

MAM-An Equivalence-based Dynamic Mass Balance Model for the Fate of Non-Volatile Organic Chemicals in the Agricultural Environment

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Abstract: A Multimedia Agricultural Model (MAM) for predicting the fate and transport of Non-Volatile Organic Chemicals (NVOCs) in the agricultural environment was presented. It is an expanded and modified version of the three compartmental model introduced by Batiha and co-authors in 2007, which is an equivalence-based level IV. MAM considered five environmental compartments to include the air, water, soil, sediment and vegetation. It calculates the complete steady-state mass budgets for the air, water and particulate organic carbon between the model compartments. MAM compartments were connected by advective and intermedia transport processes. Degradation can take place in every compartment. The mass balances for each of the compartments result in a system of five differential equations, solved numerically to yield estimates of concentrations, masses, transport fluxes and reaction rates as a function of time. All the equations required for MAM calculations were provided.

Key words: Agro-ecosystem, MAM, NVOCs, sediment, vegetation

INTRODUCTION

It is becoming evident that vegetations play an important role in the environmental fate of many organic compounds^[1-4]. It is clearly an important aspect of the agricultural environment since approximately 97% of the plantations land surface is covered by vegetation. Moreover, the total leaf surface area may exceed by factors of up to 20 the ground area on which plants grows^[5]. The total amount of cuticular material in temperate forests and agricultural plants communities may range from 180-1500 kg per hectare^[6]. As a result of the high reactivity of some compounds on vegetation surface and the array of available deposition surfaces in vegetation canopies^[7], it has been suggested that vegetation could be an important sink for organic compounds^[8].

Many authors^[9-10] have reported that the concentrations of organic chemicals in forest soils are higher than in agricultural soils. This phenomenon was explained by Horstmann *et al.*^[11] that the elevated levels of organic chemicals present in forest soils compared to agricultural soils are due to atmospheric deposition processes. Atmospheric pollutants can be transferred to vegetation canopies either through wet or

dry deposition^[12]. Wet deposition, can be expected to be similar to vegetated and non-vegetated land. Hence, the elevated deposition to vegetations must arise from dry deposition. McLachlan *et al.*^[13] have divided the dry deposition of organic chemicals to vegetations into three categories according to the volatility of the compound. For the relatively Non-Volatile Organic Chemicals (NVOCs), gaseous deposition is superseded in importance by dry-particle-bound deposition. Sehmel^[14] sub-divided the dry-particle-bound deposition into three processes: particle sedimentation, particle impaction and diffusion^[15]. Whereas, for NVOCs, the diffusion process from the surface compartments to the atmosphere is neglected^[16]. Moreover, the dominant mechanisms that convey chemicals transport from vegetation to soil are also occurring under wet (i.e., canopy throughfall) and dry (i.e., litterfall) conditions^[2].

The water-sediment interface is an active layer, which typically consists of 95% particles and is often highly in organic nature. It may consists of deposited particles and fecal material from water column^[17]. The main transport processes within water-sediment interface layer are deposition, resuspension and sediment burial. Therefore, the inclusion of vegetation

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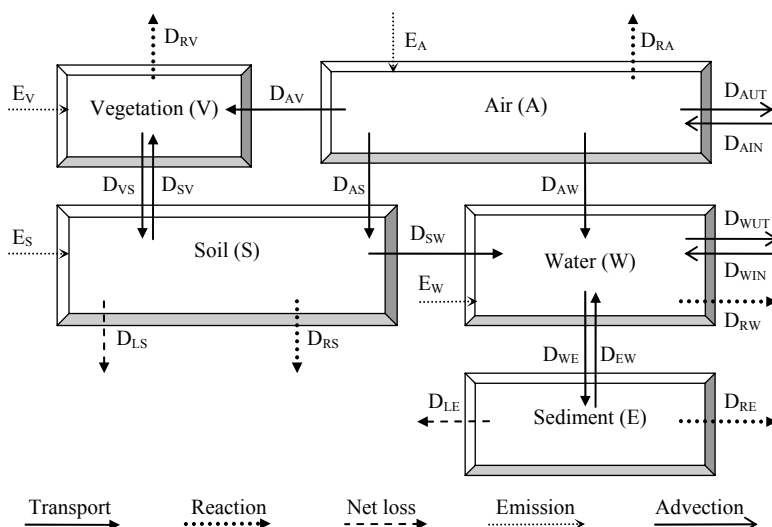


Fig. 1: Schematic representation of the environmental compartments and chemical fate processes in MAM

and sediment compartments into multimedia models for NVOCs is an important issue. This study follows up the preliminary findings, reported by Batiha *et al.*^[18] and constitute on recent attempts to include vegetation and sediment compartments into multimedia equivalence-based models at the dynamic conditions. Herewith, we have described the Multimedia Agricultural Model (MAM) and provided all the necessary equations for the model feasibility calculation.

Model structure: The main concepts of MAM have been presented in detail by Batiha *et al.*^[18]. Hence, MAM is an equivalence-based, dynamic (Level IV: unsteady-state, non-equilibrium with degradation, advection and inter-compartmental transfer) model. The MAM environment consists of up to five environmental compartments Fig. 1, namely, the Air (A), Water (W), Soil (S), Sediment (E) and Vegetation (V), which are believed to shape the agricultural environment. These compartments are linked by up to eight transport processes from *i* to *j* compartment (D_{ij} , $m^3 h^{-1}$). There are two possibilities through which NVOCs can enter the modeled environment: either by direct emission to compartment *i* (E_i mol h^{-1}) and/or by advection of air and water into the model domain (D_{AIN} and D_{WIN} , mol h^{-1}). Once NVOCs is introduced to the environment, it can move amongst compartments and can be lost from each compartment *i* through various transformation processes (D_{Ri}), leaching from soil to ground water (D_{LS}) and sediment burial (D_{LE}). In addition, NVOCs can be lost by advection of air and water out of the model domain (D_{AUT} and D_{WUT} , $m^3 h^{-1}$).

RESULTS AND DISCUSSION

NVOCs transfer fluxes: Chemical movement in the environment is strongly associated with the movement of air, water and organic matter^[19]. NVOCs advective inter-compartmental transfer fluxes are calculated as the product of a flux of a carrier phase (*F*) in units of $m^3 h^{-1}$, namely, air (AF), water (WF) and particulate organic carbon (PF) and a NVOC concentration (*C*, mol m^{-3}) in similar phase. Solving the NVOC mass balance thus requires the constructions of mass balance for air, water and Particulate Organic Carbon (POC) within the modeled system. These fluxes were assumed to be constant in time. In the following, details are provided for the construction of mass balances for air, water and POC.

Mass balance of air: As has been discussed by Batiha *et al.*^[18], the mass balance for air is calculated as the volume of atmospheric compartment divided by the atmospheric residence time.

Mass balance for water: The water mass balance consistent set of up to 11 inter-compartmental water fluxes, WF in $m^3 h^{-1}$, between the modeled compartments Fig. 2. The water flux from air to the surface compartments by precipitation, WF_{AX} (Eq. 1, 5 and 8 in Table 1), is estimated from the rain rate (U_R , m h^{-1}) and the compartment surface area (A_X , m^2). Evaporation loss from the surface compartments, WF_{XA} (Eq. 2, 6 and 9 in Table 1), is estimated by employing fractions ϕ_X of the total water flow to a compartment *x*

Table 1: Equations used to calculate the water and POC fluxes between MAM compartments in units of $m^3 h^{-1}$

Fluxes	Equations
I. Water fluxes:	
1. Precipitation from air to vegetation	$WF_{AV} = U_R A_V$
2. Evaporation from vegetation to air	$WF_{VA} = \phi_V (WF_{AV} + WF_{SV})$
3. Throughfall from vegetation to soil	$WF_{VS} = (1 - \phi_V) (WF_{AV} + WF_{SV})$
4. Rainsplash from soil to vegetation	$WF_{SV} = \phi_{RS} WF_{AS}$
5. Precipitation from air to soil	$WF_{AS} = U_R A_S$
6. Evaporation from soil to air	$WF_{SA} = \phi_S (WF_{AS} + WF_{VS})$
7. Runoff and leaching from soil to water	$WF_{SW} = (1 - \phi_S - WF_{SV}) (WF_{AS} + WF_{VS})$
8. Precipitation from air to water	$WF_{AW} = U_R A_W$
9. Evaporation from water to air	$WF_{WA} = \phi_W (WF_{AW} + WF_{SW})$
10. Water flow from water to the outside	$WF_{UT} = (1 - \phi_W) (WF_{AW} + WF_{SW}) (1 + f_{UT})$
11. Water flow from the outside to water	$WF_{IN} = (1 - \phi_W) (WF_{AW} + WF_{SW}) f_{UT}$
II. POC fluxes:	
12. POC inflow from soil to water	$PF_{SW} = WF_{SW} v_{SS} / \rho_{OC}$
13. POC production in water	$PF_{Wpro} = P_W A_W / (\rho_{OC} 8760)$
14. POC mineralization in water	$PF_{Wmin} = PF_{Wpro} \phi_{Wmin}$
15. POC concentration in water	$C_{PW} = \frac{PF_{SW} + PF_{Wpro} - PF_{Wmin} + (WF_{IN} C_{PIN}) / \rho_{OC}}{[WF_{UT} + (1 - \phi_{res}) v_{sed} A_E] / \rho_{OC}}$
16. POC sedimentations from water to sediment	$PF_{WE} = v_{sed} A_W C_{PW} / P_{OC}$
17. POC resuspension to water from sediment	$PF_{EW} = \phi_{res} v_{sed} A_W C_{PW} / P_{OC}$
18. POC burial in sediment	$PF_{LE} = A_W v_{SE} v_{bur} v_{OE}$
19. POC mineralization in sediment	$PF_{Emin} = (PF_{WE} - PF_{EW}) \phi_{Emin}$

Note: U_R is the rainfall rate, $m^3 h^{-1}$, A_X is the surface area of compartment x , m^2 , ϕ_X is the fraction of precipitation to compartment x that evaporates from that compartment, ϕ_{RS} is the fraction of raindrop water reflected after reaching the soil surface to vegetation, f_{UT} is the factor by which water is increased by inflow from the outside flux, v_{SE} , v_{OE} and v_{SS} are the volume fraction of solids in sediment, of organic carbon in sediment solids and of solids in soil, respectively, ρ_{OC} is the density of organic carbon, $g m^{-3}$, P_W is the primary productivity in water, $g carbon/m^2 a$, ϕ_{Wmin} and ϕ_{Emin} are the fraction of net POC input to water and sediment compartments, respectively, that is mineralized, C_{PIN} is the concentration of POC in the water flow from the outside, $g m^{-3}$, v_{sed} and v_{bur} are the POC sedimentation and burial velocities in sediment, respectively, ϕ_{res} is the fraction of POC deposition that is resuspended

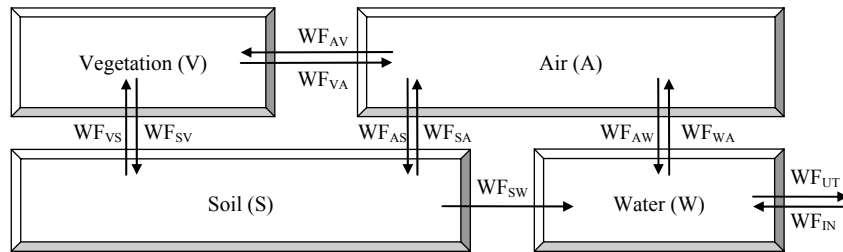


Fig. 2: Water fluxes between MAM compartments

that evaporates from that compartment. The water flux from vegetation to the soil by throughfall, WF_{VS} (Eq. 3 in Table 1), is derived as the balance of the remaining fraction of precipitation to vegetation that fall to soil from evaporation loss. The water flux from the soil to vegetation by rainsplash, WF_{SV} (Eq. 4 in Table 1), is estimated by employing fractions ϕ_{RS} of the raindrop water reflected after reaching the soil surface to vegetation. The run-off and leaching flux from soil to the water compartment, WF_{SW} (Eq. 7 in Table 1), is derived as the balance of the remaining fraction of precipitation plus water throughfall from the vegetation

to soil obtained from evaporation plus rainsplash losses. The net flow between water compartment and the outside, WF_{UT} and WF_{IN} (Eq. 10 and 11 in Table 1), is estimated employing the factor (f_{UT}) by which water is increased by inflow from the outside flux.

POC mass balance: The POC fluxes illustrated in Eq. 12-15 in Table 1, has been discussed in detail by Batiha *et al.*^[18]. Only the calculation of the new included POC fluxes over the sediment compartment needed for the construction of POC mass balance is discussed in this study Fig. 3. These fluxes are POC sedimentations from

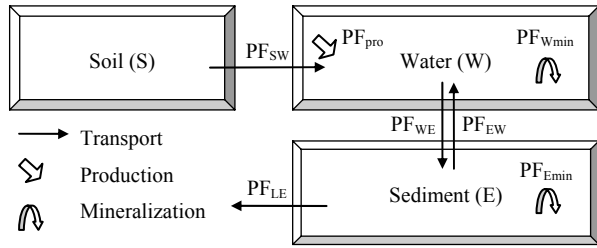


Fig. 3: POC fluxes between MAM compartments

water to sediment, POC resuspension to water from sediment, POC burial in sediment, and POC mineralization in sediment (Eq. 16-19 in Table 1, respectively). Whereas, the user-defined parameters are the POC sedimentation and burial velocities in sediment, v_{sed} and v_{bur} , respectively, the fraction of POC deposition that is resuspended (ϕ_{res}), the density of organic carbon in $g\ m^{-3}$ (ρ_{OC}), the fraction of net POC input to sediment compartment (ϕ_{Emin}), the volume fraction of solids in sediment (v_{SE}) and the volume fraction of organic carbon in sediment solids (v_{OE}).

Description of chemical fate: Chemical fate in the MAM (Level IV calculations) is expressed in the form of an unsteady-state mass balance equation for each of the five model compartments Table 2. These equations have the general form shown below and are formulated in terms of equivalence (q_i , $mol\ m^{-3}$), employing the concepts of Z-values (dimensionless) to describe the phase partitioning and D-values ($m^3\ h^{-1}$) to describe the chemical fate processes. Due to the fluctuation of some environmental parameters with season, the Z- and D-values are functions of time (t):

$$\frac{d(q_i Z_i V_i)}{dt} = E_i(t) + \sum_j (D_{ji}(t) q_j(t)) - q_i(t) \left(D_i(t) + \sum_j D_{ij}(t) \right)$$

where q_i is the equivalence in compartment i at time t in $mol\ m^{-3}$, $Z_i(t)$ the dimensionless partitioning capacity of compartment i at time t, V_i the volume of compartment i in m^3 , $E_i(t)$ the direct emission rate into compartment i at time t in $mol\ h^{-1}$, $D_{ji}(t)$ the D-value describing transport from compartment i to j at time t in $m^3\ h^{-1}$, $D_i(t)$ the D-value describing loss processes from compartment i at time t in $m^3\ h^{-1}$.

The compartments volumes are constant, therefore, the equations can be rewritten as partial differential equations:

$$\begin{aligned} \frac{\delta q_i}{\delta t} &= Z_i(t) \times V_i + \frac{\delta Z_i}{\delta t} q_i(t) \times V_i \\ &= E_i(t) + \sum_j (D_{ji}(t) \times q_j(t)) - q_i(t) \\ &\quad \left(D_i(t) + \sum_j D_{ij}(t) \right) \end{aligned}$$

Substituting the differentials by finite differences:

$$\begin{aligned} \frac{q_i(t + \Delta t) - q_i(t)}{\Delta t} \times Z_i(t) \times V_i + \\ \frac{Z_i(t + \Delta t) - Z_i(t - \Delta t)}{2\Delta t} q_i(t) \times V_i \\ = E_i(t) + \sum_j (D_{ji}(t) \times q_j(t)) \\ - q_i(t) \left(D_i(t) + \sum_j D_{ij}(t) \right) \end{aligned}$$

Z-values are independent of the equivalences and can be calculated for time $t + \Delta t$. The time course of the equivalences in all compartments can thus be calculated iteratively using:

$$q_i(t + \Delta t) = q_i(t) + \frac{\Delta t}{Z_i(t) \times V_i} \left(\begin{aligned} &E_i(t) + \sum_j (D_{ji}(t) \times q_j(t)) \\ &- q_i(t) \left(D_i(t) + \sum_j D_{ij}(t) \right) \\ &- \frac{Z_i(t + \Delta t) - Z_i(t - \Delta t)}{2\Delta t} q_i(t) \times V_i \end{aligned} \right)$$

Estimating equivalences in all MAM compartments as a function of time, the intermedia fluxes between MAM compartments, reaction rate, chemical residence time and chemical concentration in each compartment can be deduced. In the following context, the details of how the various Z- and D-values can be calculated in the MAM are provided.

Description of phase partitioning: Equilibrium phase partitioning in MAM as is typical for equivalence-based models are expressed in terms of Z-values or the compartment partitioning capacities. The Z-values for sediment and vegetation compartments (Z_E and Z_V) are described by Eq. 1 and 2, respectively:

$$Z_E = Z_W \rho_E K_{EW} / 1000 \quad (1)$$

$$Z_V = Z_W K_{CW} \quad (2)$$

where Z_W is the partitioning capacity of water compartment, ρ_E is the sediment density and K_{EW} and

Table 2: Mass balance equations for each MAM compartment

Compartment	Mass balance equations
Air	$d(V_A Z_{BA} q_A)/dt = (E_A + D_{AIN}) - (D_{AUT} + D_{RA} + D_{AV} + D_{AS} + D_{AW}) q_A$
Water	$d(V_W Z_{BW} q_W)/dt = (E_W + D_{WIN} + D_{SW} q_S + D_{EW} q_A + D_{EW} q_E) - (D_{WUT} + D_{WE} + D_{RW}) q_W$
Soil	$d(V_S Z_{BS} q_S)/dt = (E_S + D_{AS} q_A + D_{VS} q_V) - (D_{SV} + D_{SW} + D_{RS} + D_{LS}) q_S$
Sediment	$d(V_E Z_{BE} q_E)/dt = (D_{EW} q_W) - (D_{EW} + D_{RE} + D_{LE}) q_E$
Vegetation	$d(V_V Z_{BV} q_V)/dt = (E_V + D_{SV} q_S + D_{AV} q_A) - (D_{VS} + D_{RV}) q_V$

K_{CW} are the sediment- and cuticle-water partition coefficients, respectively. The K_{CW} is the parameter describing the tendency of environmental chemicals to accumulate in the cuticle phase in an ecosystem as well as on a single leaf or fruit scale. Based on the available data, one of the following quantitative structure-activity relationship models can be used to calculate the K_{CW} ^[20-21].

$$\log K_{CW} = 0.057 + 0.970 \log K_{OW} \quad (3)$$

$$\log K_{CW} = 1.118 - 0.569 \log S \quad (4)$$

$$\log K_{CW} = 0.37 + 1.31 \chi^v - 1.49 N_{aliph}^{OH} \quad (5)$$

Where K_{OW} is the octanol-water partition coefficient, S the water solubility, χ^v the valence third-order molecular connectivity index that calculated from the non-hydrogen part of the molecule and N_{aliph}^{OH} the number of aliphatic hydroxy groups.

The bulk Z -value for sediment and vegetation compartments (Z_{BE} and Z_{BV}) is calculated by Eq. 6 and 7, respectively:

$$Z_{BE} = (1 - v_E) Z_E + v_E v_{OE} Z_P \quad (6)$$

$$Z_{BV} = v_{AV} Z_A + v_{WV} Z_W + v_{CV} Z_V \quad (7)$$

where v_E is the volume fraction of solids in sediment, v_{OE} is the volume fraction of organic carbon in sediment solids, Z_P is the Z -value for particulate organic carbon and v_{AV} , v_{WV} and v_{CV} are the volume fraction of air, water and cuticle in vegetation, respectively.

Description of chemical fate processes: Transport, loss and transformation processes in equivalence-based models are described with the help of D -values in units of $m^3 h^{-1}$. The present model adds the D -values for sediment and vegetation compartments to those D -values previously described by Batiha *et al.*^[18] for air, water and soil. The additional estimated D -values are drawn upon on recent modeling published papers^[2,19,22-23]. The transport and transformation processes from

and to sediment and vegetation compartments are discussed below and D -values are listed in Table 3.

As MAM is intended to be applicable for NVOCs, the diffusion process from plant surface to air was neglected. Advective processes from air to vegetation are the wet and dry particle deposition. The D -value for wet deposition of particles to vegetation is given by Eq. 3 in Table 3. In this equation, the wet deposition interception fraction (If_w) depends on the leaf area index (LAI) in units of m^2 leaves per m^2 land, the rainfall rate (U_R , $m h^{-1}$) and the canopy water storage capacity (S_{bl}), and can be calculated from Müller and Prohl^[24] as follows:

$$If_w = S_{bl} LAI \exp\left(\frac{-\ln(2U_R)}{3S_{bl}}\right) \quad (8)$$

The D -value for dry particle deposition to vegetation is given by Eq. 4 in Table 3. The dry deposition interception fraction (If_d) is calculated from plant biomass as described by Whicker and Kirchner^[25],

$$If_d = 1 - \exp(-2.8 \text{ bio}_{inv}) \quad (9)$$

where bio_{inv} is the plant dry mass inventory (kg dry mass m^{-2}). Summation of D -values for wet and dry particle deposition (Eq. 3 and 4 in Table 3) give the overall D -value for air to vegetation.

The dominant transport mechanisms of NVOCs from vegetation to soil are also occurring under wet (canopy throughfall) and dry (litterfall) conditions. Litterfall is the process of vegetation foliage falling to the ground as a result of shedding of leaves and vegetation death and controlled by a first order rate constant (k_{LF}). The k_{LF} is assumed by Bennett *et al.*^[22] to be equal to one divided by the length of the growing season. The D -value for this process is given by Eq. 6 in Table 3. Canopy throughfall (Eq. 7 in Table 3) is the process of washing out of contaminant sorbed onto vegetations by precipitation, which is calculated as the product of the water flux from vegetation to soil (WF_{VS} , $m^3 h^{-1}$) and the vegetation bulk Z -value (Z_{BV}). Summation of D -values for canopy throughfall and litterfall yield the total D -value for the transport mechanisms from the vegetation to the soil.

Table 3: D-values formulation specific to MAM in units of m³ h⁻¹

Compartment				
From	To	Process		Equation
Vegetation	Air	1.	Chemical diffusion from foliage	$D_{VA} = 0$
Air	Vegetation	2.	Total	$D_{AV} = D_{WD} + D_{DD}$
		3.	Wet deposition of particles	$D_{WD} = W_{F_{AV}} I_{f_w} Z_{BR}$
		4.	Dry deposition of particles	$D_{DD} = A_V I_{f_d} U_Q v_Q Z_Q$
Vegetation	Soil	5.	Total	$D_{VS} = D_{CT} + D_{LF}$
		6.	Litterfall	$D_{LF} = V_V k_{LF} Z_{BV}$
		7.	Canopy throughfall	$D_{CT} = W_{F_{VS}} Z_{BV}$
Soil	Vegetation	8.	Rain splash	$D_{VS} = W_{F_{SV}} Z_{BS}$
Water	Sediment	9.	Total	$D_{WE} = D_{diff} + D_{dep}$
Sediment	Water	10.	Total	$D_{EW} = D_{diff} + D_{res}$
		11.	Diffusion across the water sediment interface	$D_{diff} = \frac{A_w}{\frac{1}{k_{EW} Z_w} + \frac{\ln(2) h_E}{Z_w [B_w (1 - v_E)^{1.5} + B_{WE}] + B_{PE} v_{OE} Z_p}}$
		12.	Deposition	$D_{dep} = P_{F_{WE}} Z_p$
		13.	Resuspension	$D_{res} = P_{F_{EW}} Z_p$
		14.	Sediment burial	$D_{LE} = P_{F_{LE}} Z_p$
		15.	Degradation in vegetation	$D_{RV} = V_V k_{RV} Z_V$
		16.	Degradation in sediment	$D_{RE} = V_E k_{RE} Z_E$

Notes: A_V and A_W are the surface area of vegetation and water compartments, m², I_{f_w} and I_{f_d} are the canopy wet and dry interception fraction, U_Q is the dry deposition velocity, m h⁻¹, v_Q , v_{OE} and v_E are the volume fraction of aerosol in air, of organic carbon in sediment and of solids in sediment, respectively, V_V and V_E are the volume of vegetation and sediment compartments, m³, k_{LF} is the litterfall rate constant, h⁻¹, k_{EW} is the mass transfer coefficient for diffusion across benthic boundary layer, m h⁻¹, h_E is the depth of sediment compartment, m, B_W is the molecular diffusivity in water, m² h⁻¹, B_{WE} is the bioirrigation diffusivity of sediment pore water, m² h⁻¹, B_{PE} is the bioturbation diffusivity of sediment solids, m² h⁻¹ and k_{RV} and k_{RE} are the vegetation and sediment degradation rate constants, h⁻¹

Rainsplash, which is the only transport mechanism from soil to vegetation considered, is based on the concept that once lifted off by the raindrop impact, the particle-sorbed contaminant in soil entrained into the splash droplets travel to vegetation. The D-value for this mechanism (Eq. 8 in Table 3) is calculated as a product of the water flux from soil to vegetation ($W_{F_{SV}}$, m³ h⁻¹) and the soil bulk Z-value (Z_{BV}).

The processes contribute the exchange of contaminants across the water-sediment interface as described by Wania *et al.*^[19] are two advective and four different diffusive processes. The advective processes are physical sedimentation or deposition and resuspension of contaminants sorbed to POC (Eq. 12 and 13 in Table 3), described using the POC transport rates $P_{F_{WE}}$ and $P_{F_{EW}}$ in m³ h⁻¹ derived in Table 1. The overall diffusive process, which may act in either direction, is described as follows. On the waterside there is a resistance to transfer through the stagnant benthic boundary layer above the sediment surface, quantified using a benthic boundary layer mass transfer coefficient, k_{EW} in m h⁻¹. Secondly, there are three parallel diffusive processes on the sediment side of the water-sediment interface. The first is the molecular diffusion through water-filled pore spaces in the sediment, quantified by the diffusivity in water B_W , corrected for the sediment porosity. Bioturbation of sediment solids and sediment pore water is treated as

two pseudo-diffusive processes invoking two equivalent bioturbation diffusivities, B_{PE} and B_{WE} in m² h⁻¹, respectively. In all three cases the diffusion path length is calculated as the log mean depth of the sediment compartment (h_E , m). The final equation for diffusive water-sediment exchange is given by Eq. 11 in Table 3. Eq. 9 and 10 in this Table show the D-values describing the exchange of the contaminants across the water-sediment interface.

Finally, the D-value for degradation processes in the vegetation and sediment compartments may be quantified as the product of compartments volume (V_V and V_E , m³), the compartment Z-value and the degradation rate constants (k_{RV} and k_{RE} , h⁻¹) as given by Eq. 15 and 16 in Table 3.

CONCLUSION

A comprehensive multimedia agricultural model, MAM, has been developed that described the processes of NVOCs transport and transformation in the agro-ecosystem. MAM is a Level IV equivalence-based model, an improved and expanded version of the model that has been described by Batiha *et al.*^[18]. Major differences from the earlier model were the increased number of environmental compartments (sediment and vegetation) which together are believed to shape the agro-ecosystem. Therefore, MAM has utilized to treat

five environmental compartments, namely, the air, water, soil, sediment and vegetation. MAM constructed complete steady-state mass balance for air, water and POC. Even though the rates of primary production and POC mineralization are not required for the contaminant mass balance, they were included in MAM calculation to complete and assure the consistency of the mass balance.

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