Theoretical Documentation

DAD drift v1.1

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1. Environmental Constants

1.1. Dynamic Viscosity of Air

The dynamic viscosity of air (kg m^{-1}s^{-1}) was calculated according to Sutherland-law:

$$\mu = \mu_0 * \frac{T_0 + S}{T + S} * \left(\frac{T}{T_0}\right)^{\frac{3}{2}} \tag{1}$$

where, μ_0 (kg m^{-1}s^{-1}) is the reference viscosity for air [1.716*10^{-5} (kg m^{-1}s^{-1})], T_0 (K) is the reference temperature for air [273 (K)], and S (K) is the Sutherland constant for air [111 (K)] (Kim et al., 2004).

1.2. Saturated Vapor Pressure of Water

The saturated vapor pressure of water (Pa) was calculated as follows:

$$p_{sat} = p_0 * 10^{\left(\frac{7.5*T}{T+237.3}\right)} \tag{2}$$

where, T (C°) is the temperature and p_0 (Pa) is the vapor pressure of water at 0 °C [610.7 (Pa)] (Holterman, 2003).

1.3. Wet-Bulb Temperature

The wet-bulb temperature (C°) is computed as follows:

$$T_w = T * \text{atan}\left(0.151977 * (Rh + 8.313659)^{\frac{1}{2}}\right) + \text{atan}(T + Rh)$$

$$- \text{atan}(Rh - 1.676331) + 0.00391838 * Rh^{\frac{3}{2}} * \text{atan}(0.023101 * Rh)$$

$$- 4.686035 \tag{3}$$

where, T (C°) is the temperature and Rh (%) is the relative humidity (Stull, 2011).

1.4. Diffusion Coefficient of Water in Air

The diffusion coefficient of water in air (m² s^{-1}) was calculated as follows:

$$D_V = D_0 * (1 + 0.0071 * T) \tag{4}$$

where, D_0 (m² s^{-1}) is the reference diffusion coefficient [21.2*10^{-6} (m² s^{-1})] and T (C°) is the temperature (Holterman, 2003).

1.5. Density of Humid Air

The density of humid air (kg m^{-3}) is calculated according to the ideal gas law:

$$\rho_{humid\ air} = \frac{p_d * M_d + P_v * M_v}{R * T}$$

<div align="right">5</div>

where, p_d (Pa) is the partial pressure of dry air, M_d (kg mol^{-1}) is the molar mass of dry air, p_v (pa) is the pressure of water vapor, M_v (kg mol^{-1}) is the molar mass of water vapor, R [J K^{-1}mol^{-1}] is the universal gas constant, and T (K) is the temperature.

1.6. Density of Water

The density of water (kg m^{-3}) is computed as follows:

$$\rho_{water} = 999.85308 + 6.32693 * 10^{-2} * T - 8.523829 * 10^{-3} * T^2$$
$$+6.943248 * 10^{-5} * T^3 - 3.821216 * 10^{-7} * T^4$$

<div align="right">6</div>

where, T (°C) is the temperature (Jones and Harris, 1992).

1.7. Absolute humidity

The absolute humidity (kg m^{-3}) is calculated as follows:

$$Ah = \frac{Rh * \rho_{sat}}{R_{h2o} * T}$$

$$[Ah] = \frac{kg}{m * s^2} * \frac{s^2 * K * kg}{m^2 * kg} * \frac{1}{K} = \frac{kg}{m^3}$$

<div align="right">7</div>

where, R_{h2o} (J kg^{-1}K^{-1}) is the specific gas constant of water vapor, p_{sat} (pa) is the saturation vapor pressure, Rh (-) is the relative humidity, and T (K) is the temperature.

1.8. Relative humidity

The relative humidity (-) is calculated as follows:

$$Rh = \frac{m_{h2o} * R_{h2o} * T}{V * \rho_{sat}}$$

$$[Rh] = kg * \frac{m^2 * kg}{s^2 * K * kg} * K * \frac{1}{m^3} * \frac{m * s^2}{kg} = -$$

<div align="right">8</div>

where, m_{h2o} (kg) is the mass of water, R_{h2o} (J kg^{-1}K^{-1}] is the specific gas constant of water vapor, T (K) is the temperature, p_{sat} (pa) is the saturation vapor pressure, and V (m^3) is the volume.

1.9. Schmidt Number

The Schmidt number of water (-) is calculated as follows:

$$Sc_{water} = \frac{\mu_{air}}{\rho_{air} * D_V}$$

$$[Sc_{water}] = \frac{kg}{m * s} * \frac{m^3}{kg} * \frac{s}{m^2} = [-]$$

where, μ_{air} (kg m^{-1}s^{-1}) is the dynamic viscosity of air, ρ_{air} (Pa) is the density of air, and D_V [m²/s] is the diffusion coefficient of water (Løfstrøm et al., 2013).

1.10. Specific Latent Heat of Water

The specific latent heat of water (kJ kg^{-1}) can be expressed as follows:

$$\lambda = \frac{H_{v_{h2o}}}{M_{h20}}$$

where, Hv_{h2o} (kJ mol^{-1}) is the enthalpy of vaporization of water and M_{h2o} (g mol^{-1}) is the molar mass of water (Brecht, 2019).

1.11. Enthalpy of Vaporization of Water

The enthalpy of vaporization of water (kJ mol^{-1}) can be estimated as follows:

$$H_{v_{h2o}} = \left(50.09 - 0.9298 * \frac{T}{1000} - 65.19 * \left(\frac{T}{1000}\right)^2\right)$$

where, T (K) is the water temperature (Brecht, 2019).

2. Micrometeorological Model

2.1. Volume

For the volume estimation of the microclimate the following assumptions where made:

1. At the bottom the volume is limited by the ground.
2. At the top the volume is limited by the boom height and vertical dispersion coefficient (σ_v).
3. In both horizontal dimensions the volume is held constant. Assuming the mass exchanges between two neighboring units of application area being reflected of each other, cancelling out any mass changes.

Hence, the volume (m³) above one unit of application area is calculated as follows:

$$V(t) = b_{height} + \sigma_v$$

where, b_{height} (m) is the boom height and σ_v (m) vertical dispersion parameter.

The change of volume is calculated as follows:

$$\delta V(t_i) = V(t_i) - V(t_{i-1}) \tag{13}$$

where, t_i is the current time-step, t_{i-1} is the previous time-step, and V (m³) is the volume.

2.2. Mass

The change in mass of water vapor (kg) is calculated as follows:

$$\delta m_{h2o} = \delta V * Ah \tag{14}$$

where, δV (m³) is the change in volume and Ah (kg m⁻³) is the absolute humidity of the global environment.

The change of air mass is calculated as follows:

$$\delta m_{air} = \delta V * \rho_{humid\ air} - \delta m_{h2o} \tag{15}$$

where, δV (m³) is the change in volume, δm_{h2o} (kg) is the mass change of water vapor, and ρ_{humid_air} (kg m⁻³) is the density of humid air.

The mass of air is calculated as follows:

$$m_{air}(t_i) = m_{air}(t_{i-1}) + \delta m_{air}(t_i) \tag{16}$$

where, $m_{air}(t_{i-1})$ (kg) is the mass of air in previous time-step and $\delta m_{air}(t_i)$ (kg) is the change of air mass in the current time-step.

The mass of water is calculated as follows:

$$m_{h2o}(t_i) = m_{h2o}(t_{i-1}) + \delta m_{h2o}(t_i) + \delta m_{h2o,evap}(t_{i-1}) \tag{17}$$

where, $m_{h2o}(t_{i-1})$ (kg) is the mass of water vapor of the previous time-step, $\delta m_{h2o}(t_i)$ (kg) is the mass change of water vapor in the current time-step, and $\delta m_{h2o,evap}(t_{i-1})$ (kg) is the mass of evaporated water in the previous time-step.

2.3. Internal Energy

The internal energy (J) of the system is described as follows:

$$E(t_0) = m_{h2o}(t_0) * c_{p_{h2o}} m_{air}(t_0) * c_{p_{air}}$$
$$E(t_i) = E(t_{i-1}) + \delta m_{h2o}(t_i) * c_{p_{h2o}} + \delta m_{air}(t_i) * c_{p_{air}} - E_{evap}(t_{i-1}) \tag{18}$$

where, m_{h2o} (kg) is the mass of water vapor, m_{air} (kg) is the mass of air, c_{p_h2o} (J kg⁻¹) is the specific heat capacity of water, c_{p_air} (J kg⁻¹⁾ is the specific heat capacity of air,

E (J) is the internal energy of the system, E_{evap} (J) is the energy used during evaporation, and δE_{drop} (J) is the change in energy of the droplets caused by the change in temperature. With t_0 indicating the first time-step, t_i indicating the current time-step and t_{i-1} indicating the previous time-step.

The energy used during evaporation (J) is calculated as follows:

$$E_{evap} = m_{h2o,evap} * H_{s_{h2o}} - m_{h2o,evap} * T_{wb} * c_{p_{h2o}} \qquad 19$$

where, $m_{h2o,evap}$ (kg) is the mass of evaporated water, Hs_{h2o} (J kg) is the specific latent heat of vaporization of water, T_{wb} (K) is the wet-bulb temperature, and c_{p_h2o} (J kg^{-1}) is the specific heat capacity of water.

2.4. Temperature

The temperature (K) of the volume is estimated as a function of the internal energy and the masses of water vapor and air:

$$T = \frac{E}{m_{h2o} * c_{p_{h2o}} + m_{air} * c_{p_{air}}} \qquad 20$$

where, E (J) is the internal energy of the control volume, m_{H2O} (kg) is the mass of water vapor, m_{air} (kg) is the mass of air, $c_{p, H2O}$ (J kg^{-1}) is the specific heat capacity of water, and $c_{p,air}$ (J kg^{-1}) is the specific heat capacity of air.

2.5. Humidity

The relative humidity (-) of the volume is estimated as follows:

$$Rh = \frac{m_{H2O} R_{H2O} T}{V p_{sat}(T)} \qquad 21$$

where, m_{H2O} (kg) is the mass of water vapor, R_{H2O} (J kg^{-1}K^{-1}) is the specific gas constant of water, T (K) is the temperature, V (m³) is the volume, and $p_{sat}(T)$ (Pa) is the saturated vapor pressure estimated by an empirical relation to temperature.

3. Droplet Model

3.1. Evaporative Flux of the Active Ingredient

The evaporative flux of the active ingredient (kg m^{-2}s^{-1}) is estimated based on the linear relationship to vapor pressure and molar mass:

$$F_{AI} = 4.07 * 10^{-7} * p_{AI} * M_{AI}$$

<div align="right">22</div>

where, p_{AI} (Pa) is the vapor pressure of the active ingredient and M_{AI} (kg mol⁻¹) is the molar mass of the active ingredient (Mackay and van Wesenbeeck, 2014).

3.2.   Solution Parameters

For the solution of AI in water, the amount of AI (kg) and the volume of water (L) is known. The volume of AI (m³) is calculated as follows:

$$V_{AI} = \frac{m_{AI}}{\rho_{AI}}$$

<div align="right">23</div>

where, m_{AI} (kg) is the mass of AI and ρ_{AI} (kg m⁻³) is the density of the AI.

The mass of water (kg) was computed as follows:

$$m_{water} = V_{water} * \rho_{water}$$

<div align="right">24</div>

where, V_{water} (m³) is the volume of water and ρ_{water} (kg m⁻³) is the density of water.

The volumetric fraction (-) of AI was calculated as:

$$x_{vol_{AI}} = \frac{V_{AI}}{V_{AI} + V_{water}}$$

<div align="right">25</div>

where, V_{water} (m³) is the volume of water and V_{AI} (m³) is the volume of active ingredient.

The density of the droplet (kg m⁻³) was calculated as:

$$\rho_{drop} = \frac{m_{water} + m_{AI}}{V_{water} + V_{AI}}$$

<div align="right">26</div>

where, V_{water} (m³) is the volume of water, V_{AI} (m³) is the volume of AI, m_{AI} (kg) is the mass of AI, and m_{water} (kg) is the mass of water.

The molar fraction of water (-) was calculated as follows:

$$x_{mo\ water} = \frac{\dfrac{m_{water}}{M_{water}}}{\left(\dfrac{m_{water}}{M_{water}}\right) + \left(\dfrac{m_{AI}}{M_{AI}}\right)}$$

<div align="right">27</div>

where, M_{water} (kg mol⁻¹) is the molar mass of water, M_{AI} (kg mol⁻¹) is the molar mass of AI, m_{AI} (kg) is the mass of AI, and m_{water} (kg) is the mass of water.

3.3. Initial Droplet Parameters

The initial droplet diameter (m) is known, and the initial volume (m³) is calculated as:

$$V_{ini} = \frac{\pi}{6} * (D_{ini})^3$$

<div align="right">28</div>

where, D_{ini} (m) is the initial droplet diameter.

The initial mass of AI (kg) and the initial mass of water (kg) are then computed as:

$$m_{ini_{AI}} = x_{vol_{AI}} * V_{ini} * \rho_{AI} = V_{ini} * c_{AI}$$

$$m_{ini_{water}} = \rho_{water} * \left(V_{ini} - \frac{m_{ini_{AI}}}{\rho_{AI}} \right)$$

<div align="right">29</div>

where, V_{ini} (m³) is the initial droplet volume, ρ_{AI} (kg m⁻³) is the density of the AI, ρ_{water} (kg m⁻³) is the density of water, x_{volAI} (-) volumetric fraction of AI, and C_{AI} (kg m⁻³) is concentration of AI in the spray solution.

The initial molar fraction of water (-) is equal to the molar fraction of water (-) calculated in equation 27.

3.4. Droplet Kinetics

The momentum equation describes the deceleration (m s⁻²) as follows:

$$\frac{\delta v}{\delta t} = g - \frac{v_{drop}}{\tau_m}$$

<div align="right">30</div>

where, g (m s⁻²) is the earth-surface gravitational acceleration, v_{drop} (m s⁻¹) is the droplet speed, and τ_m (s) is the relaxation time (Løfstrøm et al., 2013).

The relaxation time calculated as:

$$\tau_m = \frac{\rho_{drop} * (D_{drop})^2}{18 * \mu_{air} * f}$$

$$[\tau_m] = \frac{kg}{m^3} * m^2 * \frac{m * s}{kg} = [s]$$

<div align="right">31</div>

where, ρ_{drop} (kg m⁻³) is the droplet density, D_{drop} (m) is the droplet diameter, μ_{air} (kg m⁻¹s⁻¹) is the dynamic viscosity of air, and f (-) is a factor describing the deviation from the Stokes flow (Løfstrøm et al., 2013).

With f (-) being calculated as follows:

$$f = 1.0 + 0.15 * (Re)^{0.687}$$

<div align="right">32</div>

where, Re (-) is the Reynolds number (Løfstrøm et al., 2013).

The Reynolds number [-] is calculated as following:

$$Re = \frac{D_{drop} * v_{drop} * \rho_{air}}{\mu_{air}}$$

$$[Re] = m * \frac{m}{s} * \frac{kg}{m^3} * \frac{m * s}{kg} = [-]$$

<div align="right">33</div>

where, D_{drop} (m) is the droplet diameter, v_{drop} (m s^{-1}) is the droplet velocity, ρ_{air} (kg m^{-3}) is the density of air, and μ_{air} (kg m^{-1}s^{-1}) is the dynamic viscosity of air (Løfstrøm et al., 2013).

When setting the change in velocity to zero in equation 30 the settling velocity of the droplet can be described as:

$$V_{drop} = \frac{g * \rho_{drop} * (D_{drop})^2}{18 * \mu_{air} * f}$$

<div align="right">34</div>

where, D_{drop} (m) is the droplet diameter, ρ_{drop} (kg m^{-3}) is the droplet density, g (m s^{-2}) is the earth-surface gravitational acceleration, μ_{air} (kg m^{-1}s^{-1}) is the dynamic viscosity of air, and f (-) is a factor describing the deviation from the Stokes flow. This is similar to equation 4 of Holterman (2003) with the addition of the deviation from Stokes flow f (-).

3.5. Droplet Evaporation

During the initial period of droplet lifetime, the evaporation rate is mainly driven by the cooling of the droplet, until it reaches the wet-bulb temperature. After this transient process the evaporation of the droplet can be approximated by steady evaporation. Since the transient process occurs on a time scale much smaller than the total lifetime of the droplet, it can be neglected (Holterman, 2003). The mass change (kg) of AI and water in the droplet is described as follows:

$$\frac{\delta m_{AI}}{\delta t} = \pi * (D_{drop})^2 * F_{AI}$$

$$\frac{\delta m_{water}}{\delta t} = \pi * (D_{drop})^2 * F_{water}$$

<div align="right">35</div>

where, D_{drop} (m) is the droplet diameter, F_{AI} (kg m^{-2}s^{-1}) is the flux of AI through the boundary layer, and F_{water} [kg/m²s] is the flux of water through the boundary layer.

The flux of AI (kg/m²s) was estimated by equation 22 and the flux of water [kg/m²s] is computed as follows:

$$F_{water} = \frac{Sh_{water} * D_{V_{water}} * M_{water}}{D_{drop} * R * T_{wb}} * \left((p_{sat} * Rh) - \left(p_{sat_{wb}} * x_{mol_{water}} \right) \right)$$

$$[F_{water}] = \frac{m^2}{s} * \frac{kg}{mol} * \frac{1}{m} * \frac{s^2 * mol * K}{kg * m^2} * \frac{1}{K} * \frac{kg}{m * s^2} = \left[\frac{kg}{m^2 * s} \right]$$

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where, Sh_{water} (-) is the Sherwood number for water, $D_{V_{water}}$ (m² s⁻¹) is the diffusion coefficient of water, M_{water} (kg mol⁻¹) is the molar mass of water, D_{drop} (m) is the droplet diameter, R (kgm² s⁻²mol⁻¹K⁻¹) is the universal gas constant, T_{wb} (K) is the wet-bulb temperature, p_{sat} (Pa) is the saturated vapor pressure of water at ambient temperature, Rh (-) is the relative humidity, p_{satwb} (Pa) is the saturated vapor pressure of water at the wet-bulb temperature, and $x_{molwater}$ (-) is the molar fraction of water in the droplet (Løfstrøm et al., 2013).

The Sherwood number of water (-) is calculated as:

$$Sh_{water} = 1.0 + 0.276(Re)^{\frac{1}{2}} * (Sc_{water})^{\frac{1}{3}}$$

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where, Re (-) is the Reynolds number and Sc_{water} (-) is the Schmidt number (Holterman, 2003; Løfstrøm et al., 2013).

3.6. Initial Droplet velocity

The initial droplet velocity is generally assumed to be equal to the average liquid sheet velocity, with the liquid sheet velocity being equal to the liquid discharge velocity (m s⁻¹) computed as:

$$U_L = \left(\frac{2 * P_n}{\rho_L} \right)^{\frac{1}{2}}$$

$$[U_L] = \sqrt{\frac{m^3}{kg} * \frac{kg}{m * s^2}} = \sqrt{\frac{m^2}{s^2}} = \left[\frac{m}{s} \right]$$

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where, P_n (kg m⁻¹s⁻²) is the spray pressure and ρL (kg m⁻³) is the density of the spray liquid (Dorr et al., 2013).

Adjusted for the nozzle angle the initial vertical droplet velocity (m s⁻¹) can be described as:

$$V_v = \cos(\alpha) * U_L \qquad\qquad 39$$

where, U_L (m s^{-1}) is the liquid discharge velocity and α (°) is the nozzle angle.

3.7. Vertical Wind Profile

Above the canopy the vertical wind profile is described by the logarithmic law. Within the canopy the vertical wind profile is described as an exponential function of the leaf area index.

$$U(z) = \frac{U_*}{\kappa} * \ln\left(\frac{z-d}{z_0}\right) \qquad\qquad if\ z \geq Hc \qquad 40$$

$$U(z) = U_H * \exp\left(\frac{LAI}{2} * \left(\frac{z}{H_c} - 1\right)\right) \qquad\qquad if\ z < Hc \qquad 41$$

$$Hc = d + 2z_0 \qquad\qquad if\ Hc < d + 2z_0 \qquad 42$$

where, U_* (m s^{-1}) is the friction velocity, κ (-) is the von Karman constant (0.4), z (m) is the height above ground, d (m) is the zero plane displacement, z_0 (m) is the roughness length, H_c (m) is the canopy height, U_H (m) is the wind speed at the top of the canopy as calculated by equation **Fehler! Verweisquelle konnte nicht gefunden werden.**, and LAI (m² m^{-2}) is the leaf area index (Sypka and Starzak, 2013). The roughness length is the height at which the wind speed becomes zero and can be approximated as one-tenth of the height of the surface roughness elements. The zero plane displacement can be assumed to be 0.63 times the canopy height (Butler Ellis and Miller, 2010).

3.8. Cumulated Probability

The cumulated probability (-) of a normal distribution above a given value is calculated as follows:

$$p(x) = 1 - \left(\frac{1}{2}\left(1 + \mathrm{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right)\right) \qquad\qquad 43$$

where, x is the value, μ is the mean value and σ is the standard deviation.

4. Dispersion Model

The dispersion model is based around a Gaussian puff model which predicts the droplet concentration (kg m^{-3}) at a given position (x,y,z) and as function of time as follows:

$$C(x, y, z)$$
$$= \frac{M}{(2\pi)^{\frac{3}{2}}\sigma_h^2\sigma_v} \exp\left[-\frac{1}{2}\left(\frac{x - x_c(t)}{\sigma_h}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_h}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z - z_c(t)}{\sigma_v}\right)^2\right]$$

$$[C] = \frac{kg}{m^3} * \frac{m}{m} * \frac{m}{m} * \frac{m}{m} = \left[\frac{kg}{m^3}\right]$$
<div align="right">44</div>

where, x, y and z (m) are the coordinates in x, y and z direction, respectively, t (s) is the time, M (kg) is the mass release from the nozzle, σ_h and σ_v (m) are the dispersion coefficients in the horizontal and vertical directions, respectively, U (m s-1) is the wind speed, and x_c and z_c (m) are the mean puff positions in x and z directions as a function of time as predicted in the droplet model (Zannetti, 1990).

In order to stabilize the numerical prediction of this Gaussian Puff model and to avoid spray drift deposition up-wind of the application area, a skewing term in x direction and spatial integration in x and y direction were implemented.

4.1. Integration Limit Definition

The limits of the spatial integration were defined as follows:

$$x_1 = x - 0.5 * res$$
<div align="right">45</div>

$$x_2 = x + 0.5 * res$$
<div align="right">46</div>

$$y_1 = y - 0.5 * res$$
<div align="right">47</div>

$$y_2 = y + 0.5 * res$$
<div align="right">48</div>

where, res (m) is the resolution of the spatial raster, x (m) and y (m) are the mean position of the calculated cell, x1 (m) and x2 (m) are the lower and upper limit in x direction, and y1 (m) and y2 (m) are the lower and upper limit in y direction.

4.2. Skewing Term

The skewing of the Gaussian puff in downwind direction (x dimension) is defined as follows:

$$alpha = k_{skew} * U * t^{0.5} * \left(\frac{\sigma_v}{\sigma_h}\right)$$
<div align="right">49</div>

$$k_{term} = 1 + \text{erf}\left(\frac{alpha * (x - x_c(t))}{\sqrt{2} * \sigma_h}\right)$$

<div align="right">50</div>

where, k_{skew} (-) is the user defined skewing factor, U (m/s) is the wind speed, t (s) is the elapsed time, σ_v and σ_h (m) are the vertical and horizontal dispersion coefficients.

4.3. x-Dimension Term

The term of the x-dimension describes the integration from x_1 to x_2 as follows:

$$x_{term} = \text{erf}\left(\frac{(x_2 - x_c(t))}{\sqrt{2} * \sigma_h}\right) - \text{erf}\left(\frac{(x_1 - x_c(t))}{\sqrt{2} * \sigma_h}\right)$$

<div align="right">51</div>

where, x_1 and x_2 (m) are the lower and upper integration limits, x_c (m) is the mean puff position in x direction as a function of time as predicted in the droplet model, and σ_h (m) is the horizontal dispersion coefficient.

4.4. y-Dimension Term

The term of the y-dimension describes the integration from y_1 to y_2 as follows:

$$y_{term} = \text{erf}\left(\frac{(y_2)}{\sqrt{2} * \sigma_h}\right) - \text{erf}\left(\frac{(y_1)}{\sqrt{2} * \sigma_h}\right)$$

<div align="right">52</div>

where, y_1 and y_2 (m) are the lower and upper integration limits, and σ_h (m) is the horizontal dispersion coefficient.

4.5. z-Dimension Term

The term of the z-dimension is described as follows:

$$z_{term} = exp^{-\frac{1}{2}\left(\frac{z - z_c(t)}{\sigma_v^2}\right)}$$

<div align="right">53</div>

where, z (m) is the coordinates in z direction, z_c (m) is the mean puff position in z direction as a function of time as predicted in the droplet model, and σ_v (m) is the vertical dispersion coefficients

4.6. Normalization Term

The normalization term is described as follows:

$$norm_{term} = \frac{M}{(2\pi)^{\frac{3}{2}} * \sigma_h^2 * \sigma_v}$$

<div align="right">54</div>

where, M (kg) is the released mass, and σ_v and σ_h (m) are the vertical and horizontal dispersion coefficients.

4.7. Deposition Flux

The deposition flux through the horizontal deposition plane at height z is the defined as follows:

$$F_{dep}(x, y, z, t) = v_d(t) * x_{term} * y_{term} * z_{term} * norm_{term} * k_{term}$$
<div align="right">55</div>

where, v_d (m/s) is the vertical droplet velocity as a function of time as predicted in the droplet model, x_{term} as defined in equation 48, y_{term} as defined in equation 49, z_{term} as defined in equation 50, $norm_{term}$ as defined in equation 51 and k_{term} as defined in equation 47.

4.8. Dispersion Parameters

The vertical (σ_v) and horizontal (σ_h) dispersion coefficients are described by the following empirical relations to time, distance, and wind speed:

$$\sigma_h = \beta \frac{\sigma_\theta * x}{1 + 0.9\left(0.001 * \frac{x}{U}\right)^{\frac{1}{2}}}$$

$$[\sigma_h] = \beta * \frac{m}{s^{\frac{1}{2}}} = s^{\frac{1}{2}} * \frac{m}{s^{\frac{1}{2}}} = m$$
<div align="right">56</div>

$$\sigma_v = \alpha \frac{\sigma_w * x}{u * \left(1 + 0.9\left(0.02 * \frac{x}{U}\right)^{\frac{1}{2}}\right)}$$

$$[\sigma_v] = \alpha * \frac{s}{s^{\frac{1}{2}}} = \frac{m}{s^{\frac{1}{2}}} * \frac{s}{s^{\frac{1}{2}}} = m$$
<div align="right">57</div>

where, t (s) is the time, x (m) is the distance, U (m s^{-1}) is the wind speed, σ_w and σ_θ (-) are the unitless vertical and horizontal wind velocity standard deviation used as empirical calibration parameters, α (m s$^{-1/2}$) is the empirical unit-correction factor for the vertical dispersion coefficient, and β (s$^{1/2}$) is the empirical unit-correction factor for the horizontal dispersion coefficient (Draxler, 1976; Souto et al., 2001).

5. Input/Output Documentation

5.1. General Description

The DAD drift model is comprised of multiple sub-models (Figure 1). First, the droplet model and the micrometeorological model are run in parallel for all defined droplet

classes, with a droplet class representing droplets in a specific size range characterized by the mean droplet diameter. The droplet model predicts the motion and mass balance of droplets representative of their droplet class based on weather conditions (e.g., wind speed, wind direction, ambient pressure), droplet parameters (e.g., velocity, size, density), release height, and the micrometeorological model (i.e., humidity, temperature). The micrometeorological model accounts for indirect interactions between individual droplets within the spray cloud by estimating the change in humidity and temperature caused by droplet evaporation in the droplet model. Second, the dispersion model describes the atmospheric dispersion of a cloud of airborne droplets. The droplet trajectories provided by the droplet model are used to estimate the mean position of the three-dimensional puff and to predict the three-dimensional concentration field.
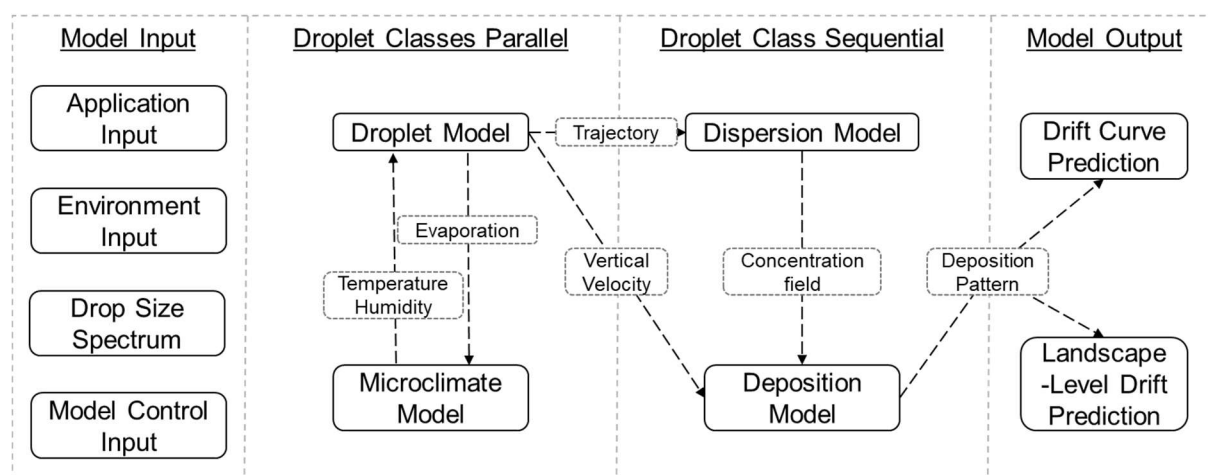

Figure 1: Schematic representation of the DAD drift model flow.

Third, the deposition model combines the vertical droplet velocity and the concentration field to predict the deposition mass flux at each deposition height, resulting in a two-dimensional deposition pattern. The dispersion model and the deposition model are executed sequentially for all droplet classes. Finally, the deposition pattern is used to predict either a drift deposition curve or a two-dimensional landscape-level drift deposition pattern as model output. The individual sub-models are described in the following sections, for additional details please refer to the theoretical model documentation.

5.2. Application Input File

In the application input file "application_input.txt" a total of 14 parameters containing information relevant to the application of the active ingredient are defined. For the

landscape mode 10 parameters are necessary, for the drift curve mode 12 parameters are necessary. Only one of the three parameters "app_rate_mh", "app_rate_mha", and "app_rate_kgha" must be defined for the model to run properly.

Table 1: application_input.txt input parameters.

Parameter Name	Unit	Description
tractor_speed	(m s^{-1})	Tractor speed, only used in combination with "app_rate_mh".
boom_width	(m)	Width of the spray boom.
boom_height	(m)	Height of the spray boom above ground.
nozzle_angle	(°)	Deviation of nozzle angle from vertically downward spraying.
application_pres	(kPa)	Spray pressure used during application.
app_rate_mh	(m³ h^{-1})	Application rate in meters cubed per hour, no data value -99.
app_rate_mha	(m³ ha^{-1})	Application rate in meters cubes per acre, no data value -99.
app_rate_kgha	(kg ha^{-1})	Application rate in kilograms per acre, no data value -99.
sol_concentration	(kg m^{-3})	Concentration of the spray solution.
AI_density	(kg m^{-3})	Density of the active ingredient.
AI_molar_mass	(kg mol^{-1})	Molar mass of the active ingredient.
AI_vapor_pressure	(Pa)	Vapor pressure of the active ingredient.
swath_number	(-)	Number of spray swaths, only used in spray curve mode.
field_length	(m)	Length of the field (swath), only used in spray curve mode.

5.3. Environmental Input File

In the environmental input file "environment_input.txt" a total of 11 parameters containing information about the environmental conditions during application are defined. The following table gives an overview of the parameters:

Table 2: environment_input.txt input parameters.

Parameter Name	Unit	Description
temperature	(°C)	Ambient temperature.
humidity	(-)	Relative humidity.
wind_speed	(m s^{-1})	Wind speed.
wind_height	(m)	Height at which the wind speed was measured.
wind_direction	(°)	Wind direction relative to the spray path.
ambient_pressure	(kPa)	Ambient pressure.
sigma_horizontal	(m)	Horizontal wind standard deviation.
sigma_vertical	(m)	Vertical wind standard deviation.
roughness_height	(m)	Surface roughness height.
canopy_height	(m)	Canopy height.
LAI	(m² m^{-2})	Leaf area index.

k_skew	(-)	Skewing factor

5.4. Control Input File

In the control input file "control_input.txt" the main parameters of model execution (i.e. mode, deposition height, maximum distance, and number of landscape files) and additional input files are defined. The "dsd_file_name" defines which file contains the drop size distribution necessary for model execution and the "landscape_file_name" defines one or more raster input files defining areas of application in the landscape mode. The following table gives an overview of the parameters:

Table 3: control_input.txt input paramteres.

Parameter Name	Unit	Description
mode	(-)	Mode of model execution: 0 = landscape mode 1 = drift curve mode
dep_height	(m)	Height at which the deposition is calculated.
max_dist	(m)	Maximum distance used during drift pattern prediction.
field_count	(-)	Number of landscape files provided, only used in landscape mode.
dsd_file_name	(-)	Name of the file containing the drop size distribution.
landscape_file_name	(-)	Name(s) of the file(s) containing the landscape raster inputs, only used in landscape mode.

5.5. Drop Size Spectrum Input File

The drop size spectrum file, defined in the control input file, contains two columns. In the first column the mean droplet diameter (m) of each droplet size class is defined, and in the second column the cumulated fraction of exceedance (-) is defined.

5.6. Landscape Input File

The landscape input files, defined in the control input file, are one or more raster files of the ".asc" file format. Containing the information on where application is happening. A raster cell where application is happening has a value of 1 assigned, all other cells should typically be assigned the no data value of -99.

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