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DripFume: A Visual Basic program for simulating distribution and atmospheric volatilization of soil fumigants applied through drip irrigation

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Abstract

A Windows-based graphical user interface program (DripFume) was developed in MS Visual Basic (VB) to utilize a two-dimensional multi-phase finite element pesticide transport model to simulate distribution and emission of volatile fumigant chemicals when applied through drip irrigation or shank injection. The program provides an intuitive user interface by linking databases with default soil and chemical properties to predict subsurface distribution patterns and surface volatilization losses of soil fumigants under selected field configurations and application regimes. The interface program was configured to simulate up to three chemicals simultaneously to accommodate the need of fumigation with multiple chemicals. Physical and chemical properties of *cis*- and *trans*-isomers of 1,3-dichloropropene and chloropicrin for a typical medium-textured soil were given as default values in the model input. Properties of other soil fumigants can be easily substituted as input options during program initialization. A database containing transport properties of 12 soil groups (from clay to sand) were created in DripFume as selectable sets of input values. Substitution is also allowed if properties of an individual soil are known. The VB output includes a normalized run-time volatilization flux display and selections in post-processing using MS Excel linked by VB. Output options from the post-processing VB/Excel program include data and graphs of cumulative volatilization loss, volatilization flux density, concentration profile by time for a selected location or by location for selected lapsed times after fumigant application. Although there are still limitations in selectable field configurations, the program should be useful in helping pesticide specialists, farm managers, or policy makers to optimize the depth, rate, and duration of fumigant application to achieve the highest possible distribution uniformity and the lowest volatilization loss.
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1. Introduction

Application methods and procedures of most established pesticides are usually strictly enforced according to federal and state regulations. The goal of pesticide use and its related regulatory requirements is to achieve effective pest control while protecting people and the environment from unintended exposures. In addition to laboratory and field experimentation, process-based computer models and simulation programs have long been used to help determine the

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relative importance of different chemical, environmental, and managerial factors that affect the efficacy and environmental impact of pesticide use (Jury et al., 1983). However, most of these process-based pesticide models are developed for scientists and engineers who are well-trained and experienced in computer programming and numerical modeling. There is a strong need to create programs that can provide an intuitive user interface to help pesticide specialists, farm managers, or policy makers who are less experienced in computer programming to fully utilize the pesticide models in selecting the best pesticide management strategies. A solution is to use recently introduced visual programming tools such as MS Visual Basic (VB) to develop graphical user programs to interface with the often complicated process models for general users. These process models are often written in other programming languages (e.g., C, FORTRAN) for computational efficiency. Visual programming provides a set of screens, object buttons, scroll bars, and menus. An intuitive visual interface program would greatly increase the usability of the research-grade pesticide models.

Soil fumigants are a special group of volatile pesticides that tend to function and be dispersed in the subsurface soil primarily through vapor phase diffusion. A major environmental concern of soil fumigation is volatilization losses to the atmosphere (Yates et al., 1997). Applying soil fumigant chemicals by (surface or subsurface) drip irrigation has an advantage over the conventional shank injection since the drip tapes may be installed and buried prior to chemical application. For chemicals with high water solubility, co-dispersion with irrigation water provides an additional means of fumigant distribution, which may help to increase the effectiveness in pest control. Field experiments and modeling studies have demonstrated the potential of drip chemigation for improving distribution uniformity and reducing volatilization loss of fumigant 1,3-dichloropropene (Wang et al., 2001) and the non-volatile insecticide imidacloprid (Leib and Jarrett, 2003).

The objective of this research was to develop an intuitive user interface program in Visual Basic to utilize a pesticide transport model to simulate distribution and volatilization of soil fumigants when applied through subsurface drip irrigation in bedded field configurations or the traditional flat fields.

2. The pesticide model

The pesticide model was modified from a generic two-dimensional finite element code CHAIN_2D, a public domain free program from the U.S. Salinity Laboratory (Simunek and van Genuchten, 1994), tailored for simulating fumigant fate and transport in the soil and volatilization into the atmosphere. Briefly, a governing equation is used for computing fumigant transport in unsaturated subsurface soil in both solution and gaseous phases. The model assumes non-equilibrium interaction between the solution and adsorbed concentrations, and equilibrium interaction between the solution and gaseous concentrations. A linear relationship was used for chemical partition between the three phases. Degradation was considered in the solution and adsorbed phases, but not in the air, using a first-order decay having the same rate constant.

3. The graphical Visual Basic program

A main requirement in developing the graphical interface program was to streamline the simulation process, including: (1) generating the input files for typical raised-bed field configurations, irrigation rates, and chemical application rates, (2) model execution and monitoring the output results, and (3) graphically presenting the simulation results for further assessment and management decisions. The key outputs are fumigant distribution patterns, concentration, and duration in the treated soil zone, and total cumulative emission loss to the atmosphere. Concentration distribution over space, time, and phases is a highly dynamic process determined by factors such as application history, water content, soil porosity, and fumigant vapor pressure and diffusivity (Leistra, 1970). Modeling is one of the most efficient ways of quantifying the distribution dynamics.

3.1. Input selections

The interface program starts with a main opening screen consisting of a series of input and output selections.

3.1.1. Application method and field configuration

Application method is the first selection for input options. Two choices are available: (1) drip irrigation, (2) shank injection. Shank injection was included for comparison with the subsurface drip irrigation method. Under drip irrigation,

Table 1
Available options for application method, field configuration, and depth of application

Application method and field configuration[a]	Application depth (cm)					
	2.5	7.6	15.2	20.3	30.5	45.7
Drip irrigation						
Flat surface	X	X	X	X	X	X
101.6 cm bed	X	X	X	X	X	X
106.7 cm bed	X	X	X	X	X	X
203.2 cm bed	X	X	X	X	X	X
Shank injection						
Flat surface					X	X
101.6 cm bed					X	X

[a] For drip irrigation, the flat surface contains one drip line placed at 203.2 cm spacing. The 101.6 and 106.7 cm bed systems also each contains one drip line placed below bed center. The 203.2 cm bed system contains two drip lines: one located 30.5 cm to the left and one at 30.5 cm to the right of the bed center. For shank injection, the flat surface has a 25 cm shank spacing, and the 101.6 cm bed receives injection below bed center.

four field configurations can be selected: a flat surface, 101.6 cm (40 in.), 106.7 cm (42 in.), or 203.2 cm (80 in.) wide bed, with the spacing referring to the center-to-center distance between beds or drip lines. Six possible depth selections are 2.5 cm (1 in.), 7.6 cm (3 in.), 15.2 cm (6 in.), 20.3 cm (8 in.), 30.5 cm (12 in.), or 45.7 cm (18 in.) for both lines. The flat surface is included for potential vineyard or orchard applications. One drip line is used and placed at 203.2 cm (80 in.) spacing. Again, there are six possible depth selections at 2.5 cm (1 in.), 7.6 cm (3 in.), 15.2 cm (6 in.), 20.3 cm (8 in.), 30.5 cm (12 in.), and 45.7 cm (18 in.). There is an option for selecting up to two soil layers for the model simulation. Under shank injection, two field configurations can be selected: 101.6 cm (40 in.) wide bed or a flat surface. Injection can be made directly below the bed center at 30.5 cm (12 in.) or 45.7 cm (18 in.) depth. A total of 28 grid files were created to facilitate selections for the application method, field configuration, and the depth of application (Table 1).

3.1.2. Soil hydraulic properties

One soil type can be selected for each soil layer for each simulation run. Arithmetic means of hydraulic properties of all 12 soil series (i.e. clay, silt, silty clay, clay loam, silty clay loam, sandy clay, sandy clay loam, silt loam, loam, sandy loam, loamy sand, and sand) were obtained from the literature data sets (Carsel and Parrish, 1988) and assimilated in a database format in DripFume as selectable sets of input values. The input soil parameters are residual and saturation water content, hydraulic conductivity under saturation, the α and n parameters used in describing the water retention and hydraulic conductivity functions, and soil bulk density. Substitution is allowed if some or all of the parameters of an individual soil are known.

3.1.3. Chemical properties

Up to three chemicals can be simulated simultaneously with the current program configuration. The user can choose any combination of one, two, or three chemicals in a simulation run. Physical and chemical properties of

Table 2
Fate and transport parameters of three selected soil fumigants used in DripFume as default values[a]

Fumigant	D_g (cm^2 day^{-1})	K_d (cm^3 g^{-1})	K_h [b]	μ (day^{-1})
E-1,3-D[c]	7199	0.30	0.056	0.087
Z-1,3-D[c]	7182	0.30	0.037	0.053
CP[d]	6684	0.73	0.103	0.346

[a] E-1,3-D = *cis*-isomer of 1,3-dichloropene, Z-1,3-D = *trans*-isomer of 1,3-dichloropene, CP = chloropicrin, D_g = diffusion coefficient in gaseous phase, K_d = adsorption coefficient, K_h = dimensionless form of Henry's constant or the ratio between gaseous and solution phase concentrations, μ = degradation coefficient.
[b] K_h values may be updated in the future using new experimental data.
[c] Data from Leistra (1970), Van Dijk (1980), and Wolt et al. (1993).
[d] Data from Dow AgroSciences (1997) and Gan et al. (2000).

the *cis*- and *trans*-isomers of 1,3-D and chloropicrin for a typical medium-textured soil are given as default values in the model input (Table 2). The chemical parameters are diffusion coefficients in air and water, Henry's constant, and adsorption and degradation coefficients for soil layers 1 and 2, respectively. Because drip irrigation is the targeted method of application, chemical concentration in the solution phase or irrigation stream is also required. These chemical parameters for other soil fumigants or in different soils can be substituted, as an input option dur-

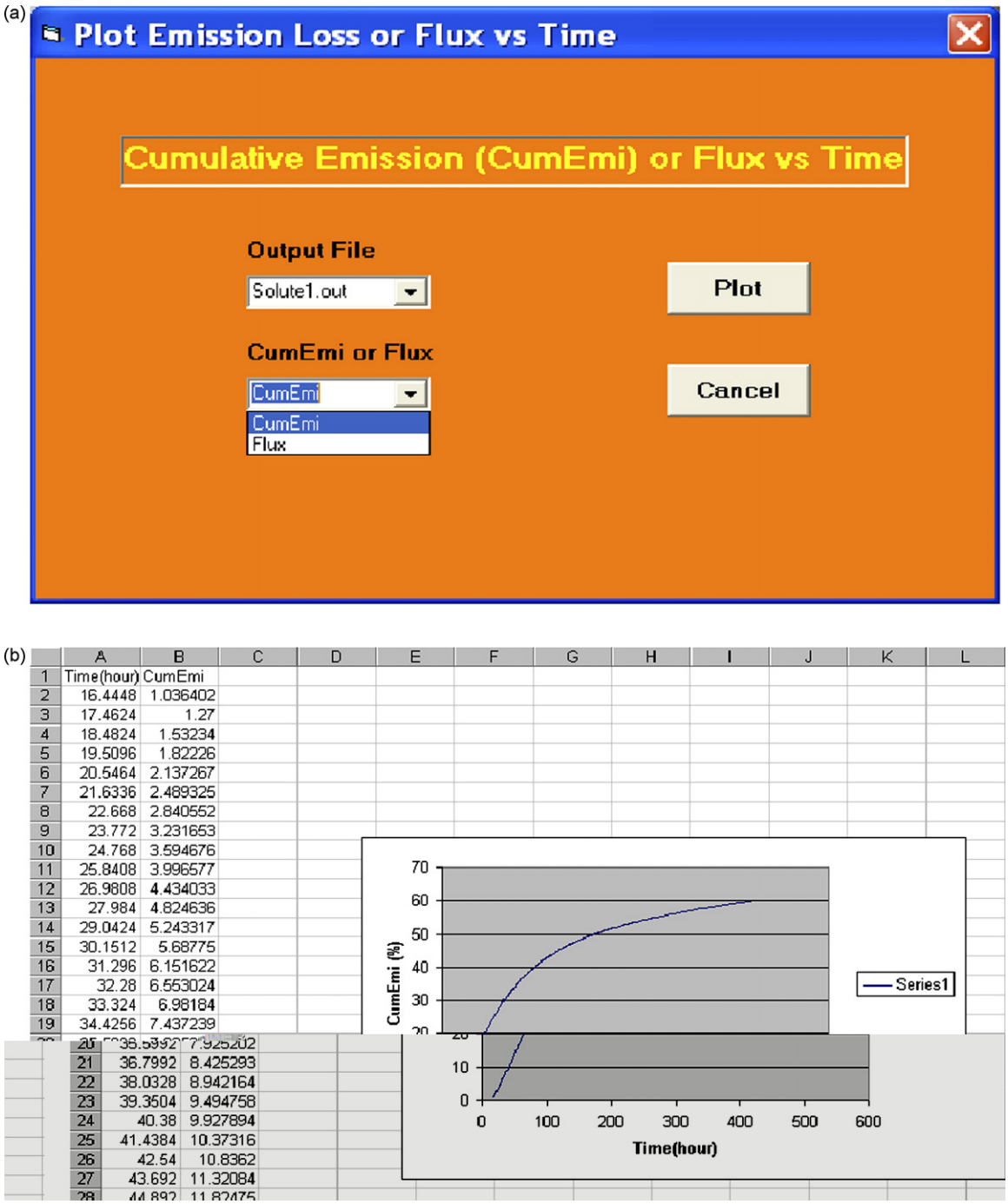
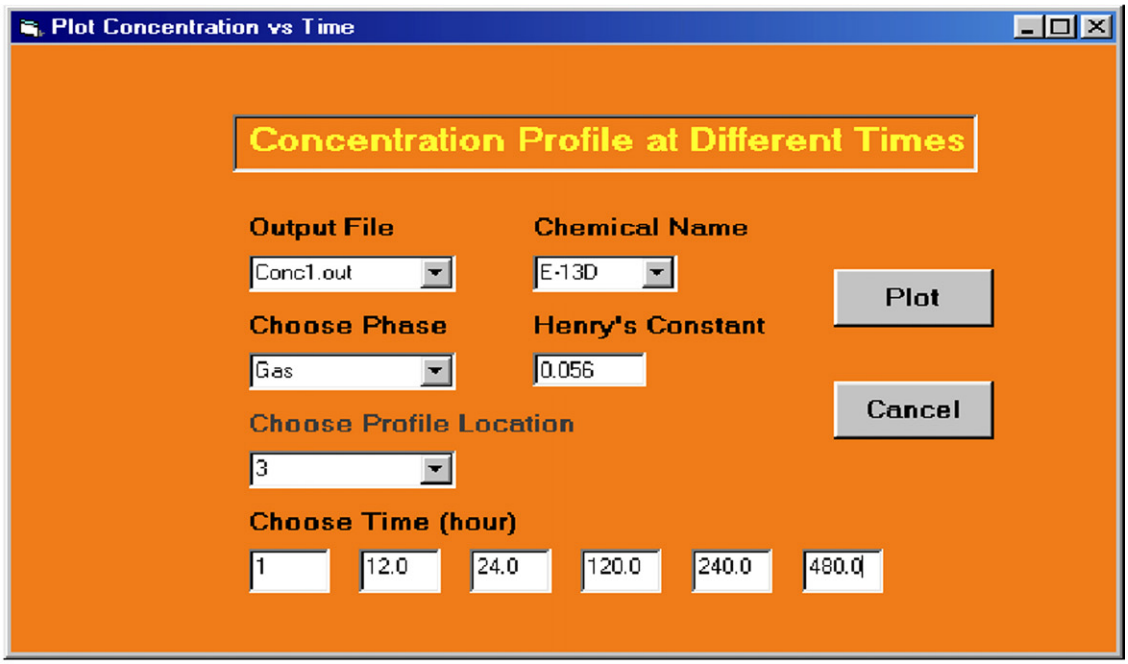


Fig. 1. Post-processing (a) screen selection of cumulative emission or emission flux, and (b) automated Excel display of cumulative volatilization loss over time.

integrated over the entire surface and displayed with a built-in automated program using Excel (Fig. 1b). This is a very useful measure for the potential fumigant loss through surface volatilization. Volatilization flux density is calculated as the mass of fumigant lost per unit surface area per unit time. This is an important variable for describing the volatilization dynamics. If total volatilization is a major concern, the above management options can be optimized to reduce the volatilization loss. The user has the option of plotting each chemical at a time for either the cumulative volatilization or the flux.

(a)



(b)

	A	B	C	D	E	F	G	H	I	J	K	L
	Tageted T	4	16	24	120	240	480	hour				
	Found T	4.8744	14.7072	19.6344	117.9024	238.1448	473.9904	(T1,T2,T3,T4,T5,T6)				
	Y (cm)	Concentration,		X =	33.8	cm						
		4.9	14.7	19.6	117.9	238.1	474.0					
	0	0.00131	0.013776	0.026684	0.017416	0.004575	0.001579					
	1	0.013513	0.147286	0.346371	0.300714	0.074866	0.024702					
	2	0.02599	0.28756	0.682545	0.585273	0.145393	0.047886					
	3	0.038948	0.440737	1.0479	0.870313	0.216076	0.071148					
	4	0.052623	0.614438	1.451005	1.155179	0.28681	0.09445					
	5	0.067082	0.816379	1.897028	1.439161	0.357498	0.11779					
	6	0.082393	1.05285	2.38829								
	7	0.098442	1.328018	2.92511								
	8	0.114559	1.64369	3.50571								
	9	0.130116	1.998909	4.12520								
	10	0.14434	2.389604	4.77544								
	11	0.156402	2.808081	5.44562								
	12	0.165536	3.241919	6.1217								
	13	0.171125	3.674787	6.7860								
	14	0.172754	4.086555	7.41911								
	15	0.170218	4.455629	8.00018								
	16	0.163621	4.759731	8.50722								
	17	0.153418	4.977051	8.91913								
	18	0.140409	5.090394	9.21632								
	19	0.125625	5.087824	9.38198								
	20	0.110146	4.964574	9.40411								
	21	0.094942	4.723617	9.27563								
	22	0.080724	4.376602	8.99603								
	23	0.067906	3.944007	8.57283								
	24	0.056644	3.452417	8.020426	5.422654	1.5197	0.538826					

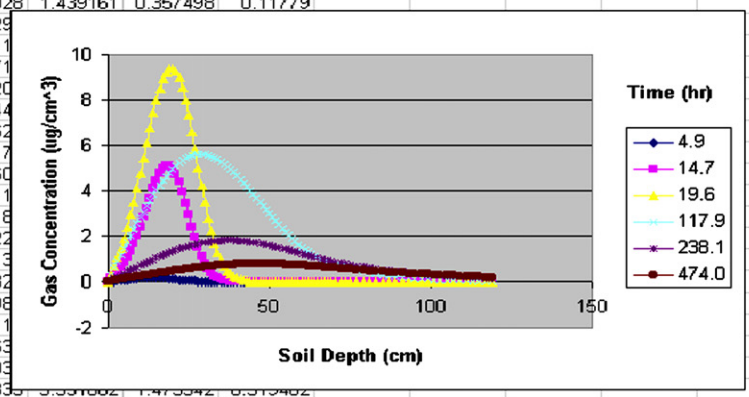


Fig. 3. Display of gaseous phase fumigant distribution at elapsed times after application: (a) screen selection of targeted times and (b) automated Excel display of gaseous phase concentrations over soil depth.

3.2.2. Concentration profiles

For each fumigant case selection, five vertical cross-sections have been pre-selected according to distribution symmetry and log-distance from the fumigant source. A schematic is shown for the 106.7 cm (42 in.) bed configuration to illustrate the profile locations (Fig. 2). For each cross-section, 100 profiles at different lapsed times after application are saved for both solution and gas phase concentrations. After choosing which chemical to display, the user can select

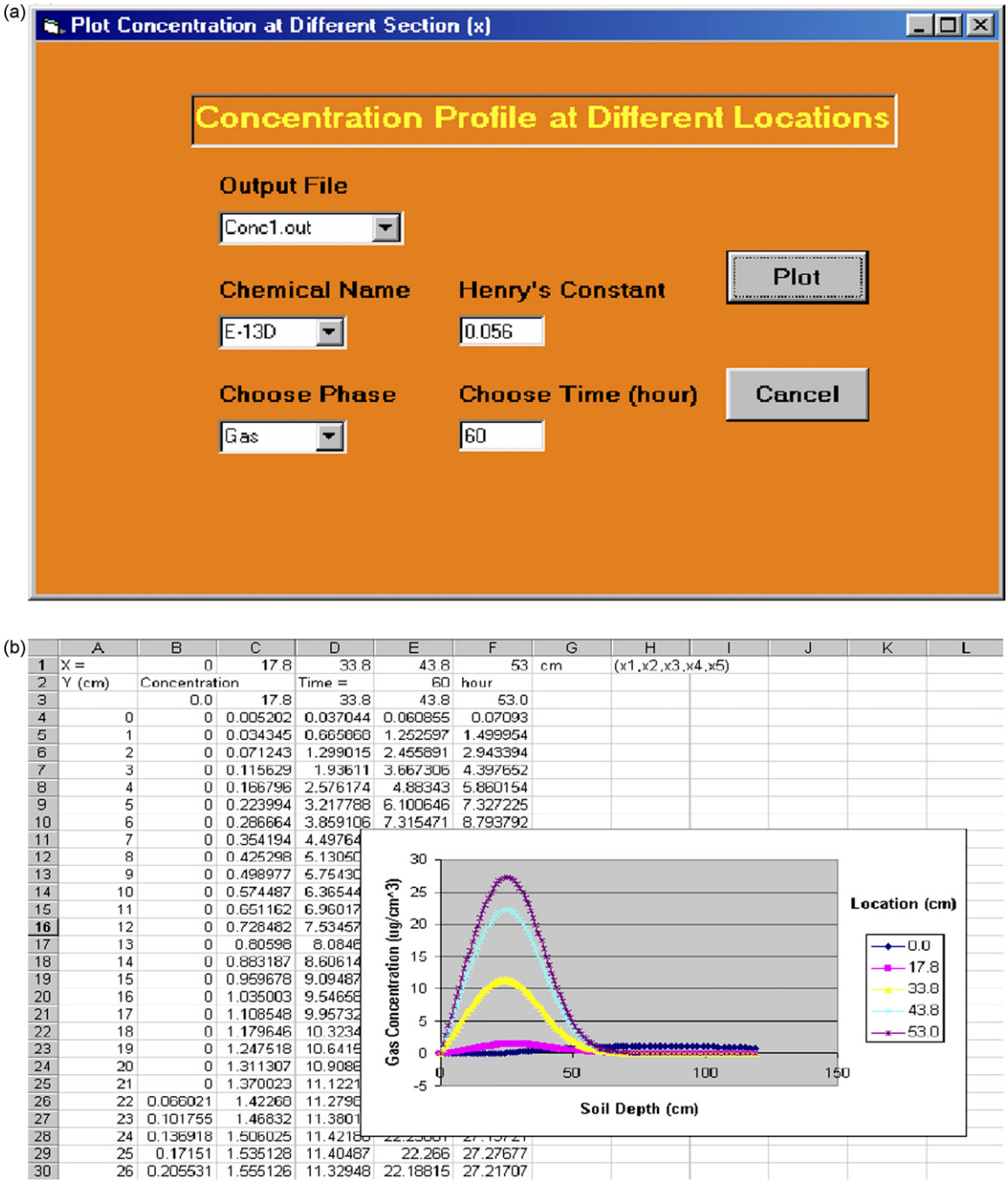


Fig. 4. Display of gaseous phase fumigant distribution at multiple locations from the source at selected times after application: (a) screen selection of targeted time and (b) automated Excel display of gaseous phase concentrations over soil depth.

to plot for either the solution phase or gas phase concentration profiles (Fig. 3a). Up to six times can be plotted on the same graph for each cross-section, and the program can internally find the nearest output time to plot the graph, which is automatically displayed in Excel (Fig. 3b). In addition to concentration profiles by elapsed times for a selected location, concentrations can also be plotted by profile location for one selected lapsed time after application (Fig. 4a and b). Therefore, the output options can provide an assessment for the spatial and temporal distributions of soil fumigants. This helps to determine the distribution uniformity in the soil. In addition to the pre-formatted graphical outputs, the output data files are saved in Excel format, so the users can further process the raw data to create other graphical presentations that fit the users' specific needs.

4. Testing the Visual Basic program

A main function of the graphical interface program is to generate input files that would otherwise be manually created for the pesticide model. The steps of generating these input files are specially designed for fumigant application by subsurface drip irrigation. Comparisons indicated that exactly the same input parameters and data format were created using either the interactive graphical interface program or manual preparation (Wang et al., 2004). Limitations on some of the soil parameters are inherent in the original code of the pesticide model, and the graphical interface program improved the pesticide model by providing warnings on parameter selections before model execution. The output selections were also tested by manually processing the raw data from model output. Exactly the same graphs were produced using the automated interface program.

5. Conclusions

A graphical user interface program was developed in Visual Basic to simulate distribution and volatilization of soil fumigants when applied through subsurface drip irrigation. The program provides an intuitive user interface by linking databases with default soil and chemical properties to predict subsurface distribution patterns and potential surface volatilization losses of soil fumigants under selected field configurations and application regimes. The output includes a normalized run-time volatilization flux display and concentration profiles that depict distribution patterns. The user can also access other windows to edit or expand available databases or further process the data for management decisions. The menus and object-driven windows were vital in making the program relatively easy to learn and operate. The program is available for free by contacting one of the authors.

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References

Carsel, R.F., Parrish, R.S., 1988. Developing joint probability distributions of soil water retention characteristics. Water Resour. Res. 24, 755–769.

Dow AgroSciences, 1997. Chloropicrin pesticide information profile. Unpublished report.

Gan, J., Yates, S.R., Ernst, F.F., Jury, W.A., 2000. Degradation and volatilization of the fumigant chloropicrin after soil treatment. J. Environ. Qual. 29, 1391–1397.

Jury, W.A., Spencer, W.F., Farmer, W.J., 1983. Use of models for assessing relative volatility, mobility, and persistence of pesticides and other trace organics in soil systems. Hazard Assess. Chem. 2, 1–43.

Leib, B.G., Jarrett, A.R., 2003. Comparing sol pesticide movement for a finite-element model and field measurements under drip irrigation. Comput. Electron. Agric. 38, 55–69.

Leistra, M., 1970. Distribution of 1,3-dichloropropene over the phases in soil. J. Agric. Food Chem. 18, 1124–1126.

Simunek, J., van Genuchten, M.Th., 1994. The CHAIN-2D code for simulating the two-dimensional movement of water, heat, and multiple solutes in variably saturated porous media. Version 1.1, Research Report No. 136. U.S. Salinity Laboratory, USDA-ARS, Riverside, CA.

Van Dijk, H., 1980. Dissipation rates in soil of 1,2-dichloropropane and 1,3- and 2,3-dichloropropenes. Pest. Sci. 11, 625–632.

Wang, D., Ernst, F.F., Yates, S.R., Knuteson, J.A., 2001. Volatilization of 1,3-dichloropropene under different application methods. Water Air Soil Pollut. 127, 109–123.

Wang, D., He, J.M., Knuteson, J.A., 2004. Concentration–time exposure index for modeling soil fumigation under various management scenarios. J. Environ. Qual. 33, 685–694.

Wolt, J.D., Holbrook, D.L., Batzer, F.R., Balcer, J.L., Peterson, J.R., 1993. Dynamics of nematicide distribution and degradation in soil subjected to long-term pineapple culture. Acta Hort. 334, 361–371.

Yates, S.R., Wang, D., Ernst, F.F., Gan, J., 1997. Methyl bromide emissions from agricultural fields: bare-soil, deep injection. Environ. Sci. Technol. 31, 1136–1143.