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Pheromones impregnated on porous PLA fibers for integrated pest management (IPM)

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Supplementary information: Model calculations and equations

Diffusivity of the pheromone in air is calculated using Chapman–Enskog theory (Equation 1) and depends on temperature. Equilibrium vapor pressure is the other temperature dependent term (Equation 2) in the model and the Sherwood number quantifies convective mass transfer and accounts for the impact windspeed (Equation 3). The Vetere approximation for latent heat of hydrocarbons (Equation 4) is used to calculate enthalpy of vaporization. The initial rate of evaporation that the model calculates using these terms (Equation 5) is equivalent to free surface evaporation.

$$D_{AB} = 0.0018583T^{3/2}\sqrt{\left(\frac{1}{M_A}+\frac{1}{M_B}\right)\frac{1}{\sigma_{AB}^2\Omega P}} \qquad \textit{Equation 1}$$

$$P = P_b^{\left(\frac{-\Delta H_{vap}}{R}\left(\frac{1}{T}-\frac{1}{T_b}\right)\right)} \qquad \textit{Equation 2}$$

$$S_h = 14.5 + 0.65R_e^{1/2}S_c^{1/3} \qquad \textit{Equation 3}$$

$$H_{vap} = 4.1868T_b + \left(9.08 + 4.36\log T_b + \frac{0.0068T_b}{M_B} + \frac{0.0009T_b^2}{M_B}\right) \qquad \textit{Equation 4}$$

$$Q = \frac{S_h D_{AB}}{L}\frac{P}{RT}\frac{1}{SA} \qquad \textit{Equation 5}$$

$D_{AB} = Diffusivity\ [cm^2/s]$

$T = \ Temperature\ [K]$

$M_A = Molar\ mass\ of\ air\ [g/mol]$

$M_B = Molar\ mass\ of\ pheromone\ [g/mol]$

$\sigma_{AB} = Average\ collision\ diameter\ [\dot{A}]$

$\Omega = \ Collision\ integral\ solution$

$P = Vapor\ pressure\ [atm]$

$H_{vap} = Enthalpy\ of\ vaporization\ [J/mol]$

$T_b = Boiling\ point\ [K]$

$P_b = Vapor\ pressure\ at\ boiling\ point\ [atm]$

$R_e = Reynold's number$

$S_c = Schmidt\ number$

$S_h = \ Sherwood\ number$

$Q = Mass\ loss\ rate\ [g/s \cdot cm^2]$

$L = \ Characteristic\ length\ [\ cm]$

$SA = Surface\ area\ [cm^2]$

$R = Ideal\ gas\ contant\ [J/mol \cdot K]$

The decay function uses the mass of pheromone remaining in the pores as its independent variable and contains a constant that was determined empirically by fitting logarithmic functions to 10 sets of experimental mass loss tests (Equation 6). In theory this constant should be the same for all compounds since the rate of decrease in available surface area as pores deplete should be dependent only on the structure of the porous network. During the slower stage of evaporation a linear model whose parameters were also determined by fitting with experimental mass loss tests is used (Equation 7)

$$Q_1 = R_1 * Q_0 \left(\ln\left(1 - \frac{C}{C_0}\right)\right) \qquad \textit{Equation 6}$$

$$Q_2 = R_2 * Q_{1\,end} \left(1 - \frac{C}{C_0}\right) \qquad \textit{Equation 7}$$

$Q_1 = Evaporation\ rate\ during\ first\ stage\ [g/s \cdot cm^2]$

$Q_2 = Evporation\ rate\ during\ second\ stage\ [g/s \cdot cm^2]$

$Q_{1\,end} = Evaporation\ rate\ for\ a\ surface\ concentration\ of\ 12\ g/m^2\ [g/s \cdot cm^2]$

$Q_0 = Initial\ evapoartion\ rate\ [g/s \cdot cm^2]$

$C = Surface\ concentration\ [g/m^2]$

$C_0 = Initial\ surface\ concentration\ [g/m^2]$

$R_1 = Rate\ constant\ for\ first\ stage\ of\ evaporation\ equal\ to\ -1.11$

$R_2 = Rate\ constant\ for\ secodn\ stage\ fo\ evaporation\ equal\ to\ 0.6$