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# Software Tools for Weed Seed Germination Modeling

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The next generation of weed seed germination models will need to account for variable soil microclimate conditions. To predict this microclimate environment we have developed a suite of individual tools (models) that can be used in conjunction with the next generation of weed seed germination models. The three tools that will be outlined here are GlobalTempSIM, GlobalRainSIM, and the soil temperature and moisture model ($STM^2$). Each model was compared with several sets of observed data from worldwide locations. Overall, the climate predictors compared favorably. GlobalTempSIM had a bias between −2.7 and +0.9 C, mean absolute errors between 1.9 and 5.0 C, and an overall Willmott *d*-index of 0.79 to 0.95 (where $d = 1$ represents total agreement between observed and modeled data) for 12 global validation sites in 2007. GlobalRainSIM had a bias for cumulative precipitation ranging from −210 to +305 mm, a mean absolute error between 29 and 311 mm, and a corresponding *d*-index of 0.78 to 0.99 for the sites and years compared. The high *d*-indices indicate that the models adequately captured the annual patterns for the validation sites. $STM^2$ also performed well in comparisons with actual soil temperatures with a range of −2 to +4.6 C biases and mean absolute errors between 0.7 and 6.8 C, with the *d*-index ranging from 0.83 to 0.99 for the soil temperature comparisons. The soil moisture prediction annual bias was between −0.09 and +0.12 $cm^3\ cm^{-3}$, mean absolute errors ranging from 0.02 to 0.16 $cm^3\ cm^{-3}$, and possessed a *d*-index between 0.32 and 0.91 for the validation sites. These models were developed in JAVA, are simple to use, operate on multiple platforms (e.g., Mac, personal computer, Sun), and are freely available for download from the U.S. Department of Agriculture Agricultural Research Service website (http://www.ars.usda.gov/Services/docs.htm?docid=11787).

**Nomenclature:** Environmental modeling, climate, simulation, JAVA.

Effective weed management is and will continue to be an integral component of a profitable, competitive, and sustainable agricultural production. The economic consequences of weed infestations are established well via reduced yields (e.g., Cousens 1985; Lindquist et al. 1994) and diminished quality (e.g., Kleinhenz and Cardina 2003). Annual losses from weeds in agricultural commodities in the United States were estimated at billions of dollars in 1991 (Bridges 1992). Such expensive losses are not restricted to the United States, as recent estimates suggest annual billion-dollar agricultural losses in Australia too (Sinden et al. 2004). Even with the recent proliferation of herbicide-resistant crops (Dill 2005), application timing still is vital in the prevention of important yield losses (Cox et al. 2005).

Ironically, application timing is one of the most critical aspects in the selection pressure for development of weed resistance to herbicides like glyphosate (Neve et al. 2003). Furthermore, improperly timed mechanical control measures (tillage) can actually increase weed pressure by providing the environmental stimulus for germination or bringing additional seeds into optimum emergence depths (Chancellor 1985; Lamour and Lotz 2007; Spokas et al. 2007). This clearly signifies the need for improved decision-making tools for weed management that are applicable globally.

Predominantly, agricultural production systems rely upon synthetic herbicides for weed control. This is demonstrated by predictions that financial losses in the agricultural sector would increase 500% (from \$4 billion to \$20 billion per year in the United States) without the use of herbicides (Bridges 1992). Other anecdotal evidence of herbicide use is the growing trend in the increasing acreage of glyphosate-resistant crops (Dill 2005). To minimize unnecessary application, protect the environment from excessive chemical applications, and curtail evolution of resistant weeds, efficacy and timeliness of selected weed control measures need to be maximized (Oriade and Forcella 1999). To achieve this goal, knowledge of weed behavior is needed, in particular germination, emergence, and early seedling growth. We propose that this can be gained through the use of weed emergence models that mechanistically relate the weed seed bank to emerged seedlings using soil microclimate simulations.

Numerous models already exist in the literature for the simulation of daily climatic variables. The most widely used weather simulation model has been the model introduced by Richardson (1981) and subsequent revisions (e.g., Richardson and Wright 1984). This has led to the development of a large number of meteorological simulation models: CLIGEN (Nicks and Lane 1989), USCLIMATE (Hanson et al. 1994), WXGEN (Nicks et al. 1990; Williams 1995), and CLIMGEN (Stockle and Nelson 1999). The major purpose of these models is to provide data to supplement existing meteorological measurements or to provide climate information where measured data are not available (Johnson et al. 2007). The major drawbacks are that a majority of these models have been solely developed for the continental United States (Phillips et al. 1992) and some also have large input data requirements (e.g., training data for fitting statistical coefficients; Dubrovský et al. 2004; Wilks and Wilby 1999). In addition, Harmel et al. (2002) discovered that these models result in simulated monthly temperature populations that do not represent the distribution of measured temperature data sets. They hypothesized that that was due to substantial seasonal and geographic variability in actual temperatures, leading to skewness that violates the normality assumption of the weather generators. Furthermore, these models are written in several different computer languages and are platform specific (e.g., personal computer, Mac, mainframe). These factors hamper their direct incorporation into existing as well as future weed germination and emergence models.

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Several coupled soil moisture and temperature models have been validated in the literature (e.g., Ács et al. 1991; Flerchinger 1987; Hammel et al. 1981; Nagai 2002; Xiao et al. 2006). However, a major user-oriented difficulty with these models is the large input requirements both for soil properties and climatic data. Our goal was to develop a theoretical soil moisture and temperature model that utilized validated empirical relationships to ease the soil input requirements and required only maximum and minimum daily air temperature along with precipitation as the sole climatic inputs. A soil water simulation model developed by Chanzy et al. (2008) represents a step in this direction. However, our developed soil temperature and moisture model has even fewer user inputs, allows infinitely small depth increments, and has an improved user interface.

All of these tools have been programmed in JAVA. The JAVA language is gaining popularity in the scientific and commercial software programming arenas (Bull et al. 2003; Fox and Furmanski 1998), despite a few drawbacks in terms of availability of variable types and mathematical functions (Gudenberg 1998). Furthermore, a program's execution speed difference between JAVA and older languages (e.g., C, FORTRAN) is becoming less of an issue, especially for desktop computers (Bull et al. 2003).

## Materials and Methods

**GlobalTempSIM.** The purpose of this tool is to estimate daily maximum and minimum air temperatures for a yearly cycle at any location on the globe. GlobalTempSIM predicts the daily average air temperature on the basis of 30-yr (1961–1990) temperature records that were compiled and interpolated by Legates and Willmott (1990a,b), with further improvements by Willmott and Matsuura (1995). This 30-min (0.5° grid [361 by 721 elements]) interpolated data set is based upon 24,941 independent surface air temperature and oceanic grid point estimates from a variety of sources (Legates and Willmott 1990a). Diurnal temperature ranges ($T_{\mathrm{DTR}}$) were interpolated from monthly averages from data collected from 1961 to 1990 and cross-validated by New et al. (1999). These also were interpolated to the 30-min (0.5°) grid.

Both the average monthly temperatures and diurnal temperature ranges were fitted to separate spline extrapolations to estimate daily values. Extrapolation was performed using day of year, with each month assigned to the respective day of year for half of the month. The extrapolated values from the spline resulted in the estimation of daily average air temperatures. Average daily temperature ($T_{\mathrm{mean}}$) was used together with the daily temperature ranges (again extrapolated through a spline) to calculate daily maximum ($T_{\mathrm{max}}$) and minimum temperatures ($T_{\mathrm{min}}$) as given in Equation 1:

$$T_{\max} = T_{mean} - \frac{1}{2} T_{DTR}. \qquad [1]$$

and

$$T_{\min} = T_{mean} - \frac{1}{2} T_{DTR}.$$

The sole input from the user is the geographical latitude and longitude as well as whether or not the daily temperatures should account for random diurnal variability. This random variability was assumed to be a function of the annual temperature amplitude at the location. This random factor produces a more variable output. However, statistically this random factor may or may not result in improved statistical measures since it is a random calculation. For the analyses conducted here, the random factor was not selected. The output file is a comma-spaced value (CSV) file that has the following format: day of year, maximum temperature, minimum temperature. GlobalTempSIM is a JAVA jar file. To execute the model, the JAVA run-time library from Sun Microsystems (www.java.com) is required to be installed on the appropriate computer platform. Once JAVA is installed the model can be run. The user input for the model is limited to solely the geographical information (latitude, longitude) and then the year for the simulation. The year is only used in establishing the daily output for the output file (i.e., leap year). This output file can be loaded into a spreadsheet program or directly incorporated into another model through the use of the JAVA JAR file (library).

**GlobalRainSIM.** The purpose of this tool is to estimate daily precipitation patterns for a yearly cycle at any location on the globe. GlobalRainSIM forecasts the daily rainfall on the basis of two databases. The first was the average number of days in a month with precipitation (wet days) that were compiled and interpolated by Legates and Willmott (1990a,b) with further improvements by Willmott and Matsuura (1995). This 30-min (0.5° grid) interpolated data set is based upon 26,858 independent precipitation stations and oceanic grid point estimates from a variety of sources (Legates and Willmott 1990a). The second database was the global average monthly precipitation data collected from 1961 to 1990, cross-validated by New et al. (1999), and also interpolated to the 0.5° grid. These two data sets then were used to establish the monthly precipitation totals and the frequency of precipitation in a month. The average precipitation event was calculated as the monthly mean divided by the number of wet days. This mean value was then randomly assigned to a day of the month looping through the number of wet days. In other words, if the average monthly rainfall was 10 mm with 5 average wet days, each rain event was 2 mm. This amount (2 mm) then was assigned randomly to 5 days of that month. The advantage of this tool is that a typical pattern of precipitation can be simulated for any global location arriving at an average year as a baseline case for comparison. This tool also outputs the daily rainfall as a CSV file or can be embedded easily within another program.

**Soil Temperature and Moisture Model ($STM^2$).** Despite the fact that there are several soil physics models for water and heat transport (e.g., SWIM [Verburg et al. 1996], SHAW [Flerchinger 1987], HYDRUS [Šimůnek et al. 2008], UNSAT-H [Fayer 2000)]), the major difficulty limiting the widespread use of these models is the large input requirement in terms of soil physical constants and climatic variables. In addition, numerical stability problems can occur on the basis of these user-supplied soil parameters. Some of these soil properties are unknown to the general user and this hampers widespread user acceptance of soil temperature and moisture models. The purpose of the $STM^2$ model was to keep these required inputs to a minimum. Therefore, to achieve this reduced input requirement, empirical models were used to estimate fundamental soil physical parameters to improve the usability of the model. The model also possesses an advanced tab to enable experienced users to input these soil physical values directly or adjust the calculated empirical parameters (Figure 1). Briefly, field capacity water content was estimated on the basis of soil pedotransfer functions (PTF) of Saxton and Rawls (2006). Overall correlation coefficient for the volumetric water content at field capacity was 0.63, with a standard error of $\pm 0.05$ m$^3$ m$^{-3}$ for over 2,000 soil samples (Rawls et al. 1982; Saxton and Rawls 2006). For soil parameters, basically the user need only select the desired soil to be simulated from a screen version of the soil textural triangle and then select organic matter content from a sliding bar (Figure 1). No other physical soil characteristics need be known.

Bulk density was estimated by taking the average of four PTFs on the basis of soil texture and organic matter classifications from Federer (1983), Kaur et al. (2002), Leonavičiutė (2000), and Saxton and Rawls (2006). Saturated volumetric moisture content for the soil is calculated from Saxton and Rawls (2006). Saturated hydraulic conductivity was estimated on the basis of the average of Saxton and Rawls (2006) and Kaur et al. (2002). The estimated hydraulic conductivity was then used to estimate the air entry potential and the slope of the $\ln\Psi$ vs. $\ln\theta$ graph (Campbell B), with the empirical relationships developed on the basis of the available data from all soil textural classes (Rawls et al. 1982; Saxton and Rawls 2006). Unsaturated conductivity is estimated on the basis of Campbell (1985):

$$K_{\mathrm{u}} = K_{\mathrm{s}}\left(\frac{\psi_{\mathrm{air}}}{\psi_{\mathrm{m}}}\right)^{2+\frac{3}{B}}, \quad [2]$$

where $K_{\mathrm{u}}$ is the unsaturated conductivity, $K_{\mathrm{s}}$ is the saturated conductivity, $\Psi_{\mathrm{air}}$ is the air entry potential, $\Psi_{\mathrm{m}}$ is the current soil moisture potential, and $B$ is the slope of the $\ln\Psi$ vs. $\ln\theta$ graph (Campbell B). The formula for water potential (Campbell 1985) is:

$$\psi_{\mathrm{m}} = \psi_{\mathrm{air}}\left(\frac{\theta}{\theta_{\mathrm{s}}}\right)^{-B}, \quad [3]$$

where $\Psi_{\mathrm{m}}$ is the current soil moisture potential, $\Psi_{\mathrm{air}}$ is the air entry potential, $\theta$ is the current moisture content, $\theta_{\mathrm{s}}$ is the saturated soil moisture, and $B$ is the slope of the $\ln\Psi$ vs. $\ln\theta$ graph (Campbell B). Thermal properties of the soil are calculated from de Vries (1963) and Farouki (1986) relationships. Solar radiation is modeled using a previously validated hourly solar radiation model (Spokas and Forcella 2006). Water transport is solved through a finite-difference solution to Richard's equation accounting for both liquid and vapor fluxes and a coupled finite-difference solution for heat flow.

Besides the soil texture and organic matter input, the other input from the user is the climatic data (weather file). The inputs required are day of year, maximum air temperature, minimum air temperature, and precipitation amounts in a CSV file (no headers).

**Statistical Model Validation.** Model performance was analyzed by several measures. Bias was calculated following the formula of Daly et al. (1994):

$$bias = \frac{1}{n}\sum_{i=1}^{n}(M_i - O_i), \quad [4]$$

where $M_i$ is the model output and $O_i$ is the observed quantity (rain, temperature, soil moisture content, etc.), and $n$ is the total number of comparisons. As indicated by Willmott and Matsuura (2005), bias is also simply the mathematical difference between the two means ($\bar{M} - \bar{O}$). Bias can be used as an indication of systematic over- or underprediction by the model (Willmott and Matsuura 2005). Mean absolute error (MAE) was also calculated by the following:

$$MAE = \frac{1}{n}\left[\sum_{i=1}^{n}|M_i - O_i|\right], \quad [5]$$

where $O_i$ are the measured values and $M_i$ are the modeled values (Willmott 1982). An "index of agreement" or modeling index ($d$) was calculated with the following expression:

$$d = 1 - \left[\frac{\sum_{i=1}^{n}(O_i - M_i)^2}{\sum_{i=1}^{n}\left(\left|O_i - \overline{O}_i\right| + \left|M_i - \overline{O}_i\right|\right)^2}\right], \quad [6]$$

where $O_i$ are the observed values (i.e., air temperature, rainfall, soil temperature, soil moisture) with a mean of $\bar{O}_i$, and $M_i$ are the modeled values (Mayer and Butler 1993; Willmott 1981). The value of $d$ will vary between 0 and 1, with a value of 1 indicating perfect model agreement (Willmott 1981). The coefficient of modeling efficiency (ME) was calculated by the following formula:

$$ME = 1 - \left[\frac{\sum_{i=1}^{n}(O_i - M_i)^2}{\sum_{i=1}^{n}\left(O_i - \overline{O}_i\right)^2}\right], \quad [7]$$

where $O_i$ are the measured values with a mean of $\bar{O}_i$ and $M_i$ are the corresponding modeled values (Legates and McCabe 1999; Mayer and Butler 1993). ME will vary between $-\infty$ and 1, with higher values (closer to 1) indicative of superior model performance (Willmott 1982). These indices have been used in other modeling comparisons (e.g., Diekkrüger et al. 1995; Eitzinger et al. 2004; Legates and McCabe 1999; Spokas and Forcella 2006) and are recommended measures in assessing model performance (Willmott 1982; Willmott and Matsuura 2005).

Relative percentage difference (RPD) was also calculated for the precipitation modeling, since the millimeters of rainfall are variable for each location. RPD was calculated by the following:

$$RPD = \frac{|M_{\mathrm{yr}} - O_{\mathrm{yr}}|}{(O_{\mathrm{yr}} + M_{\mathrm{yr}})} \times 200, \quad [8]$$

where $O_{\mathrm{yr}}$ is annual measured rainfall (mm) for the comparison year and $M_{\mathrm{yr}}$ is the modeled cumulative annual rainfall (mm). This provides a relative means to compare the precipitation predictions from various climates.

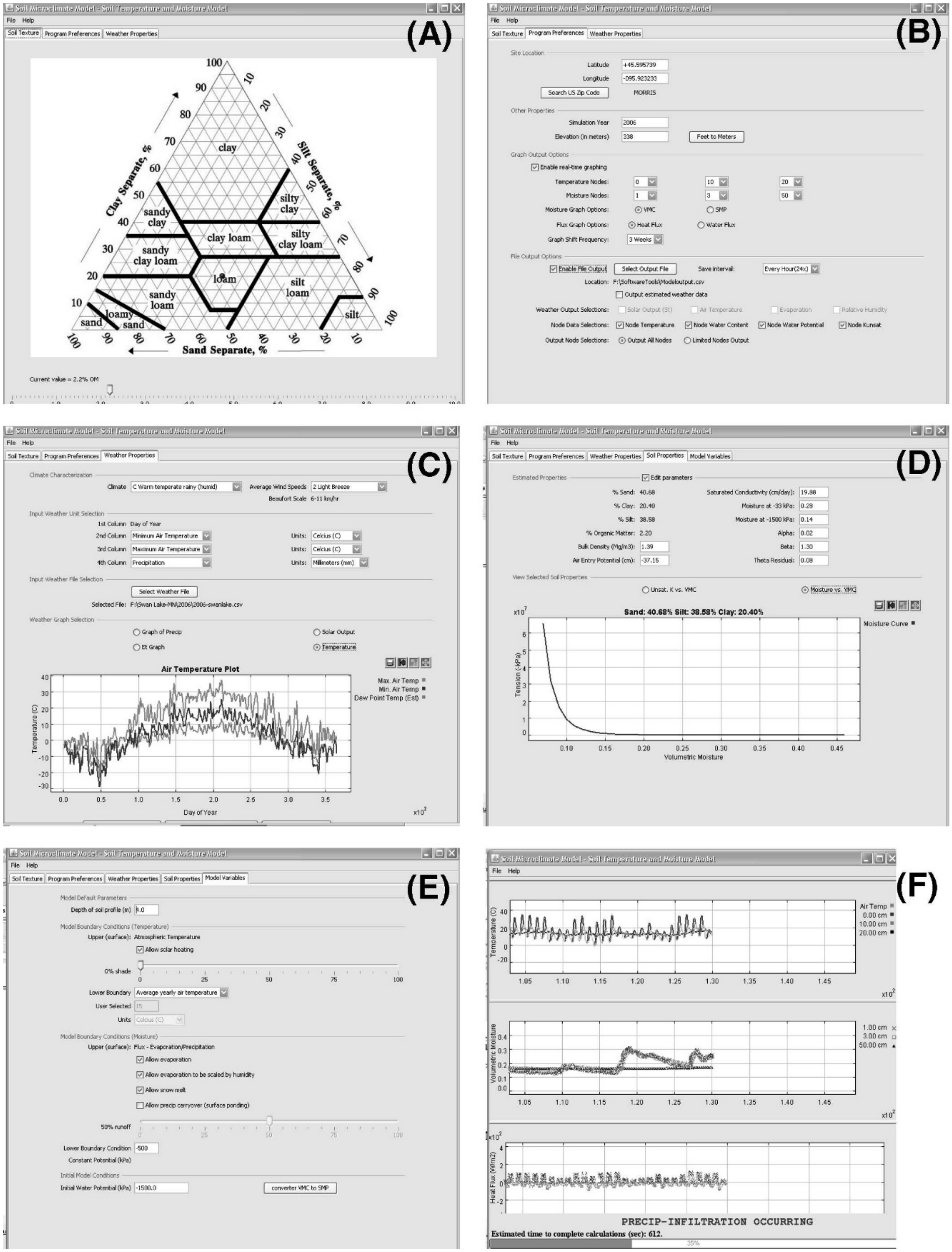


Figure 1. Example screen captures of the STM$^2$ JAVA program. (A) Soil selection and organic matter input screen, (B) program preferences tab, (C) weather data input tab, (D) advanced soil properties tab, (E) advanced model parameters tab, and (F) screen shot of the model during calculations.

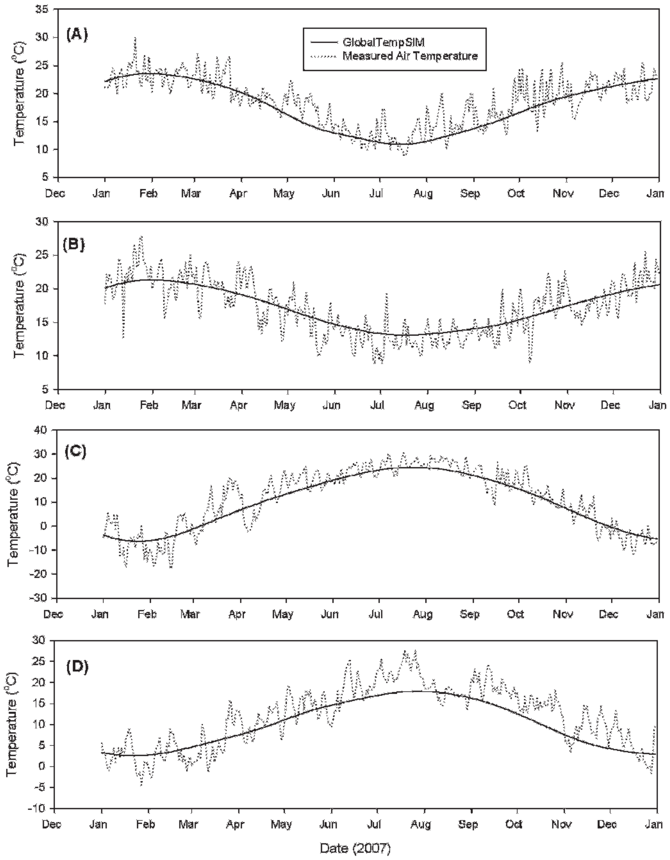


Figure 2. Comparisons of the output from GlobalTempSIM to measured air temperatures from (A) Sydney, Australia; (B) Cape Town, South Africa; (C) Omaha, NE; and (d) Paris, France. Measured data were retrieved from *Weather Underground* (www.wunderground.com) for 2007.

## Results and Discussion

**GlobalTempSIM.** Graphical comparisons of output from GlobalTempSIM and corresponding measured air temperature values for four selected locations are given in Figure 2. The model output from GlobalTempSIM is actually predicted maximum and minimum temperatures for each day. For these comparisons, just the mean temperature predictions are actually compared. Table 1 presents the statistics of all the validation comparisons. As seen in Figure 2 and Table 1, GlobalTempSIM does simulate the annual temperature wave. Model bias ranged from −4.3 to +0.5 C, with the model possessing a slight negative bias (average = −1.55 C) . Mean absolute errors ranged from 1.87 to 4.95 C; average MAE was 3.06 C. The *d*-index ranged from 0.8 to 0.95 (average 0.90), with corresponding ME ranging from 0.10 to 0.71 (average 0.52). These errors are within the same order of magnitude of other more complex weather simulators (e.g., Semenov et al. 1998). These measures indicate that the model did match the annual temperature pattern at all 12 sites evaluated.

**GlobalRainSIM.** Output from GlobalRainSIM also was compared with seven sites with precipitation data and the results are summarized in Table 2 as well as a graphical comparison of selected sites in Figure 3. Overall, there was good agreement between the GlobalRainSIM output and the precipitation records for the evaluation sites. The bias for all the sites and years ranged between −210 and +305 mm of annual rainfall and mean absolute errors were between 60 and 311 mm of rain. However, despite these high apparent errors, the model did simulate the precipitation patterns at the sites as indicated by the *d*-index values ranging from 0.836 and 0.995 (average = 0.94), and corresponding modeling efficiencies were between 0.034 and 0.980 (average = 0.75). Figure 3 illustrates some of the comparisons graphically, and in Figure 2d multiple years of precipitation data and the output

Table 1. Statistical measures of the GlobalTempSIM for 12 global sites.

| Site and Year | Latitude/longitude | Bias (C) | Mean absolute error (C) | *d*-index | ME |
|---|---|---|---|---|---|
| Sydney, Australia | 33.9°S, 151.2°E | | | | |
| 2007 | | −0.94 | 1.98 | 0.907 | 0.642 |
| Paris, France | 48.7°N, 2.3°E | | | | |
| 2005 | | −1.82 | 3.38 | 0.885 | 0.396 |
| 2006 | | −2.01 | 3.45 | 0.892 | 0.409 |
| 2007 | | −1.99 | 3.16 | 0.873 | 0.472 |
| Hong Kong, China | 22.3°N, 113.9°E | | | | |
| 2007 | | −2.16 | 2.62 | 0.902 | 0.612 |
| Düsseldorf, Germany | 51.2°N, 6.8°E | | | | |
| 2007 | | −1.65 | 2.88 | 0.910 | 0.455 |
| Cape Town, South Africa | 34.0°S, 18.6°E | | | | |
| 2007 | | +0.05 | 1.87 | 0.877 | 0.298 |
| Reykjavik, Iceland | 64.1°N, 21.9W | | | | |
| 2007 | | −0.99 | 2.47 | 0.887 | 0.473 |
| Los Angles, CA | 34.1°N, 118.2°W | | | | |
| 2007 | | −2.74 | 2.90 | 0.800 | 0.101 |
| Houston, TX | 29.7°N, 95.2°W | | | | |
| 2007 | | −0.71 | 2.84 | 0.922 | 0.639 |
| New York, NY | 40.8°N, 74.0°W | | | | |
| 2007 | | −4.3 | 4.95 | 0.898 | 0.538 |
| Omaha, NE | 41.3°N, 95.9°W | | | | |
| 2007 | | −1.2 | 3.90 | 0.953 | 0.779 |
| Ames, IA | 42.0°N, 93.6°W | | | | |
| 2007 | | −0.41 | 3.82 | 0.954 | 0.786 |
| Jay, FL | 30.8°N, 87.1°W | | | | |
| 2007 | | −0.85 | 2.62 | 0.923 | 0.672 |
| Average | | −1.55 | 3.06 | 0.90 | 0.52 |

Table 2. Statistical measures of the GlobalRainSIM for seven global sites and various years.

| Site and year | Bias (mm) | Mean absolute error (mm) | *d*-index | ME [a] | RPD (%) |
|---|---|---|---|---|---|
| Paris, France | | | | | |
| 2007 | 60.3 | 60.3 | 0.985 | 0.821 | 23 |
| Seattle, WA | | | | | |
| 2005 | 76.3 | 76.3 | 0.965 | 0.865 | 9 |
| 2006 | −66.4 | 75.0 | 0.964 | 0.852 | 18 |
| 2007 | 105.1 | 107.4 | 0.931 | 0.753 | 14 |
| Minneapolis, MN | | | | | |
| 2005 | −39.0 | 49.7 | 0.980 | 0.902 | 1.8 |
| 2006 | −3.2 | 28.6 | 0.995 | 0.980 | 4 |
| 2007 | −35.9 | 72.5 | 0.970 | 0.846 | 19 |
| Dallas, TX | | | | | |
| 2004 | −68.2 | 71.9 | 0.974 | 0.885 | 17 |
| 2005 | 132.1 | 159.4 | 0.777 | 0.439 | 59 |
| 2006 | −66.7 | 72.9 | 0.966 | 0.859 | 15 |
| 2007 | −209.6 | 209.6 | 0.863 | 0.034 | 38 |
| Jay, FL | | | | | |
| 2004 | 92.5 | 99.4 | 0.983 | 0.926 | 1 |
| 2007 | 304.5 | 311.1 | 0.836 | 0.419 | 25 |
| London, UK | | | | | |
| 2007 | 59.79 | 62.66 | 0.938 | 0.799 | 30 |
| Sydney, Australia | | | | | |
| 2007 | −27.6 | 68.8 | 0.980 | 0.901 | 8 |
| Average | 20.9 | 101.7 | 0.940 | 0.752 | 19 |

[a] Abbreviations: ME, modeling efficiency; *d*-index is described in the statistical section; RPD, relative percentage difference.

of GlobalRainSIM visually demonstrate the ability of the model to match the annual precipitation cycle. At a majority of the validation sites RPD fell within a ±30% bracket. High values of RPD are a direct result of the variability of precipitation and the difficulties encountered in attempting to duplicate nature in mathematical models (Airey and Hulme 1995). Other more mathematically complex precipitation models are able to make precipitation predictions to within ±20% RPD (Thornton et al. 1997). However, these models require extensive user inputs and training sets. GlobalRainSIM provides a simple model to predict a typical annual cycle of precipitation for any location.

**STM².** The ability to model the natural system is paramount to weed seed germination prediction. However, environmental modeling is also important in several other research areas. The next generation of weed seed germination models will need to account for soil microclimate conditions. To predict this microclimate environment, we have developed a suite of models. The major emphasis for this work was to provide a typical year of climatic data along with the generation of soil microclimate conditions from limited meteorological and site data. Granted, the year-to-year variability will not be captured with these tools, like the weather simulators mentioned above. However, the ability to generate a typical year of climatic data (air temperature and precipitation) from only a latitude and longitude input does have a wide range of applications. Many important weed species have worldwide distributions (Holm

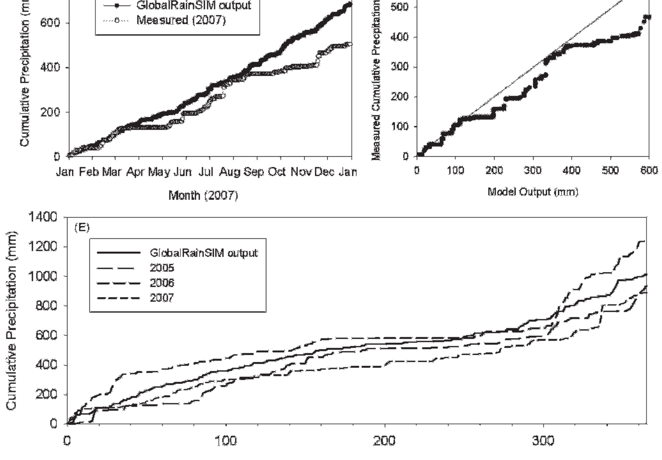


Figure 3. Graphical comparison of (A) and (B) cumulative vs. GloablRainSIM output for Jay, FL (2004); (C) and (D) cumulative vs. GlobalRainSIM output for London, UK (2007); and (E) a comparison of the output for Seattle, WA against 3 yr of precipitation data (2005, 2006, and 2007).

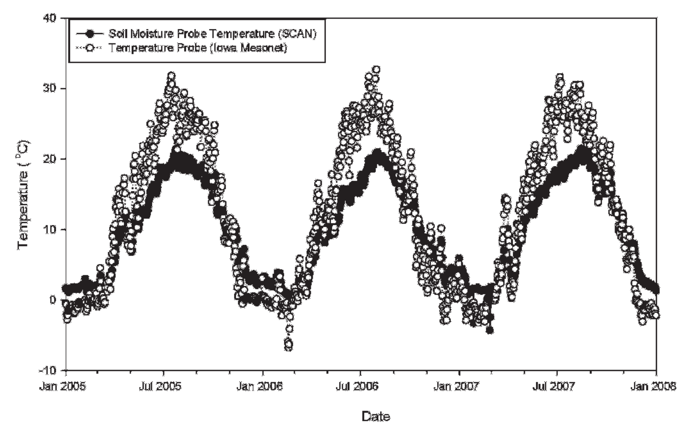


Figure 4. Comparison of soil temperature from the SCAN network compared with the independent measurement of soil temperature (Mesonet) at 10 cm in Ames, IA.

Table 3. Statistical measures of the temperature simulations with soil temperature and moisture model ($STM^2$) for 15 global sites.

| Site and soil depth | Latitude/longitude | $n$ | Bias (C) | Mean absolute error (C) | $d$-index | ME[a] |
|---|---|---|---|---|---|---|
| Amargosa Desert Research Site[b] (Beatty, NV) | 36.77°N, 116.69°W | | | | | |
| 2005 – 1 cm | | 8,760 | 0.90 | 5.34 | 0.927 | 0.687 |
| Odessa, WA[c] | 47.31°N, 118.88°W | | | | | |
| 2007 – 2.5 cm | | 333 | −1.80 | 4.39 | 0.943 | 0.815 |
| 2007 – 5 cm | | 333 | −1.86 | 2.87 | 0.970 | 0.884 |
| 2007 – 20 cm | | 333 | −1.78 | 2.65 | 0.958 | 0.788 |
| 2007 – 100 cm | | 333 | −1.68 | 2.65 | 0.886 | 0.178 |
| Aberdeen, ID[c] | 42.95°N, 112.83°W | | | | | |
| 2000 – 10 cm | | 366 | −2.07 | 2.65 | 0.964 | 0.873 |
| Padua, Italy | 45.34°N, 11.97°E | | | | | |
| 2006 – 5 cm | | 221 | 0.57 | 1.31 | 0.991 | 0.962 |
| Everglades, Fl[d] (ARS SCAN site) | 25.5°N, 80.55°W | | | | | |
| 2006 – 5 cm | | 363 | 1.64 | 1.93 | 0.829 | 0.231 |
| Ames, IA[d,e] | 42.02°N, 93.73°W | | | | | |
| 2005 – 5 cm | | 362 | −0.12 | 3.89 | 0.919 | 0.791 |
| 2005 – 10 cm | | 362 | 0.17 | 3.74 | 0.922 | 0.797 |
| 2005 – 10 cm (Mesonet) | | 365 | −2.05 | 2.92 | 0.966 | 0.865 |
| 2006 – 5 cm | | 365 | 2.25 | 3.70 | 0.923 | 0.786 |
| 2006 – 10 cm | | 365 | 1.02 | 2.99 | 0.944 | 0.840 |
| 2006 – 10 cm (Mesonet) | | 365 | −0.73 | 2.12 | 0.980 | 0.909 |
| 2007 – 5 cm | | 365 | 4.59 | 6.83 | 0.835 | 0.587 |
| 2007 – 10 cm | | 365 | −0.37 | 3.99 | 0.920 | 0.796 |
| 2007 – 10 cm (Mesonet) | | 365 | 1.69 | 2.70 | 0.937 | 0.820 |
| White Bear Lake, MN | 45.12°N, 92.95°W | | | | | |
| 2006 – 5 cm | | 57 | 0.04 | 0.72 | 0.988 | 0.950 |
| 2007 – 5 cm | | 122 | 0.52 | 1.52 | 0.934 | 0.944 |
| Morris, MN (Swan Lake Research Farm) | 45.68°N, 95.80°W | | | | | |
| 2007 – 1 cm | | 333 | −1.80 | 4.39 | 0.943 | 0.815 |
| 2007 – 2 cm | | 333 | −1.86 | 2.87 | 0.970 | 0.884 |
| 2007 – 5 cm | | 333 | −1.78 | 2.65 | 0.958 | 0.788 |
| 2007 – 10 cm | | 333 | −2.10 | 3.55 | 0.911 | 0.688 |
| Beasley Lake, MS[d] | 33.83°N, 90.65°W | | | | | |
| 2006 – 5 cm | | 8,639 | 1.10 | 2.02 | 0.977 | 0.916 |
| 2006 – 10 cm | | 8,639 | 1.50 | 1.77 | 0.983 | 0.931 |
| Sellers Lake, FL[d] | 29.10°N, 81.63°W | | | | | |
| 2006 – 5 cm | | 8,757 | 0.03 | 1.85 | 0.966 | 0.862 |
| 2006 – 10 cm | | 8,757 | −0.19 | 1.69 | 0.967 | 0.855 |
| Crossroads, NM[d] | 33.53°N, 103.23°W | | | | | |
| 2006 – 5 cm | | 8,758 | 0.150 | 5.76 | 0.864 | 0.440 |
| 2006 – 10 cm | | 8,758 | 0.190 | 3.67 | 0.933 | 0.700 |
| Dexter, MO[d] | 36.78°N, 89.93°W | | | | | |
| 2006 – 5 cm (hourly) | | 8,182 | 1.41 | 3.74 | 0.940 | 0.773 |
| 2006 – 10 cm (hourly) | | 8,182 | 1.36 | 2.60 | 0.970 | 0.875 |
| 2006 – 5 cm daily | | 342 | 1.35 | 1.77 | 0.985 | 0.940 |
| 2006 – 10 cm daily | | 342 | 1.25 | 1.57 | 0.987 | 0.949 |
| Lye Brook, VT[d] | 43.05°N, 73.03°W | | | | | |
| 2006 – 5 cm | | 6,346 | 2.14 | 3.29 | 0.902 | 0.708 |
| 2006 – 10 cm | | 6,266 | 1.91 | 2.69 | 0.932 | 0.789 |
| FermiLab, IL | 41.86°N, 88.22°W | | | | | |
| 2007 – 10 cm | | 363 | 1.12 | 1.90 | 0.981 | 0.934 |
| 2007 – 50 cm | | 361 | 1.91 | 2.07 | 0.952 | 0.802 |
| St. Paul, MN University of MN Weather Station | 44.99°N, 93.18°W | | | | | |
| 2007 | | | | | | |
| Bare soil – 1 cm | | 8,760 | 0.19 | 4.68 | 0.955 | 0.844 |
| Bare soil – 5 cm | | 8,760 | 0.29 | 3.69 | 0.967 | 0.887 |
| Bare soil – 10 cm | | 8,760 | 0.39 | 3.45 | 0.970 | 0.895 |
| Grass (turf) – 1 cm | | 8,760 | −1.44 | 4.52 | 0.928 | 0.789 |
| Grass (turf) – 5 cm | | 8,760 | −1.25 | 3.64 | 0.945 | 0.831 |
| Grass (turf) – 10 cm | | 8,760 | −1.10 | 3.20 | 0.952 | 0.848 |
| *Without frozen soil period* | | | | | | |
| Grass (turf) – 1 cm | | 5,412 | 0.46 | 2.99 | 0.928 | 0.762 |
| Grass (turf) – 5 cm | | 5,412 | 0.43 | 2.06 | 0.957 | 0.839 |
| Grass (turf) – 10 cm | | 5,412 | 0.42 | 1.61 | 0.971 | 0.883 |

[a] Abbreviaton: ME, modeling efficiency.
[b] Data from Johnson et al. (2007).
[c] Data from AgriMet: The Pacific Northwest Cooperative Agricultural Weather Network (http://www.usbr.gov/pn/agrimet/webarcread.html).
[d] Data from Soil Climate Analysis Network (SCAN) (http://www.wcc.nrcs.usda.gov/scan/).
[e] Secondary Soil Temperatures from Iowa Environmental Mesonet (http://mesonet.agron.iastate.edu/agclimate/hist/dailyRequest.php).

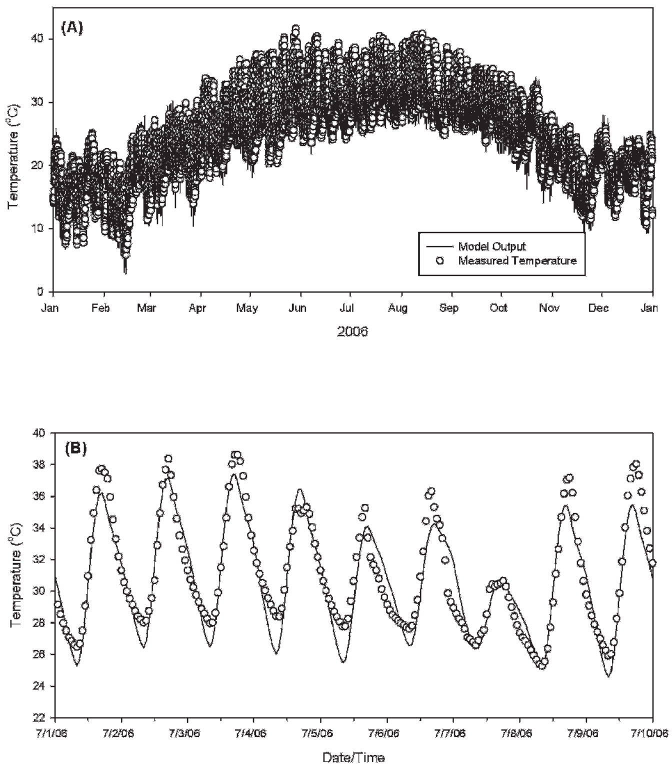


Figure 5. Example of graphical comparison for Sellers Lake, FL, for (A) modeled vs. measured 5-cm soil temperatures throughout 2007 and (B) during the first 15 d in July 2007.

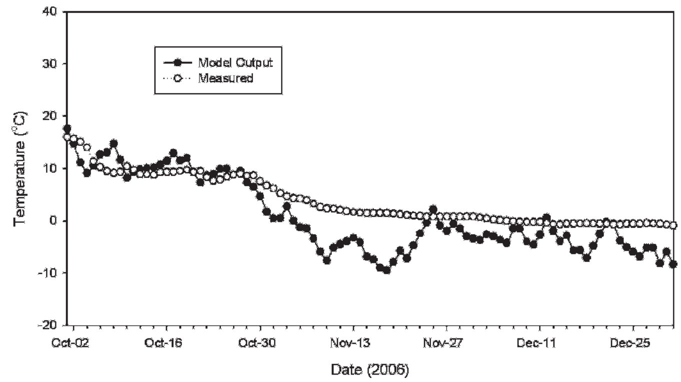


Figure 6. Example of underestimation of soil temperatures (5 cm) during the winter for Aberdeen, ID in 2006.

et al. 1977, 1997), and the chemical and mechanical tactics used to control these plants may have equally broad or broader ranges. Consequently, when studying topics spanning from weed ecology to pesticide fate, weed scientists, environmental scientists, and perhaps even regulatory agencies may have need to simulate daily temperature and rainfall conditions in locations where measured meteorological data are not readily available. GlobalTempSIM and GlobalRainSIM assist users in approximating these variables easily and on a worldwide basis.

$STM^2$ results were compared for multiple sites and locations. One of the databases utilized for this comparison came from the U.S. Department of Agriculture National Resources Conservation Service—Soil Climate Analysis Network (SCAN: www.wcc.nrcs.usda.gov/scan/). This allowed a selection of sites across various climates and soils to be evaluated. Results of the temperature and soil moisture simulations will be discussed individually below.

**Soil Temperature Modeling.** Improved model fits for soil temperature were achieved when there were independent soil temperature sensors (thermistor or thermocouple) opposed to the use of temperature data from the enclosed soil moisture probe from the SCAN network. This is seen clearly in the Ames, IA comparison where the 10-cm soil temperature was compared with the SCAN data (enclosed temperature sensor) and the Iowa Environmental Mesonet (independent temperature probe). There was a consistent reduction in the mean absolute error as well as a corresponding increase in the $STM^2$ comparison as measured by the *d*-index and the modeling efficiency for the 3 yr compared at Ames, IA when the independent soil temperature data were used (Table 3). When the data between the soil moisture probe (SCAN) and the independent soil temperature probe (Mesonet) were compared, a negative bias in the SCAN data in the summer months and a positive bias in the winter months was observed (Figure 4). However, these two sources of temperature data were from different sites (even though in proximity) and multiple factors could contribute to observed differences. Curiously, the SCAN soil moisture probe does not report negative soil temperatures, even in the winter months for the northern climate sites (Figure 4). For the remainder of the SCAN sites, independent data for the soil temperature were not located and the soil moisture probe temperature data were used as the basis of the model comparisons.

Improved temperature model fits occurred when daily average temperatures were used as opposed to hourly values (Table 3). This can largely be attributed to the difficulty in simulating the diurnal temperature pattern (Cesaraccio et al. 2001). The site at Dexter, MO demonstrates this improvement: mean absolute error changed from 3.7 C for the hourly values to 1.8 C for the daily averages, with corresponding improvement also observed in the *d*-index (0.940 to 0.985) and modeling efficiency (0.773 to 0.940). However, hourly data also fit extremely well, such as at Sellers Lake, FL (bias = 0.3 C and modeling efficiency of 0.865), the values for which are shown in Figure 5.

Also in Table 3 are statistics on the basis of the data from the St. Paul, MN weather station, which offered an opportunity to compare the ability to simulate temperatures below sod (grass) as well as bare soil. The model performed similarly in both situations, indicating that it is capable of simulating temperatures below surface vegetation, which would be important for modeling weed behavior in turf of golf courses, etc. The difficulty encountered was with the insulating properties of the snow + grass system that was not considered during model development (Figure 6). When the snow-covered period (frozen soil) is eliminated from the comparison, the statistical assessments are virtually identical to the bare soil simulation (Table 3).

For comparison of model performance, a more detailed physical process model (SHAW) possessed an average bias of 0.6 to 0.9 C and a model efficiency of 0.94 (Flerchinger et al. 1998). Therefore, even with the empirical simplifications, $STM^2$ performed well at simulating soil temperatures and resulting statistical measures are virtually equivalent to the more sophisticated soil temperature models.

Table 4. Statistical measures for the soil moisture simulations with soil temperature and moisture model ($STM^2$) for 12 global sites.

| Site and soil depth | $n$ | Bias ($cm^3\ cm^{-3}$) | Mean absolute error ($cm^3\ cm^{-3}$) | *d*-index | ME[a] |
|---|---|---|---|---|---|
| Calibrated soil moisture sensors | | | | | |
| Amargosa Desert Research Site (Beatty, NV) | | | | | |
| 2005 – 1 cm | 8,760 | 0.01 | 0.02 | 0.911 | 0.572 |
| White Bear Lake, MN | | | | | |
| 2008 | 288 | 0.03 | 0.05 | 0.914 | 0.655 |
| FermiLab, IL | | | | | |
| 2007 – 10 cm | 362 | 0.01 | 0.03 | 0.668 | −0.637 |
| Watkins, GA | | | | | |
| 2007 – 5 cm | 8,730 | 0.01 | 0.03 | 0.905 | 0.463 |
| Morris, MN | | | | | |
| 2005 – 5 cm | 146 | −0.01 | 0.16 | 0.757 | 0.710 |
| 2006 – 5 cm | 259 | −0.08 | 0.15 | 0.799 | 0.620 |
| Soil moisture sensors using default calibration | | | | | |
| Everglades, Fl[b] | | | | | |
| 2006 5 cm[c] | 365 | 0.05 | 0.07 | 0.622 | −0.287 |
| Ames, IA | | | | | |
| 2005 – 5 cm | 364 | 0.02 | 0.05 | 0.667 | −2.63 |
| 2005 – 10 cm | 364 | −0.06 | 0.06 | 0.450 | −4.40 |
| Beasley Lake, MS | | | | | |
| 2006 – 5 cm | 8,758 | −0.06 | 0.06 | 0.535 | −1.58 |
| 2006 – 10 cm | 8,758 | −0.05 | 0.05 | 0.603 | −1.63 |
| Sellers Lake, FL | | | | | |
| 2006 – 5 cm | 8,754 | 0.05 | 0.07 | 0.366 | −16.5 |
| 2006 – 10 cm | 8,754 | 0.12 | 0.12 | 0.392 | −4.687 |
| Crossroads, NM | | | | | |
| 2006 – 5 cm | 8,758 | 0.11 | 0.11 | 0.354 | −9.58 |
| 2006 – 10 cm | 8,758 | 0.11 | 0.11 | 0.321 | −12.40 |
| Dexter, MO | | | | | |
| 2006 – 5 cm (hourly) | 8,180 | 0.04 | 0.06 | 0.777 | −0.349 |
| 2006 – 10 cm (hourly) | 8,180 | 0.01 | 0.05 | 0.765 | −0.199 |
| 2006 – 5 cm daily | 342 | 0.04 | 0.06 | 0.781 | −0.322 |
| 2006 – 10 cm daily | 342 | 0.01 | 0.04 | 0.775 | 0.145 |
| Santarem Forest, Brazil (logged) | | | | | |
| 2001 – 20 cm | 340 | −0.09 | 0.14 | 0.430 | −7.147 |

[a] Abbreviation: ME, modeling efficiency.
[b] Data from Johnson et al. (2007).
[c] Precipitation data was not available from the site (instrumentation error), used precipitation data from Naples, Fl (70-km distance).

**Soil Moisture Modeling.** The $STM^2$ model performed well in duplicating the annual cycle of changes in soil moisture at the sites. One of the difficulties in comparing model soil moisture performance is the large errors due to installation and measurement issues (e.g., Plauborg et al. 2005). Soil moisture potential was measured with Watermark sensors both at the Padua, Italy and Morris, MN sites. Despite numerous laboratory efforts at developing universal calibration equations (e.g., Thomson and Armstrong 1987; Thomson et al. 1996), existing calibration equations underestimate when they are compared with actual soil moisture potentials for some soils (Irmak and Haman 2001), and responses for each sensor are variable and not necessarily reproducible (Spaans and Baker 1991). Therefore, the readings without regular individual calibration and corrections should be considered only a relative indicator of soil moisture status rather than an absolute measurement (Leib et al. 2003). The other important factor is that the soil moisture data for the SCAN network is processed with the manufacturer's provided calibration and no site-specific calibration is performed on the data (D. Harms, personal communication). Evett et al. (2006) indicated that the lack of soil-specific calibration is a potential source of error in soil moisture measurements.

Despite these sources of error, the model did compare favorably with the soil moisture measurements (Tables 4 and 5; Figure 7). Overall, the soil moisture bias was between −0.09 to 0.12 $cm^3\ cm^{-3}$, with mean absolute errors between 0.02 and 0.16 $cm^3\ cm^{-3}$. Overall, the mean absolute errors for the soil moisture model are well within the range of errors

Table 5. Statistical measures for the soil moisture potential simulations with soil temperature and moisture model ($STM^2$) for two sites.[a]

| Site and soil depth | $N$ | Mean error (kPa) | Mean absolute error (kPa) | *d*-index | ME[b] |
|---|---|---|---|---|---|
| Padua, Italy | | | | | |
| 2007 – 10 cm | 177 | −41 | 54 | 0.861 | 0.11 |
| Morris, MN (Swan Lake Research Farm) | | | | | |
| 2007 – 3 cm | 169 | −54.8 | 62.4 | 0.531 | 0.02 |
| 2007 – 5 cm | 191 | −40.3 | 56.6 | 0.400 | −1.50 |
| 2007 – 10 cm | 214 | −34.1 | 35.7 | 0.648 | −0.02 |

[a] Frozen soil periods were eliminated from the comparisons.
[b] Abbreviations: ME.

expected with field soil moisture measurements (Evett et al. 2006; Vitel 1994; Yu et al. 1999). The model did duplicate the annual cycle in soil moisture at the sites with a *d*-index between 0.32 and 0.91 (average = 0.64) and a modeling efficiency between −16.5 and 0.71 (average −2.96). As seen in Table 4, there is a slight improvement in the statistical measures of the model in the comparisons with soil moisture data that were calibrated to the specific soil. For comparison, Hymer et al. (2000) observed that detailed soil physics models had errors that typically fell within 0.03 to 0.07 $cm^3\ cm^{-3}$, whereas our simplified model had errors in the range of 0.02 to 0.16 $cm^3\ cm^{-3}$. Therefore, our developed model is close to the more detailed theoretical models despite the simplified user inputs.

For soil moisture potential, data from two sites were compared (Table 5). The model had a consistent negative bias from −55 to −34 kPa and a mean absolute error between 36 and 63 kPa. However, the model predicted the annual cycle with *d*-index values ranging between 0.40 and 0.86, and modeling efficiencies were between −1.5 and 0.11 for the soil moisture potential comparisons. In contrast to the soil temperature data, comparing hourly vs. daily values did not improve the statistical measures (Dexter, MO; Table 5). This is probably linked to the reduced diurnal fluctuations in soil moisture as compared with soil temperatures.

Another source of error with $STM^2$ is the lack of exact timing of precipitation events. The model extrapolates the daily precipitation evenly over the 24-h period. This is a source of error in the modeling and is hypothesized for the lag in the timing of the soil moisture response in the measured vs. model data. In addition, the positive bias of the model could be due to improved infiltration as a consequence of the reduced intensity of the rainfall. Rainfall intensity greatly affects runoff vs. infiltration amounts (e.g., Pruski and Nearing 2002). A potential scenario is where the rainfall might have occurred solely within a 1-h time period in the morning (1:00 to 2:00 A.M.), whereas the model will distribute this rainfall amount evenly over a 24-h period. A correction factor (% runoff) has been incorporated in the model to aid in reducing the impact of this bias by reducing the available precipitation by the runoff percentages (Figure 1). Despite these simplifications, the predictions still are within a usable range of values to be used for model purposes.

$STM^2$ has admitted shortcomings due to the simple handling of the soil moisture retention curve as well as the empirical relationships in deriving the soil physical constants. Soil porosity and residual soil moisture contents have been cited as vital properties for proper modeling efforts, since these values largely control the ability of the model to match soil moisture contents during extreme wet or dry periods (Walker et al. 2001). This impact of residual soil moisture can be seen in Figures 7b and 7c, where the model simulations do not drop as low as the actual soil moisture measurements. Finke et al. (1996) already documented the fact that the uncertainty in the empirical relationships can play an important role in specific aspects of soil moisture behavior. Despite these shortcomings, empirical relationships provide values comparable with actual spatial means of soil properties (Soet and Stricker 2003). A further simplification was the fact that the model handles only one type of soil. This can be seen as a large source of error both for moisture and temperature comparisons at depth since alterations in bulk density, structure, or texture are not considered. However, for the majority of studies on weed seeds and seedlings, and perhaps even pesticide fate, where the emphasis is on shallow soil depths, this error should not be a significant factor.

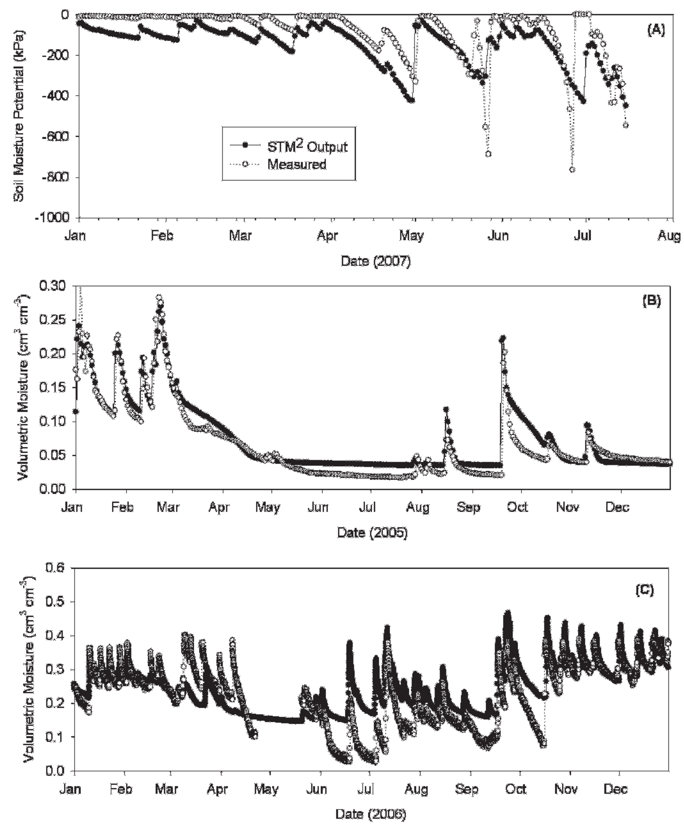


Figure 7. Graphical comparisons of (A) soil moisture potential from Padua, Italy in 2007 at 10 cm, (B) volumetric moisture comparison at the Amargosa Desert Research Site in Beatty, NV for surface soil moisture in 2005, and (C) volumetric moisture comparison at 5 cm in Dexter, MO during 2006. Gaps in the figure indicate time periods where no measured data were available.

The insulating properties of snow are ignored in the current version of $STM^2$. Consequently, the model underpredicts the winter soil temperatures as a result of this omission (Figure 7). Despite the simplifications taken in the model, as well as ignoring other soil moisture modeling complexities (e.g., O'Connell and Todini 1996), the model still predicts the annual cycles in soil microclimate conditions well (Tables 3 to 5), particularly the simulation of surface soil temperature and moisture profiles needed for weed seed germination models.

As seen in the above comparisons, $STM^2$ did have more difficulty in modeling soil moisture than soil temperature, which is related to the use of the empirical models for the simplification of data input requirements. $STM^2$ also had a slight positive bias for soil moisture (Table 3) for the sites evaluated. This results from assumptions and shortfalls, such as the one-dimensional nature of the model, underestimating runoff, alterations of soil texture and structure with depth, or neglecting horizontal moisture redistribution. Despite these limitations, the model provides a more user-friendly tool for predicting soil moisture and temperature profiles than existing models and has already proved useful in weed germination studies (e.g., McGiffen et al. 2008; Schutte et al. 2008).

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