STRATEGIES FOR INCLUDING THE PADDY FIELD COMPARTMENT IN MULTIMEDIA MODELS

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Introduction

Multimedia models that describe the environmental fate of organic contaminants are proposed as tools to rank chemicals based on their environmental persistence (P) and long-range transport potential (LRTP). However, on most multimedia models, for instance, the Equilibrium Criterion Model (EQC)[1], Coastal Zone Model for Persistent Organic Pollutants (CoZMo-POP)[2] and Global Distribution Model (Globo-POP)[3], the paddy field is not included. There may be a reason of relatively few paddy fields in America and European countries. While being used for estimation of the environmental fate of organic chemicals such as pesticides and POPs emitted from the Asian region, multimedia models are justifiably criticized for not including paddy field. The criticism comes due to: 1) approximately two thirds of the earth's paddy field area is located in the Asian region, and 2) large quantities of pesticides are applied to paddy fields for agricultural uses in Asian countries. For instance, in Japan, the amount of pesticides applied to the paddy fields reaches about two thirds of the total amount spent over a year.

Even so, it is not obvious, if and how, the rice plant should be treated while the paddy field is incorporated as a compartment into the multimedia models because of its relatively smaller canopy volume. It is also uncertain that how the different growth stages of the rice plant affect the overall environmental fate of targeted chemicals.

By reference to conventional works on multimedia models, we have newly set out a promising framework for inclusion of the paddy field compartment in a new multimedia fugacity model, named NIAES-MMM. This model is developed to estimate the long-term fate in global environment of pesticides and POPs emitted from Japan and the whole Asian region. One objective of this paper is therefore to confirm whether the rice plant that generally has only small canopy volume should be considered or not when the paddy field is included in multimedia models, by examining the effects of the rice plant on the environmental fate of pesticides and POPs, such as α-HCH (hexachlorocycrohexane), γ-HCH and PCB-28 (polychlorobiphenyl) based on the computed values of MRC (maximum reservoir capacity) with and without the inclusion of the rice plant. Another objective is to establish a schematic representation of the paddy field and thus detailed scenario expressions on the inter-medium mass transfer processes between air and the rice canopy, when incorporating the paddy field compartment into the NIAES-MMM.

Maximum reservoir capacity (MRC) of the paddy field compartment

Definition of the MRC of the paddy field compartment

The MRC is defined as the ratio of the inventory in an underlying medium (um, such as water, soil and vegetation soil) that contacts with the atmosphere to the inventory in the atmospheric mixed layer at equilibrium, namely, $f_{um} = f_{air}$, as proposed by Dalla Valle et al.[4] (Equation (1)).

$$MRC_{um} = \frac{C_{um}V_{um}}{C_{air}V_{air}} = \frac{f_{um}Z_{um}Ah_{um}}{f_{air}Z_{air}Ah_{air}} = \frac{Z_{um}h_{um}}{Z_{air}h_{air}} \quad \text{............(1)}$$

where, C_{um} and C_{air} are the concentrations in the underlying medium and air, respectively, A is the surface area, h_{air} is the air thickness (assumed to be 1000 m), and h_{um} is the thickness of the underlying medium. MRC > 1 indicates more targeted chemicals are partitioned to the underlying medium than to the air, while, MRC < 1 indicates that the overlying atmosphere contains more chemicals than the underlying layer. In this study, we expressed the paddy field compartment as one box containing three sub-compartments of rice plant (*r*), flooding water (*fw*) and soil (*rs*). These sub-compartments were assumed to be well-mixed, and the soil sub-compartment (*rs*) was further assumed to be composed of soil air (*rs-air*), soil water (*rs-water*) and soil particle (*rs-solid*). By substituting equations described in Figure 1 for equation (1), the variable MRC_{paddy} for the paddy field compartment at a given temperature *T* could be described as equation (2).

$$MRC_{paddy}(T) = 0.0003 \times (\frac{2}{3} \times (0.00615 K_{OA}(T) + 0.5 \times \frac{1}{K_{AW}(T)}) + \frac{1}{3} \times \frac{1}{K_{AW}(T)} + \frac{0.4 VF_r \times K_{OA}(T)}{(1 - VF_r)}) \quad \text{.........(2)}$$

$$Z_{um} = Z_{paddy} = (VF_{rs} Z_{rs} + VF_{fw} Z_{fw} + VF_r Z_r)$$
$$VF_{rs} + VF_{fw} + VF_r = 1$$
$$V_{rs} + V_{fw} + V_r = V_{box}$$
$$h_{um} = h_{paddy} = h_{fw} + h_{rs} + h_r$$
$$Z_{rs} = VF_{rs-solid} Z_{rs-solid} + VF_{rs-water} Z_{water} + VF_{rs-air} Z_{air}$$
$$Z_{rs-solid} = 0.41 m_{oc-soil} K_{OW}(T) \rho_{soil} Z_{air}$$
$$Z_r = m_{oc-rice} K_{OA}(T) Z_{air}$$
$$Z_{fw} = Z_{air} / K_{AW}(T)$$
$$\log K_{OA}(T) = \log K_{OA}(T_{ref}) + \frac{H_{OA}}{2.303 R} \times (\frac{1}{T_{ref}} - \frac{1}{T})$$
$$\log K_{AW}(T) = \log K_{AW}(T_{ref}) + \frac{H_{AW}}{2.303 R} \times (\frac{1}{T_{ref}} - \frac{1}{T})$$

where,

A: paddy field area (m^2), assumed to be 1 m^2

T: temperature of terrestrial environment (K), T_{ref}: reference temperature of terrestrial environment (298K)

V_{rs}, V_{fw}: volumes of paddy field soil and flooding water (m^3), respectively; $V_{rs} = A \times h_{rs}$; $V_{fw} = A \times h_{fw}$

V_r, V_{box}: volumes of the rice plant and total paddy field (m^3), respectively; $V_r = A \times h_r$; $V_{box} = A \times h_{box}$

V_r value at heading time was calculated as 0.33 using the following relationship between the total rice plant volume V_{box} and the total dry weight M: $M = 0.0133 \times V_{box} + 4.62$

VF_{rs}: volume fraction of paddy field soil V_{rs} in total volume of the total paddy field V_{box} (m^3 / m^3)

VF_{fw}: volume fraction of flooding water V_{fw} in total volume of the total paddy field V_{box} (m^3 / m^3)

VF_r: volume fraction of rice plant V_r in total volume of the total paddy field V_{box} (m^3 / m^3)

VF_r value at heading time was computed as 0.03, the values of other times before heading date were respectively assumed to be 0.01 and 0.02 to reflect the seasonal changes of the rice plant

Z_{rs}: bulk Z value of paddy field soil ($mol \cdot m^{-3} \cdot pa^{-1}$), Z_r: Z value of rice plant ($mol \cdot m^{-3} \cdot pa^{-1}$)

Z_{fw}: Z value of flooding water ($mol \cdot m^{-3} \cdot pa^{-1}$), equals to Z value of water

$Z_{rs-solid}$: Z value of solid in the paddy field soil ($mol \cdot m^{-3} \cdot pa^{-1}$)

h_r: length of the rice plant

h_{fw}: depth of the flooding water, 0.1m; h_{rs}: thickness of the paddy field soil, 0.2 m

K_{OW}: octanol-water partition coefficient ($mol \cdot m^{-3} / mol \cdot m^{-3}$), K_{OA}: octanol-air partition coefficient ($mol \cdot m^{-3} / mol \cdot m^{-3}$)

K_{AW}: air-water partition coefficient ($mol \cdot m^{-3} / mol \cdot m^{-3}$)

H_{AW}, H_{OA}: heats of phase transfer between air and water, air and octanol, respectively (J/ mol)

ρ_{soil}: bulk density of paddy soil (kg / m^3), 1500

$m_{oc-soil}$: mass fraction of organic carbon in soil, 0.02; $m_{oc-rice}$: mass fraction of organic carbon in rice plan, 0.4

Fig. 1 Equations and parameters used to estimate the MRC_{paddy} values of the paddy field compartment

Seasonal trends of the MRC_{paddy}

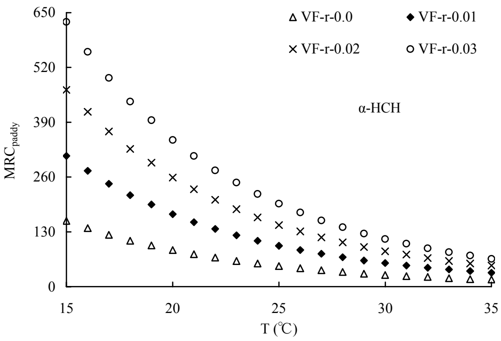

Fig. 2 MRC_{paddy} for α-HCH in paddy field

Based on equation (2), the values of MRC_{paddy} were calculated. As shown in Figure 2 that, for α-HCH at 25 °C, the magnitude of MRC_{paddy} in consideration of the rice plant differed markedly from that without the consideration of the rice plant. And, even for the same rice plant, the values of MRC_{paddy} were also found to differ considerably in accordance with the different growth stages of the plant: a general trend of increases of MRC_{paddy} with the growth of the rice plant was confirmed. Besides this, the MRC_{paddy} was also found to vary markedly with the variation of the environmental temperature. Similar trends were also obtained for chemicals γ-HCH and PCB-28, and for 34 pesticides generally used in paddy fields. It is thus inferable that the rice plant is a very important factor that should be considered when the paddy field is incorporated to the multimedia model, so that to execute reliable prediction of the environmental fate of organic chemicals. As another important finding, the results also suggested that the seasonal change of the rice plant should be reflected in the models when the rice plant is considered.

Scenario description for incorporation of the paddy field compartment into multimedia models

Figure 3 is a schematic illustration of various transport and transformation processes of the targeted chemicals between the paddy field compartment and its surrounding media, such as air and water when the paddy field is considered in the multimedia model. Of all parameters appeared in Figure 3, since the parameters of D_{AR}, D_{RA}, $D_{AP\text{-}D}$, $D_{AP\text{-}R}$ and $D_{deg\text{-}r}$ devised for reflecting the primary transport and degradation processes between air and the paddy field undergo large changes in time as a result of the seasonal change of the rice canopy, the methodologies for definition of their values are thus described here in details; while the descriptions for the remaining parameters including G_{in}, G_{out} and $D_{deg\text{-}fw}$ are omitted.

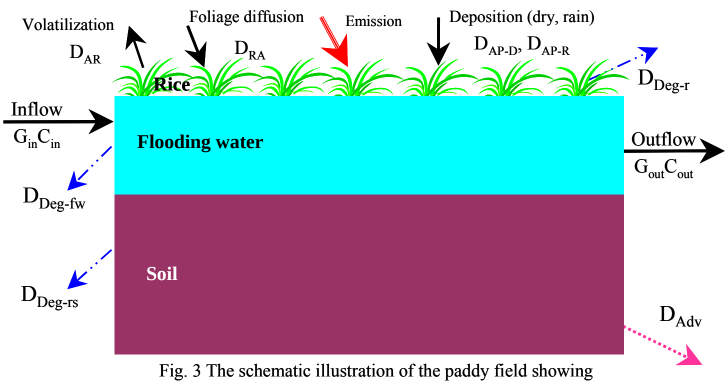

Fig. 3 The schematic illustration of the paddy field showing transport and transformation processes

Table 1 Equations used to calculate D values for processes related to rice canopy

Process		Equation
chemical evaporation from foliage		$D_{RA}=A_P v_{D\text{-}G} Z_A$
foliar uptake of chemical from the atmosph	foliage diffusion	$D_{AR}=A_P v_{D\text{-}G} Z_A$
	dry deposition	$D_{AP\text{-}D}=A_P v_{D\text{-}P} v_Q Z_Q$
	wet deposition	$D_{AP\text{-}R}=A_P frU_P U_R Z_{rain}$, $Z_{rain}=1/H + Qv_Q Z_Q$
chemical degradation in foliage		$D_{deg\text{-}r}=Z_P V_R k_R$

Descriptors

A_P: paddy field area; V_R : rice volume.
$v_{D\text{-}G}$ (m/h) : dry gaseous deposition velocity. $v_{D\text{-}Gmax}$: 5 (summer), $v_{D\text{-}Gmin}$: 2 (winter).
$v_{D\text{-}P}$ (m/h) : dry particle deposition velocity. $v_{D\text{-}Pmax}$: 1.71 (summer), $v_{D\text{-}Pmin}$: 1.03 (winter).
frU_P: interception loss,
v_Q: volume fraction of aerosols, 2×10^{-12}.
U_R (m/h) : rain rate, 0.85 m/y.
Q: particle scavenging ratio by precipitation, 68000.

The complete descriptions of the five D-values mentioned above are summarized in Table 1. Environmental variables related to the wet deposition parameter of $D_{AP\text{-}R}$, for example, the rain rate U_R, the particle scavenging ratio Q, the interception loss frU_P and the volume fraction of aerosols in air v_Q, do not affect the environmental behavior of chemicals, as indicated by previous results of sensitivity analysis, so their values were assumed by referencing to existing materials[1,2,5] and are summarized in Table 1. On the other hand, since gaseous and dry particle-bound deposition velocities of $v_{D\text{-}G}$ and $v_{D\text{-}P}$ used for estimation of D_{RA} and D_{AR}

demonstrate a significant seasonal change as shown (Figure 4a), the minimum and maximum values of these two parameters were adopted (Table 1) as was done by Wania et al[5]. For the rice volume V_R, a remarkable change of its magnitude over the seasons was also displayed (Figure 4b). We thus take it as a product of the area A_R occupied by the rice plant vegetation with the length of the rice plant.

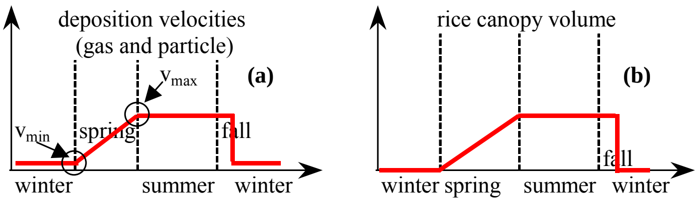

Fig. 4 Schematic diagram of the seasonal change of the volume of the rice canopy V_R and the deposition velocities to the rice canopy. During summer, values are maximum. Spring values are derived from liner interpolation beteen winter and summer values.

Rice plant area A_R

According to Shibata et al.[6], an exponential relationship existed between the coverage ratio, defined as the rice plant area A_R divided by the ground area A_P, and the leaf area index (LAI). Because LAI could be obtained from satellite data, the rice occupation area A_R at different growth steps can be readily and reasonably estimated.

Length of the rice plant

As reported by Sasaki et al.[7], the length of the rice plant is the sum of the plant length of no transplanting or the rice plant length after being transplanted at arbitrary times and the extended amount of the plant length *PLER* (*n*) (cm) after *n* days from the initial measurement date. *PLER* (*n*) was found to be affected by the highest temperature T_{max} and the lowest temperature T_{min} of every day, and could be simply computed using the following equations.

$$PLER(n) = [ERH(n) + ERL(n)]/2 \qquad (PLER \geq 0)$$

$$ERH(n) = ERT_S + a[T\max(n) - T_S] + b[T\max(n) - T_S] \quad (if \quad T\max \geq T_S \quad then \quad b = 0, if \quad T\max < T_S \; then \quad a = 0)$$

$$ERL(n) = ERT_S + a[T\min(n) - T_S] + b[T\min(n) - T_S] \quad (if \quad T\min \geq T_S \quad then \quad b = 0, if \quad T\min < T_S \; then \quad a = 0)$$

where, *ERH* and *ERL* are the plant length extension speeds (cm/day) at the highest temperature and the lowest temperature, respectively. ERT_S is the plant length extension speed at the temperature T_S, of the conversion point, and *a* and *b* refer to the temperature coefficients (cm /day /°C).

Conclusions

The incentives for incorporating the paddy field compartment in the new multimedia model "NIAES-MMM" were discussed. Since the rice plant sub-compartment is shown to have a significant effect on the environmental fate of targeted chemicals, the scenario description for incorporation of the paddy field compartment in multimedia models was established, and needed equations and parameters for undertaking calculations related to the incorporation of the rice plant were suggested. In coming research, parameters that describe the air-rice canopy mass transfer processes are to be refined so as to generate more reliable estimations for the environmental fate of concerned chemicals.

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