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

Journal of Polymer and the Environment

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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.

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

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

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

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

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

D_{AB} = Diffusivity [cm^2/s]	T_b = Boiling point [K]
T = Temperature [K]	P_b = Vapor pressure at boiling point [atm]
M_A = Molar mass of air [g/mol]	R_e = Reynold's number
M_B = Molar mass of pheromone [g/mol]	S_c = Schmidt number
σ_{AB} = Average collision diameter [Å]	S_h = Sherwood number
Ω = Collision integral solution	Q = Mass loss rate [$\text{g/s} \cdot \text{cm}^2$]
P = Vapor pressure [atm]	L = Characteristic length [cm]
H_{vap} = Enthalpy of vaporization [J/mol]	SA = Surface area [cm^2]

$$R = \text{Ideal gas constant [J/mol} \cdot \text{K]}$$

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)

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

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

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

$$Q_2 = \text{Evaporation rate during second stage [g/s} \cdot \text{cm}^2]$$

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

$$Q_0 = \text{Initial evaporation rate [g/s} \cdot \text{cm}^2]$$

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

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

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

$$R_2 = \text{Rate constant for second stage of evaporation equal to } 0.6$$