l = total concentration in the liquid phase, g/m^3
D_i = diffusion coefficient of component i, m^2/s
k_i = overall mass-transfer coefficient of component i, m/s
k_g = film mass-transfer coefficient of species i in gas side, m/s
k_l = film mass-transfer coefficient of species i in liquid side, m/s
K_i = equilibrium ratio for component i
M_i = molecular weight, g/mol
P_i^{sat} = vapor pressure of component i, Pa
$\boldsymbol{r}$ = three-dimensional position vector
$\boldsymbol{r}_0$ = source moving path vector
t = time, s
t_I = initial time, s
v_s = velocity of the moving source, m/s
y_i = molar fraction of the gas phase
x_i = molar fraction of the liquid phase
x, y, z = Cartesian coordinates, m
x_0, y_0, z_0 = Cartesian coordinates of the source, m
z_i = initial position of the source, m

Greek letters

δ = film thickness, m
$\delta(z - z_0) \, \delta(t - t_I)$ = Dirac impulse source at position z_0 and time t_I.
μ_i^{mass} = releasing rate (mass) of component i, g/m^{2}s
μ_i^{molar} = releasing rate (molar) of component i, mol/m^{2}s
ρ_i = density of component i, g/mL
τ = integration variable

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