Predicting Methyl Iodide Emission, Soil Concentration, and Pest Control in a Two-Dimensional Chamber System

Lifang Luo,* Scott R. Yates, and Daniel J. Ashworth

Due to ever-increasing state and federal regulations, the future use of fumigants is predicted on reducing negative environmental impacts while offering sufficient pest control efficacy. To foster the development of a best management practice, an integrated tool is needed to simultaneously predict fumigant movement and pest control without having to conduct elaborate and costly experiments. The objective of this study was (i) to present a two-dimensional (2-D) mathematical model to describe both fumigant movement and pest control and (ii) to evaluate the model by comparing the simulated and observed results. Both analytical and numerical methods were used to predict methyl iodide (MeI) transport and fate. To predict pest control efficacy, the concentration-time index (CT) was defined and a two-parameter logistic survival model was used. Dose–response curves were experimentally determined for MeI against three types of pests (barnyardgrass [*Echinochloa crus-galli*] seed, citrus nematode [*Tylenchulus semipenetrans*], and fungi [*Fusarium oxysporum*]). Methyl iodide transport and pest control measurements collected from a 2-D experimental system (60 by 60 cm) were used to test the model. Methyl iodide volatilization rates and soil gas-phase concentrations over time were accurately simulated by the model. The mass balance analysis indicates that the fraction of MeI degrading in the soil was underestimated when determined by the appearance of iodide concentration. The experimental results showed that after 24 h of MeI fumigation in the 2-D soil chamber, fungal population was not suppressed; >90% of citrus nematodes were killed; and barnyardgrass seeds within 20-cm distance from the center were affected. These experimental results were consistent with the predicted results. The model accurately estimated the MeI movement and control of various pests and is a powerful tool to evaluate pesticides in terms of their negative environmental impacts and pest control under various environmental conditions and application methods.

Due to the potential to pollute air, water, and soil resources, the use of pesticides has been strictly regulated to protect public and environmental health. Since 2005, only three fully registered chemical fumigants have been brought to the market place. Under federal and state regulations, pesticide application has to achieve efficient pest control while having fewer negative environmental effects (UNEP, 2006). For highly volatile pesticides (e.g., fumigants), emission to the atmosphere is the most important process adversely affecting human and environmental health. Numerous efforts have been made to reduce fumigant emission into the atmosphere using various application methods such as less-permeable films, surface irrigation, deep injection, and the addition of organic matter and ammonium thiosulfate (e.g., Gan et al., 1998; Yates et al., 2003; Gao et al., 2008; Ashworth et al., 2009). The optimum fumigant dose is one that has the least human and environmental health risks while offering sufficient pest control. However, few studies have been done that examine fumigant emission and pest behavior simultaneously (Wang and Yates, 1999). It would be ideal but practically impossible to conduct laboratory and field experiments to determine the pesticide transport and pest survivability for every soil, pesticide, cultural management practice, application method, and environment condition.

Process-based mathematical models can be cost-effective and powerful alternatives to expensive laboratory and field experiments. Simulation models have been successfully used to determine fumigant transport, fate, and the influences of different emission reduction methods and environmental factors (Jury et al., 1984; Wang et al., 2007; Yates et al., 2002; Yates, 2006; Ha et al., 2009). Numerous computer programs such as CHAIN-2D (Šimunek and van Genuchten, 1994), HYDRUS 1/2/3-D (Šimunek et al., 2006), SOLUTE (Yates, 2006), and DripFume (Wang et al., 2007) are able to simulate volatile pesticide transport while coupling water and heat transport processes. These models include a description of the volatilization process and are capable of simulating a volatile surface boundary condition. When soils are relatively homogeneous due to deep plowing and fumigants are applied to relative dry soil (e.g., for hot-gas and shank fumigation), water movement and chemicals carried by water can be ignored since gas-phase transport is the dominant process. For such cases, an analytical solution has been developed to estimate

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*Corresponding author (lifang.luo@ars.usda.gov).
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5585 Guilford Rd., Madison, WI 53711 USA

L. Luo, S.R. Yates, and D.J. Ashworth, U.S. Salinity Lab., 450 W. Big Springs Rd., Riverside, CA 92507; L. Luo, Dep. of Environmental Sciences, Univ. of California, Riverside, CA.
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Abbreviations: 1,3-D, 1, 3-dichloropropene; 2-D, two-dimensional; CT, concentration-time index.

the fumigant volatilization rate to air, concentration and degradation in soils, and concentration-time index (CT) by simplifying the governing equations (Yates, 2009).

While many programs are available to predict fumigant fate and transport, few peer-reviewed research studies exist that predict pest control after pesticide application. Wang et al. (2004) numerically simulated 1, 3-dichloropropene (1,3-D) transport and pest control efficacy under different soil types, bed shapes, and application depths and rates using a concentration-time exposure index. However, the model was not validated because of a lack of experimental data. Logistic dose–response curves have been used to describe the mortality of organisms at different concentration-time levels (i.e., the integral of concentration over time) (Becker et al., 1998; Hutchinson et al., 2000), but these studies did not include model simulations. However, even with the same dose or application rate, pesticide concentration in soil varies with different application methods, procedures, soil properties, and environmental conditions. Some emission reduction methods, such as the addition of organic matter, tend to increase soil degradation and lower emissions from the soil surface but may lead to reduced concentration and pest control efficacy in the amended soil layer. Therefore, after application, pesticide concentrations in the soil have to be determined to predict the mortality kinetics of soil-borne pests.

A new and easy-to-use tool is needed to simultaneously predict pesticide transport, fate, and pest control to help growers apply new and improved fumigation methods into their operations without conducting elaborate and costly experiments. The objectives of this study were (i) to present a 2-D mathematical model to describe fumigant volatilization, degradation, resident concentration, and pest survivability in soils and (ii) to evaluate the model by comparing the results from prediction and measurement.

Materials and Methods

Simulation Model

For a volatile organic compound (VOC), the 2-D governing equation to simulate vapor diffusion, liquid dispersion, degradation, partitioning in soils is

$$\eta\frac{\partial C_g}{\partial t}+\theta\frac{\partial C_l}{\partial t}+\rho_b\frac{\partial C_s}{\partial t}=\frac{\partial}{\partial x}[D_g\frac{\partial C_g}{\partial x}+D_l\frac{\partial C_l}{\partial x}-q_xC_l] \\ +\frac{\partial}{\partial z}[D_g\frac{\partial C_g}{\partial z}+D_l\frac{\partial C_l}{\partial z}-q_zC_l]-\eta\mu_gC_g-\theta\mu_lC_l-\rho_b\mu_sC_s \quad [1]$$

where C_g, C_l, and C_s are gas-, liquid-, and solid-phase concentrations (μg mL^{-1}), respectively; D_g and D_l are liquid- and gas-phase diffusion coefficients (cm^2 s^{-1}), respectively; μ is a first-order degradation coefficient (s^{-1}); θ, ρ_b, and η, respectively, are water content (cm^3 cm^{-3}), bulk density (g cm^{-3}), and air content (cm^3 cm^{-3}); q is the Darcian flux density; and the subscripts: l, s, and g indicate liquid-, solid-, and gas- phases, respectively.

The partitioning is assumed to obey the following relationships:

$C_g = K_HC_l$ Henry's law, liquid-gas partitioning [2]

$C_s = K_dC_l$ equilibrium adsorption,liquid-solid partitioning [3]

where K_H is the Henry's law constant (dimensionless) and K_d is the linear equilibrium sorption coefficient (cm^3 g^{-1}). Volatilization at the soil–atmosphere boundary is described as

$$(D_e\frac{\partial C_l}{\partial z}-qC_l)\bigg|_{Z=0}=h(C_g-C_{air})\bigg|_{Z=0} \quad [4]$$

where h is a mass transfer coefficient (cm s^{-1}), C_{air} is gas concentration in the atmosphere (μg mL^{-1}), and $D_e = D_l + K_HD_g$ is effective dispersion coefficient (cm^2 s^{-1}).

The total concentration, C_T, is defined as

$$C_T=\theta C_l+\eta C_g+\rho_bC_s=R_sC_s=R_lC_l=R_gC_g \quad [5]$$

where R_s, R_l, and R_g are retardation coefficients of solid, liquid, and gas phases, respectively. According to Eq. [5], Eq. [1] and [4] can be rewritten as

$$\frac{\partial C_T}{\partial t}=D_e\frac{\partial^2C_T}{\partial x^2}+D_e\frac{\partial^2C_T}{\partial z^2}-\mu_TC_T \quad [6]$$

$$\frac{\partial C_T}{\partial z}\bigg|_{Z=0}=\frac{h_e}{D_e}C_T(x,0,t)\quad \text{with } C_{air}=0 \text{ and } q=0 \quad [7]$$

where $h_e = (h/R_g)$ is effective mass transfer coefficient (cm s^{-1}).

When water movement can be neglected, analytical solutions to Eq. [1] and [4] are possible. The analytical solution for fumigant transport in a 2-D vertical plane can be obtained from multiplying the solutions to the associated 1-D problems (Yates, 2009):

$$C_T(x,z,t)=C_x(x,t)C_z(z,t) \quad [8]$$

An advantage of analytical solution is that simple relationships for some transport quantities can be obtained. For example, using analytical solution, the total volatilization can be written as (Yates, 2009)

$$\text{Total volatilization}=\frac{C_0h_ee^{-\frac{-z_0\sqrt{\mu}}{\sqrt{D_e}}}}{h_e+\sqrt{D_e}\sqrt{\mu}} \quad [9]$$

where C_0 is the applied mass (μg cm^{-1}) and z_0 is the depth of fumigant application. The analytical solution of concentration at a certain point and time, $C(x,z,t)$, volatilization fluxes, and total CT were also derived by Yates (2009).

To quantitatively evaluate organisms' exposure to pesticides, a concentration-time index, CT, the integral of concentration over time, is defined as

$$\mathrm{CT}(t)=\int_0^tC_T(x,z,t)\mathrm{d}t \quad [10]$$

A logistic dose–response curve was used to describe the relationship between organism mortality, y, and CT:

$$y=\frac{100\%}{1+\left(\mathrm{CT}/\mathrm{CT}_{50}\right)^{-b}} \quad [11]$$

where b is the slope at the inflection point of the logistic curve and CT_{50} is the effective CT required to give a 50%

of mortality. Fitting Eq. [11] to experimental measurements was conducted using SigmaPlot version 10.0 (Systat Software Inc., Point Richmond, CA).

Application to Experimental Data and Model Parameters

The model accuracy was tested using the data for MeI movement and pest control determined in a 2-D chamber system. The 2-D soil chamber with a surface-mounted flux chamber was 60 cm wide, 60 cm long, and 6 cm thick. The soil type used was a Milham sandy loam (fine-loamy, mixed, superactive, thermic Typic Haplargids), consisting of 60% sand, 30% silt, 10% clay, and 2.5% organic matter content. The soil with a water content of 7.9% by weight was mixed thoroughly with fungi (*F. oxysporum*)-infested millet seeds (*Panicum miliaceum*), barnyardgrass seeds (*E. crus-galli*), and citrus nematode (*T. semipenetrans*)-infested roots, as described below. Methyl iodide was injected into the center of the 2-D soil chamber at an application rate of about 56.4 kg ha^{-1}. Methyl iodide volatilization rates were determined by pulling air in the flux chamber using a vacuum and collecting MeI in the air flow using the charcoal filters at the outlet. Spatial and temporal distributions of soil gas-phase concentration were determined by drawing soil air samples using gas-tight 100-μL syringes. Methyl iodide degradation was determined by measuring iodide concentration in the soil at different positions in the chamber after 24 h. The survivability of three pest types, after 24 h of exposure, was also determined. A detailed discussion of experimental conditions and protocols is provided by Luo et al. (2010).

The parameters of the experimental conditions and simulation models are listed in Table 1. The first-order degradation rate constant was 0.0779 h^{-1} (Luo et al., 2010). Henry's constant, K_H, was 0.22 at 23°C according to a reported value of 0.21 at 21°C (Gan and Yates, 1996). The binary gas diffusion coefficient, D_{ab}, was estimated using Fullar correlation (Reid et al., 1987). The soil gas diffusion coefficient, soil liquid diffusion coefficient, and solid-, liquid-, and gas-phase retardation coefficients were calculated as described by Jury et al. (1983). For a volatile boundary condition, stagnant boundary layer theory with a boundary layer thickness (b) of 0.5 cm was used to calculate the mass transfer coefficient (h) (Jury et al., 1983):

$$h = \frac{D_g^{air}}{b} \qquad [12]$$

where D_g^{air} is the binary gas diffusion coefficient in the air. The other three boundaries were described as nonflow boundary:

$$\left.\frac{\partial C_T}{\partial x}\right|_{x=0} = \left.\frac{\partial C_T}{\partial x}\right|_{x=L} = \left.\frac{\partial C_T}{\partial z}\right|_{Z=F} = 0 \qquad [13]$$

where L and F are the width and depth of the 2-D soil chamber. The volatilization fluxes, concentration in the soil, degradation, and CT were calculated using the analytical solutions (Yates, 2009) and the numerical solutions in Hydrus 2-D version 2.05 (Šimunek et al., 1999).

Dose–Response Measurements

The response of three types of pests (barnyardgrass seed, citrus nematode, and fungi) to MeI were determined by using a stainless steel cell (10 cm i.d., 8 cm in depth in total). This device has two gas sampling ports and allows fumigant injection and gas-phase concentration measurement in real time. A detailed description of the test cells was given in Papiernik et al. (2001). *Fusarium oxysporum* was incubated on millet seeds following the method introduced by Ma et al. (2001a). The citrus nematodes were collected from the citrus roots of an infested orchard at the University of California, Riverside Citrus Research Center. The barnyard grass seeds were purchased from Valley Seed Service, Fresno, CA. Thirty millet seeds, 100 barnyardgrass seeds, or 15 g of citrus nematode–infested roots were thoroughly mixed with 107.9 g of soil (Milham sandy loam) with a soil water content of 7.9% by weight and placed in the cell. The cell was well sealed with epoxy resin (Permalite Plastics Corp., Costa Mesa, CA) and aluminum tape, a configuration that has been shown to be gas-tight (Papiernik et al., 2001).

A preliminary experiment was conducted for each organism to determine the concentration range that would lead to a range of 0 to 100% mortality. The survivability of citrus nematodes was tested at initial MeI concentrations of 0.0, 0.6, 1.8, 2.6, 3.9, 5.8, 7.7, 9.8, 1.3.5, 19.3, 27.0, and 38.6 μM. The response of barnyardgrass seeds to MeI was tested at initial concentrations of 0.0, 6.4, 12.7, 21.2, 42.4, 63.6, 84.8, 106.6, 148.4, and 190.7 μM. The response of fungi to MeI was tested at initial concentrations of 0.0, 134.9, 168.6, 202.3, 236.0, 269.7, 303.5, 337.1, 404.6, 472.0, 539.5, and 674.3 μM. Two replicates were used at each concentration. After MeI injection, the gas samples were measured at least six time points during the 24-h fumigation using a gas-tight syringe. After 24 h, the chambers were opened under a hood. The barnyardgrass seeds and millet seeds were quickly picked from the soil. Citrus nematodes were extracted using a Baermann funnel method (Viglierchio and Schmitt, 1993). Ten millet seeds were placed onto a potato dextrose agar (PDA) media in a petri dish at 22°C. The growth of fungi was monitored daily, and the millet seeds colonized with fungi were counted after 5 d. The

Table 1. The parameters of experimental conditions and simulation model.

Parameters	Value
Bulk density, ρ_b	1.34 g cm^{-3}
Water content, θ	0.11 cm^3 cm^{-3}
Porosity, ϕ	0.49
Air content, θ_a	0.38
Organic matter content, f	2.50%
Temperature, T	23°C
Sorption coefficient, K_d	0.1 cm^3 g^{-1}
Degradation rate constant, u	0.0779 h^{-1}
Henry's constant, K_H	0.22
Binary gas diffusion coefficient, $D_{G,air}$	377.18 cm^2 h^{-1}
Binary liquid diffusion coefficient, $D_{L,water}$	0.12 cm^2 h^{-1}
Soil gas diffusion coefficient, D_G	64.65 cm^2 h^{-1}
Soil liquid diffusion coefficient, D_L	0.00003 cm^2 h^{-1}
Effective soil diffusive coefficient, D_e	43.84 cm^2 h^{-1}
Retardation coefficient of gas, R_g	1.47
Retardation coefficient of water, R_l	0.32
Retardation coefficient of solid, R_s	3.24
Boundary layer thickness, d	0.5 cm
Effective mass transfer coefficient, h	511.46 cm h^{-1}
Mass applied	37620 μg cm^{-1}

germination of 81 barnyardgrass seeds placed in a petri dish containing a moist blotter was tested at 22°C, and germinated seeds were counted after 5 d. The degradation rate constant was determined by fitting the first-order kinetic equation to the concentration data. Based on the first-order kinetic equation, a degradation-corrected CT was calculated for each MeI application rate.

Results and Discussion

Prediction of Methyl Iodide Transport and Fate

The observed and predicted MeI volatilization fluxes from the soil surface to air are shown in Fig. 1. The predicted volatilization fluxes using both the analytical method and numerical method showed a very similar pattern to that experimentally determined. The MeI volatilization flux increased rapidly until around 3 h (Fig. 1). After this, the flux decreased gradually. The peak fluxes were 1289, 1272, and 1359 μg min^{-1} for the observed value and predicted values by the analytical method and numerical method, respectively. Total volatilizations estimated by the analytical and numerical methods were about 28.3 and 29.7% of the total applied mass, respectively, close to the measured value (28.9%). Overall, both methods predicted the behavior of MeI volatilization. The fraction of total emission was lower than the value reported in the literature (78% for nontarped application after 20 d; Gan et al., 1997) partially due to the higher degradation rate in the soil studied. The differences were also due to geometry of the experimental systems. When water movement can be neglected, despite the same soil, application rate, and environmental conditions, the concentration gradient in a 2-D system (e.g., this study) is approximately radial, leading to a greater fumigant dissipation in the lateral direction, thus a lower fraction of total emission than that in a 1-D system (e.g., Gan et al., 1997) where the concentration gradient is approximately vertical and vertical movement of fumigant is dominant.

The simulation model also predicted the soil gas-phase concentrations in terms of its spatiotemporal distribution despite some discrepancies between the two sets of data. Only the simulated results from the analytical method are shown here (Fig. 2). Compared to the simulation predictions, observed MeI dissipated slightly more rapidly during the first 3.5 h but more slowly afterward. The discrepancy could be caused by several factors. For example, to simulate fumigant transport, the degradation rate constant determined from the batch experiment (Luo et al., 2010) was used for the whole domain in the 2-D soil chamber. The experimental condition in the batch experiment may not fully represent that in the 2-D soil chamber even with the same soil, application rate, and temperature since MeI concentration in the 12-mL vials for the batch experiment is relatively homogenous shortly after injection, whereas MeI concentration varied dramatically in the 2-D soil chamber during the experiment (Fig. 2). The degradation rate constant is also affected by initial concentration (Ma et al., 2001b). Some discrepancy could be partially due to the sampling time. It still took about 6 min to sample 49 ports from the center to outer. To map and compare the measured and simulated soil gas-phase concentration at a certain time, we assumed the time was the same for all the 49 ports. This could result in the

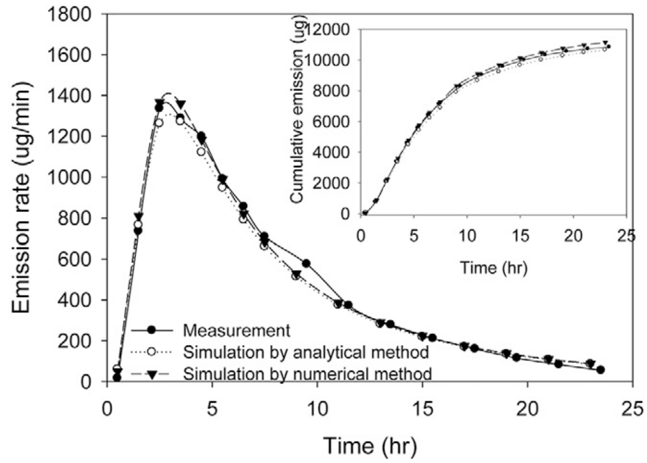

Fig. 1. The observed and simulated MeI emission rate and cumulative emission from the soil surface (with a surface area of 60 cm^2).

higher concentration in the soil chamber (Fig. 2). In addition, the experimental measurements are subject to error and uncertainty caused by possible blockage of the syringe needles, even with side opening to avoid it, which could lead to the nonsymmetrical and erratic contours (Fig. 2). Similar to total volatilization, the observed and simulated values of MeI residue in the soil after 24 h were consistent, about 6.8% of applied mass.

On the basis of the prediction results, more than 60% of applied MeI degraded within 24 h, about 20% greater than the observed value (43.6%) (Table 2). About 79.3% of applied mass was recovered by experimental measurement of volatilization, degradation, and residue (Table 2). According to the comparison between the predicted and observed results, the observed MeI degradation in the soil was probably underdetermined and mainly contributed to the uncovered mass (20.7%). When MeI is exposed to the light, generation of I_2 (gas) is possible (Gan and Yates, 1996). Besides possible photodegradation, the high variation of the measured iodide concentration distribution might also lead to experimental uncertainty (Luo et al., 2010). Yates et al. (1996) reported that drastic variation of the bromide concentration after shank injection in a field study led to the high uncertainty in determining MeBr degradation ratio. They suggested that a large number of samples was required to reduce the uncertainty and increase accuracy of the results. The above mass balance analyses are helpful to examine the experimental uncertainty and accuracy when both measured and simulated results are available.

Dose–Response Curves of Methyl Iodide against Barnyardgrass Seed, Fungi, and Citrus Nematode

Figure 3 shows the dose–response curves of barnyardgrass seed, citrus nematode, and fungi. Citrus nematodes immediately responded to low concentration of MeI. According to the fitted equation (r = 0.99), the CT_{50} of citrus nematodes was 13.1 μg h mL^{-1}. More than 90% control of citrus nematodes was reached when the CT was >40 μg h mL^{-1}. The mortality was slightly underestimated when the CT > 30 μg h mL^{-1}. The CT_{50} for barnyardgrass seeds was estimated to be 185.9 μg h mL^{-1}. A CT > 400 μg h mL^{-1} was needed to completely control barnyardgrass seeds. Fungi (*F. oxysporum*) were not influenced by MeI until the CT > 500 μg h mL^{-1}.

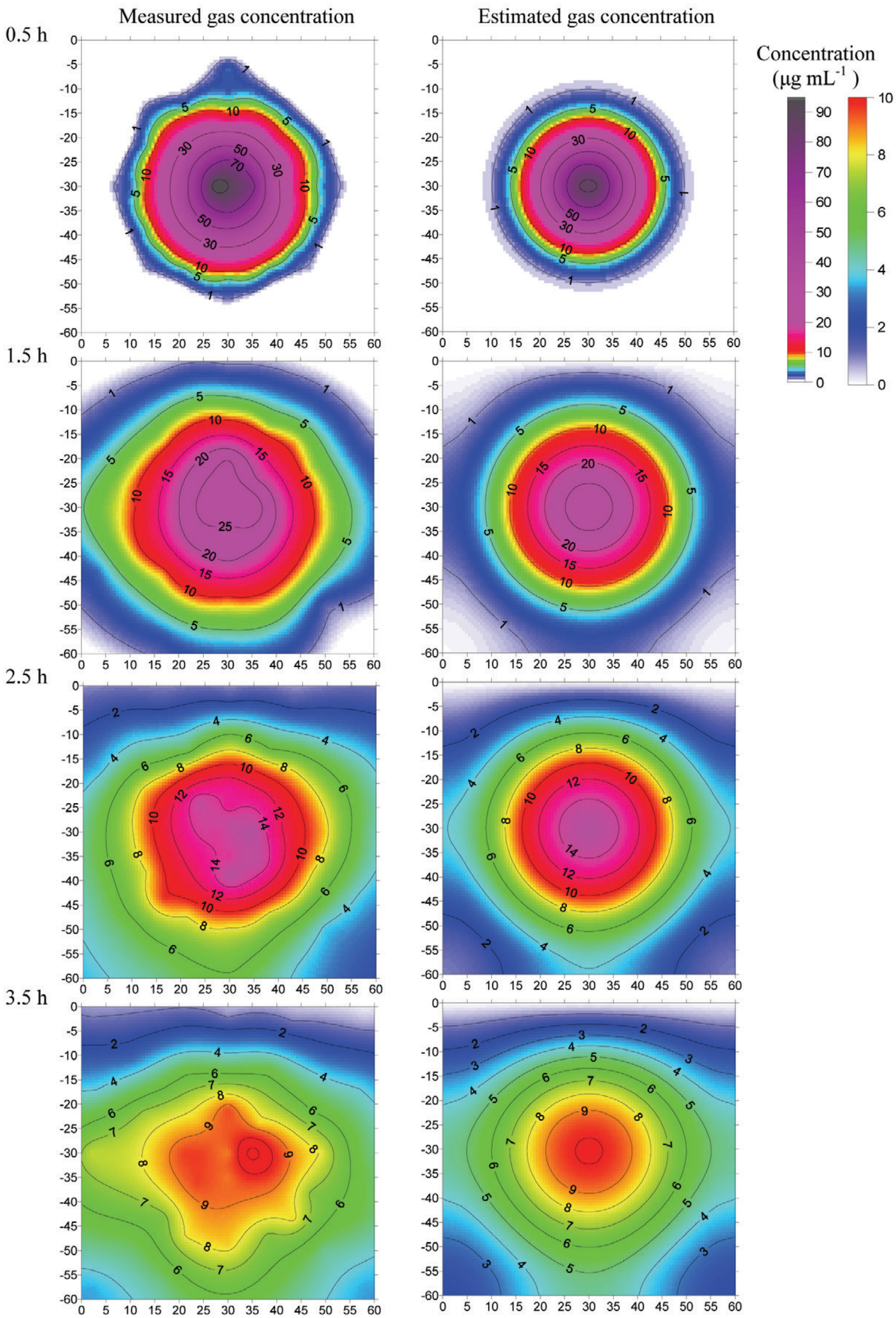

Fig. 2. The observed and estimated (by the analytical method) spatial distribution of MeI gas-phase concentration (μg mL^{-1}) over time in the soil (60 × 60 cm).

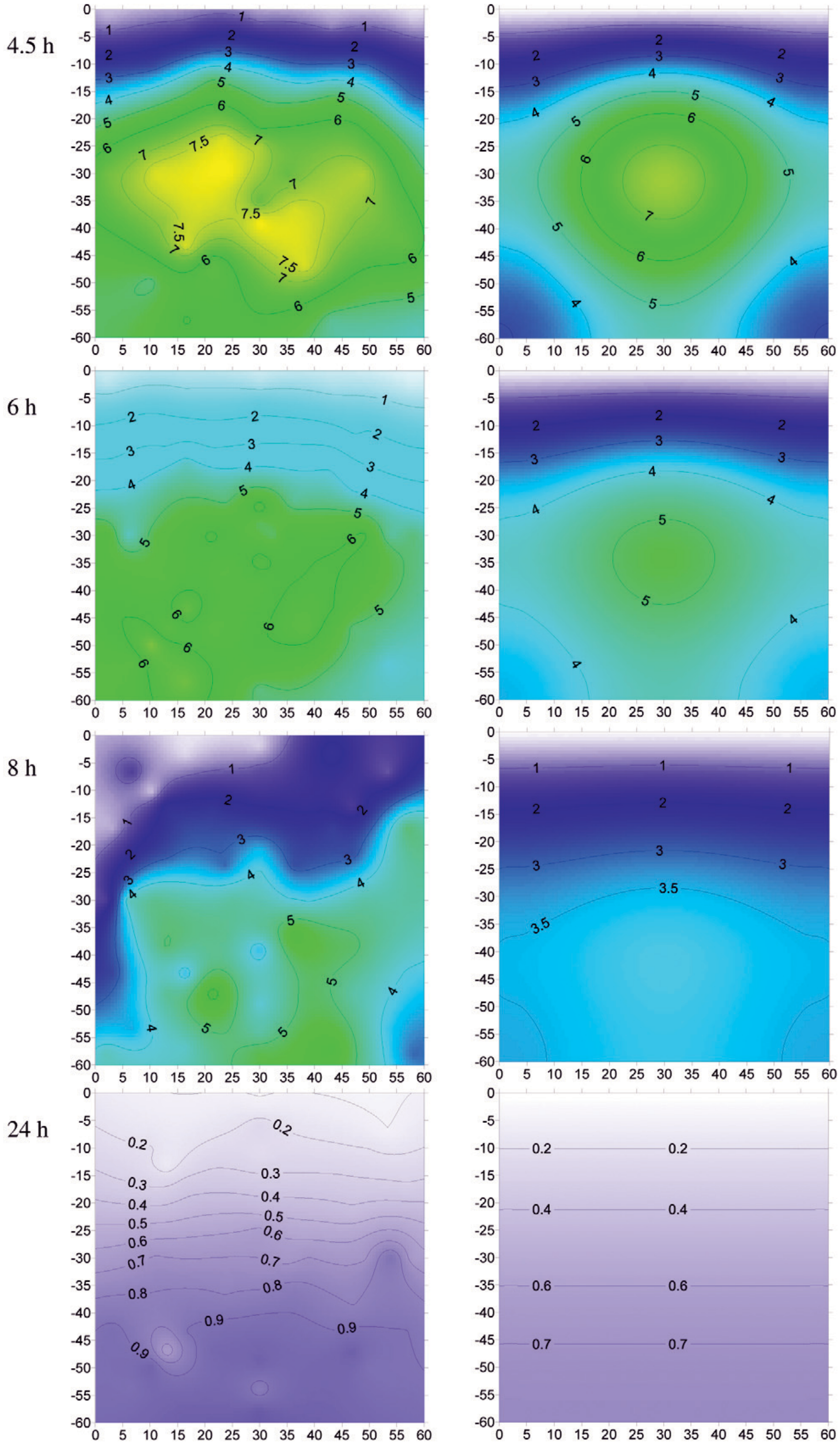

Fig. 2. Continued.

The mortality increased rapidly until the CT > 1000 μg h mL^{-1} and a CT of 1500 μg h mL^{-1} was required to obtain full control of *F. oxysporum*. The CT_{50} of *F. oxysporum* was 1194.6 μg h mL^{-1}, similar to the value (~1012 μg h mL^{-1}) from Hutchinson et al. (2000). The fitted curve for *F. oxysporum* underestimated the mortality when CT was around 800 μg h mL^{-1} and 1400 μg h mL^{-1}. The goodness-of-fit could contribute to the discrepancy between the observed and simulated pest mortality in the 2-D soil chamber. In short, dose–response curves indicate that MeI can control citrus nematodes when dosage is relatively low (CT > 70 μg h mL^{-1}) and can control barnyardgrass seeds if the CT is > 400 μg h mL^{-1}. But a high application rate of MeI is required to control *F. oxysporum.*

Prediction of the Responses of Barnyardgrass Seed, Fungi, and Citrus Nematode after Methyl Iodide Fumigation

As expected, the maximum CT was about 900 μg h mL^{-1} at the application point (Fig. 4). The CT decreased rapidly to about 155 μg h mL^{-1} at a radius of 10 cm and gradually decreased toward the outer of the soil chamber. The CT was lowest near the soil surface (<20 μg h mL^{-1}) due to the volatilization. Based on the dose–response curve (Fig. 3) and estimated CT distribution (Fig. 4) within the soil, the mortality distributions for three types of pests were estimated and compared with the measured values.

The estimated mortalities of citrus nematodes were consistent with those of the measured values for most of the area within the 2-D soil chamber except for the area close to the soil surface (Fig. 5); that is, more than 90% of citrus nematodes were killed in the soil chamber. However, overall, the measured mortalities of citrus nematodes were greater than the simulated values, especially in top 15-cm soils. As mentioned above, one possible reason for the discrepancy was that the fitted dose–response curve used in the simulation underestimated the measured mortality when the CT was >30 μg h mL^{-1}. These results confirm that MeI is an excellent nematicide on previous studies (Becker et al., 1998).

All of *F. oxysporum* in the soil chamber survived after fumigation. This was consistent with the measured dose–response curve. *Fusarium oxysporum* was not influenced until the CT was >500 μg h mL^{-1}. The application rate of MeI was not sufficient to kill *F. oxysporum.* Previous studies also showed that, generally, *F. oxysporum* is difficult to control with fumigants (Minuto et al., 1999; Hutchinson et al., 2000; Ma et al., 2001a). The combination of chloropicrin and MeI is necessary to improve the efficacy on fungi such as *F. oxysporum* (Hutchinson et al., 2000).

The measured and simulated mortalities of barnyardgrass seeds also had a similar pattern. Around the injection point, >80% of the barnyardgrass seeds were controlled by MeI (Fig. 6). The mortality of barnyardgrass seeds decreased rapidly with the distance to the center due to the rapid decline in the CT. When the radius was about 10 cm, the mortality was about 40%. Few seeds were influenced by the applied MeI when the radius was >20 cm. However, similar to *F. oxysporum*, the mortality of barnyardgrass seeds was slightly underestimated throughout the whole chamber. At the regular rate (about three times greater than the MeI rate applied in this study), the weeds should be better controlled.

Table 2. Mass balance analyses for MeI transport and fate.

Method	Volatilization	Degradation	Residue	Total
	%			
Measured	28.9	43.6	6.8	79.3
Simulated (analytical)	28.3	64.9	6.8	100
Simulated (Hydrus)	29.7	63.8	6.5	100

Summary and Conclusions

New reduced-emission methods have been proposed to reduce human and environmental health risks. However, little has been known about their effects on pest control efficacy. Due to high cost, it may not be practical to obtain this information experimentally for long-term field testing. To assist in this activity, new and easy-to-use tools are needed to help integrate new and improved fumigation methods into agricultural operations. The motivation of this study was to describe a 2-D mathematical model that simulates volatile pesticide transport including volatilization, degradation, and resident concentration as well as pest control.

We tested the model accuracy by comparing the predicted and measured fumigant transport, fate, and pest control using the data collected from a 2-D system. The models provided good estimations of MeI volatilization and soil gas-phase concentration in the soil. The total emission ratio was 28.9, 28.3, and 29.7% according to the measurement, the analytical simulation method, and the numerical simulation method, respectively. Mass balance analysis showed that the uncertainty was involved to determine the degradation by measuring the iodide concentration produced in the soil and was possibly due to MeI photodegradation and experimental error. Conducting a mass balance, especially coupled with simulation models, helps to examine the accuracy and uncertainty of experimental measurements. Similarly, the model estimated reasonably well the mortalities of the three types of pests with different levels of sensitivity to MeI. The estimated and simulated results were consistent within the 2-D soil chamber: more than 90% of citrus nematodes were controlled for most of the area; more than 40% of barnyardgrass seeds were controlled at 10-cm distance from the injection point; the dose was too low to control fungi. Compared with the measured results, the mortality tended to be underestimated in this study.

The above results demonstrate that the model described in this study has great potential as a predictive tool to evaluate the different pesticides in terms of their environmental impacts

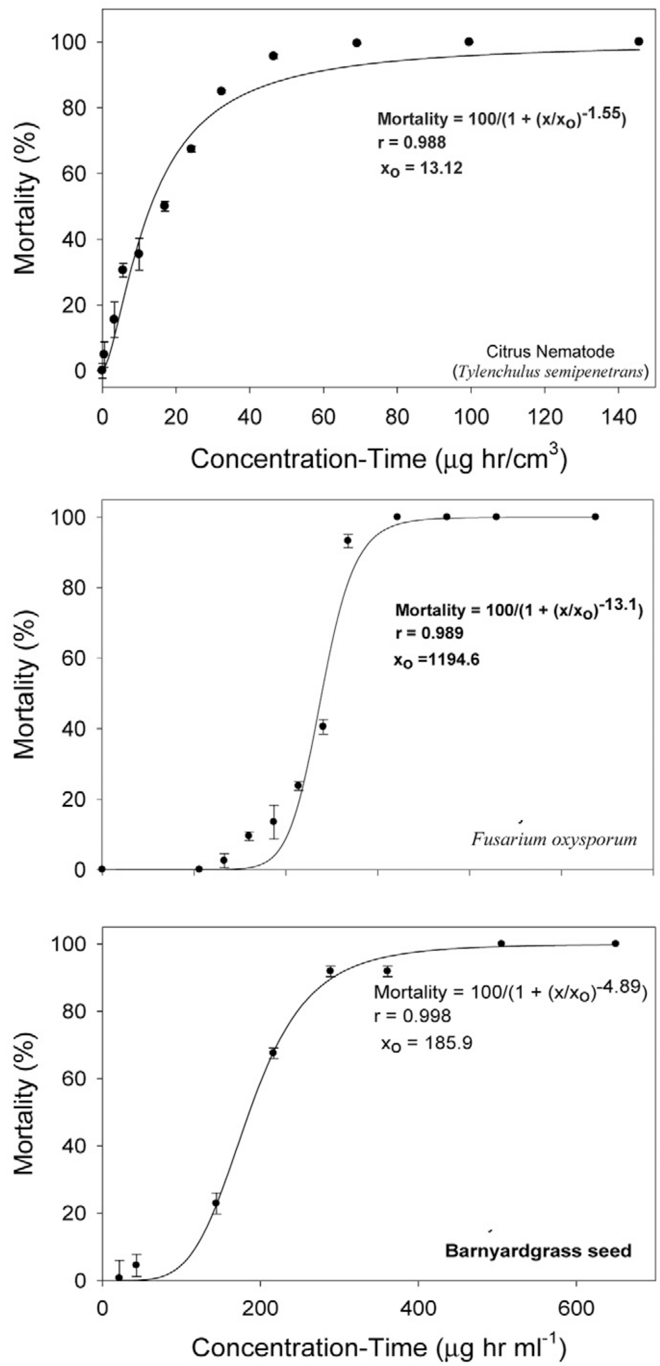

Fig. 3. The response curves of citrus nematodes, barnyardgrass seeds, and fungi (*F. oxysporum*) to MeI fumigation after 24 h.

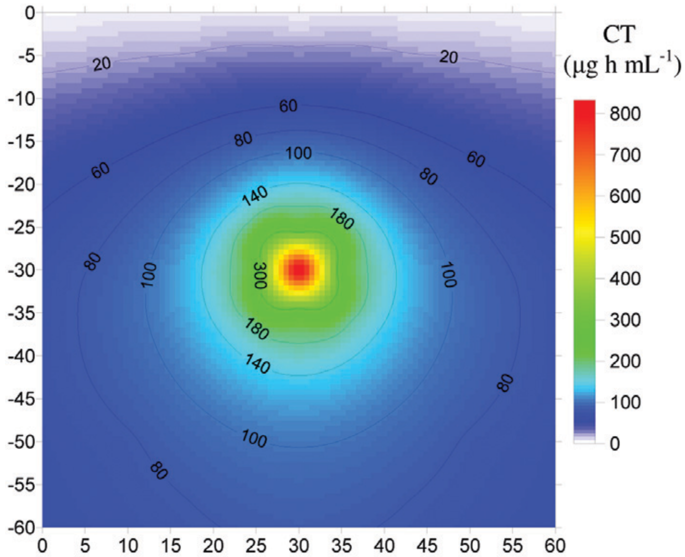

Fig. 4. The estimated spatial distribution of MeI concentration-time index (CT) in the soil (60 × 60 cm) after MeI injection for 24 h (by the analytical method).

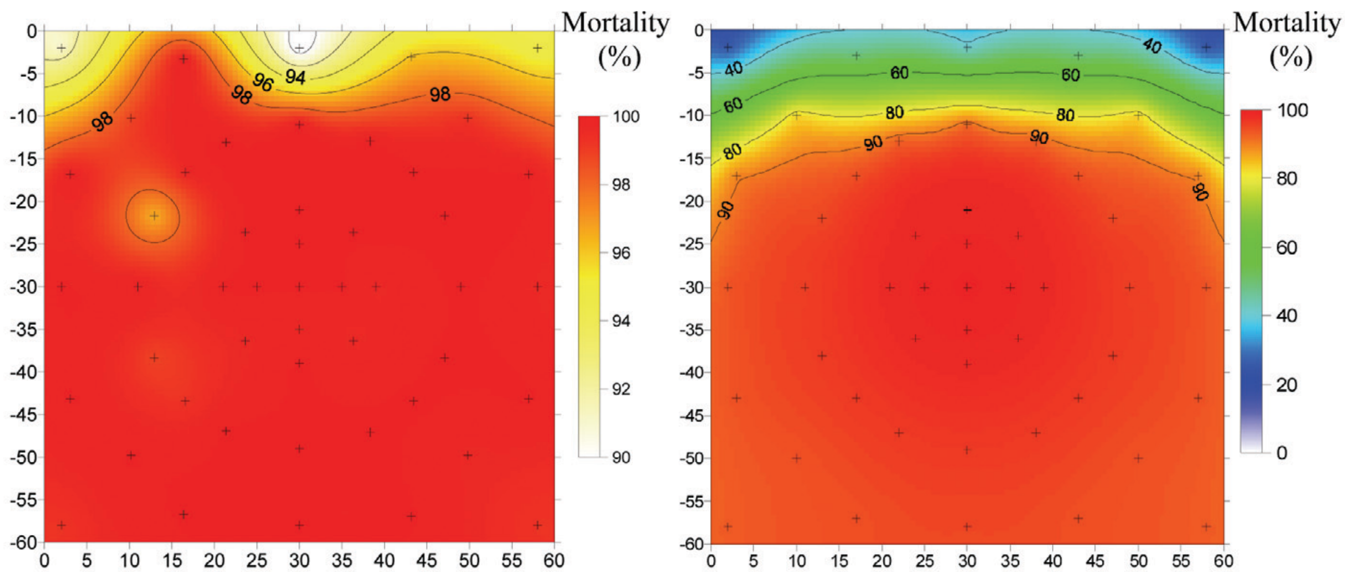

Fig. 5. The observed (left) and simulated (right) spatial distribution of citrus nematode mortality (%) in the soil (60 × 60 cm) after MeI fumigation for 24 h.

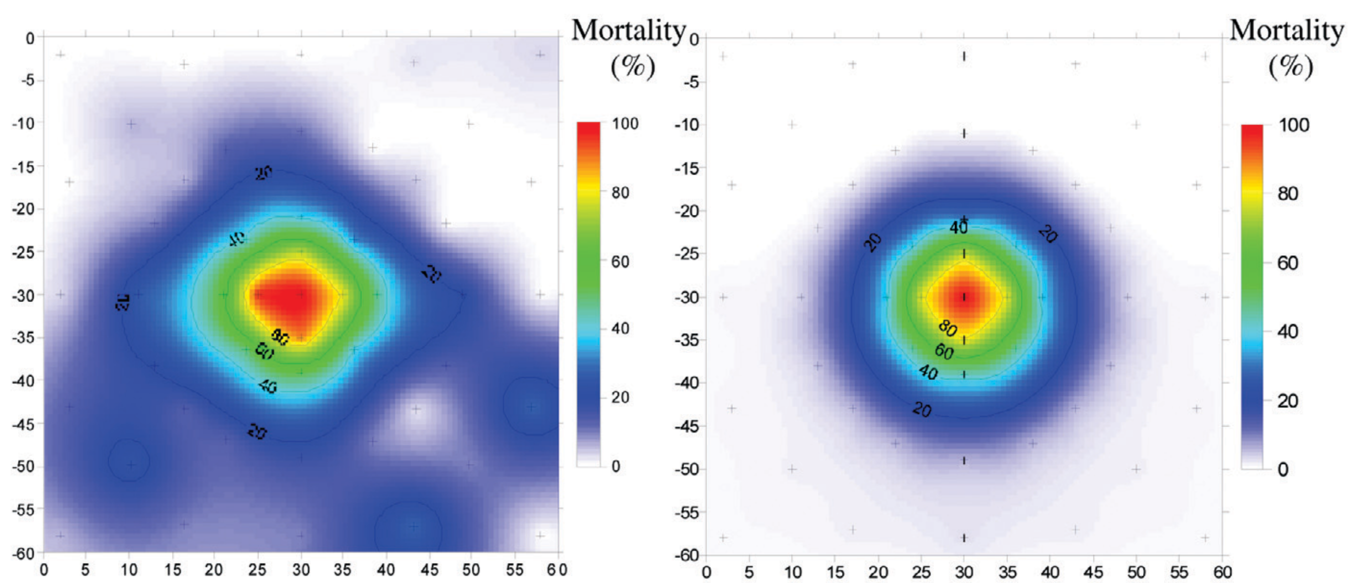

Fig. 6. The observed (left) and simulated (right) spatial distribution of barnyardgrass seed mortality (%) in the soil (60 × 60 cm) after MeI fumigation for 24 h.

and pest control under various environmental condition and application methods. When water movement can be neglected, that is, when soil is relatively dry and homogenous, the analytical solution provides an accurate prediction of fumigant transport and it is also easier to use, compared with the numerical method. Otherwise, the numerical solution is available in some computer programs such as HYDRUS 1/2/3-D (Šimunek et al., 2006). Soil and pesticide properties such as degradation rate, Henry's constant, sorption coefficient, and gas diffusion coefficient (listed in order of sensitivity; Ha et al., 2009) are needed for predicting fumigant transport and fate. To predict pest control, the dose–response curve of the soil pest organism is essential. For fumigants, the concentrations in gas, liquid, or solid phase are quite different. The mode of action is also different for various pathogens and weeds (Allaire et al., 2004). We believe that the use of the same type of concentration for prediction as used for the dose–response curve is necessary to get accurate prediction.

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