2DSOIL - A Modular Simulator of Soil and Root Processes

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EXECUTIVE SUMMARY

Because of the complexity of the various linkages in agricultural systems, research questions are often best studied via simulation modeling. The goal of this project was to develop the framework for a generic, two-dimensional soil simulator that could easily be modified and incorporated into crop models. Most agricultural crops are grown in rows and operations are carried out parallel with rows. As a consequence, root growth, wheel traffic, tillage fertilizer banding, furrow and drip irrigation, among other operations, all produce variations in soil conditions in two dimensions, perpendicular to the rows. Soil modeling is now increasingly being focused at these two dimensions. Plant modelers, however, wishing to incorporate comprehensive soil models into their plant models require soil code that can be easily interfaced with a plant model and subsequently modified to incorporate different management practices. The development and upgrading of detailed models requires a large investment of time and resources. The tools developed as part of this project will simplify the process of building the model and incorporating modifications as research finds new information to include.

The 2DSOIL model is a modular, comprehensive two-dimensional soil simulator that is specifically designed to be combined with existing plant models. Modules of the present release, 2DSOIL.03, simulate water, solute, heat and gas movement, as well as root activity of plants, nitrogen dynamics, and chemical interactions in a two-dimensional soil profile. An uneven soil surface, mulching, and local applications of water and chemical can be easily modeled. The modules interact by means of soil state variables that are important for plants and the environment. The modules are highly independent because details of a particular module's activity are unknown to other modules. Several modules were adapted from existing models; others were developed specifically for 2DSOIL. 2DSOIL is written in FORTRAN and may be run on 486 or more advanced MS-DOS or MS-WINDOWS based computers.

The modular structure of 2DSOIL allows users to add their own modules of soil and plant processes, and soil management practices. The users can also easily replace modules of 2DSOIL.03 with more appropriate ones for their specific problems, or with more accurate modules as they become available.

Potential users are soil and plant modelers, environmental scientists, agronomists, crop scientists and others who are interested in investigating environmental quality and crop productivity as affected by management practices and possible climate changes.

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ABSTRACT

2DSOIL - A New Modular Simulator of Soil And Root Processes. Release 03 (March, 2001) Dennis Timlin, Yakov Pachepsky, and Martinus Th. van Genuchten, Eds.

The various linkages in agricultural systems are so complex that research questions are often studied most effectively with the help of simulation modeling. The development and upgrading of detailed models requires a large investment of time and resources. Therefore, it is necessary to simplify the process of building the model and incorporating modifications as research finds new information to include. The goal of this study was to develop the framework for a generic soil simulator that could easily be modified and incorporated into crop models. Soil and root processes in the simulator are represented by modules that interact on the spatial-temporal grid covering the soil profile and the simulated time interval. Data were divided into public and private components to minimize information passing between modules. This modular structure and information hiding simplifies replacement or addition of modules and promotes code reuse. The classes of modules include: (a) control modules that oversee interactions between processes, (b) water, solute, heat, and gas transport modules, (c) interphase chemical transformation modules, (d) biochemical transformation modules, and (e) root growth and uptake modules. A representative simulator, 2DSOIL, was assembled according to the proposed design. Examples include the incorporation of 2DSOIL into a simple crop model and the expansion of 2DSOIL with a management module to simulate chemical application. The documentation includes instructions for adding customized modules.

TECHNICAL REQUIREMENTS AND TECHNICAL SUPPORT

A 486 MS-DOS based personal computer is recommended. A DOS extender will be necessary if the program code size exceeds the conventional memory available (generally about 600K).

The authors of 2DSOIL used a FORTRAN77 compiler developed by the Salford Software Systems[1]. This software uses DBOS as a DOS extender. There are several calls to non-standard routines that are supported only by University of Salford compilers; these are present in only one subroutine to control screen output. The program can be linked without including this subroutine. We have used VISUAL FORTRAN, for details please contact the authors.

Work on 2DSOIL is a continuous effort. We encourage users to contact us if they have comments or suggestions, or if they find any problems. Two of the developers (Yakov Pachepsky and Dennis Timlin) are located at:

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[1]Mention of a trade name or product does not constitute a recommendation or endorsement for use by the USDA

LIST OF SYMBOLS

α	parameter in soil water retention model, cm^{-1}
α_M	characteristic time of mature root mass growth, day^{-1}
α_Y	characteristic time of root maturity, day^{-1}
$\alpha_\diamond$	solar altitude, rad
$\alpha_\diamond'$	apparent solar elevation, rad
β	angle between row orientation and solar azimuth, rad
γ	psychrometric constant, kPa·$(^oC)^{-1}$
γ_1	activity coefficient of univalent non-associated ion
Γ_e	boundary of element e
δ	solar declination
$\Delta\varepsilon$	water vapor pressure deficit, kPa
Δl_Y	length of young roots that appear in a soil cell during a time step, cm
Δm_R	initial mass of roots in a soil cell when roots grow from another cell, g
$\Delta P_{M,D}$	turgor pressure available to expand a root after overcoming soil mechanical resistance, bar
Δt	time interval, day
Δu	threshold water uptake by new roots, g day^{-1}
ϵ	canopy extinction coefficient
ϵ_t	time weighing factor
ε	actual water vapor pressure for day, kPa
ε_w	saturated water vapor pressure at wet bulb temperature, kPa
ζ	solar azimuth, rad
η	cloud cover factor
θ	volumetric soil moisture content, cm^3 cm^{-3} of soil
θ_1	volumetric soil moisture content minus the exclusion volume of univalent anions, cm^3 cm^{-3}
θ_a	parameter in soil water retention model, cm^3 cm^{-3} of soil
θ_k	parameter in soil water retention model, cm^3 cm^{-3} of soil
θ_m	parameter in soil water retention model, cm^3 cm^{-3} of soil
θ_r	residual water content, cm^3 cm^{-3}
θ_s	soil moisture content at saturation, cm^3 cm^{-3}
ϑ_a	air-filled porosity, cm^3 cm^{-3} of soil
$\vartheta_{a,Tr}$	threshold value of air-filled porosity below which gas diffusion does not occur, cm^3 cm^{-3}
κ_i	weight coefficients showing proportion of actual root growth to potential growth in soil cell i
$\varkappa_i$	weight coefficients showing proportion of actual root water uptake to potential water uptake
Λ	thermal conductivity of the soil, J cm^{-1} C^{-1} day^{-1}
Λ_a	thermal conductivity of air, J cm^{-1} C^{-1} day^{-1}
Λ_{cl}	thermal conductivity of clay, J cm^{-1} C^{-1} day^{-1}

Λ_{om}	thermal conductivity of soil organic matter, J cm^{-1} C^{-1} day^{-1}
Λ_{da}	thermal conductivity of dry air, J cm^{-1} C^{-1} day^{-1}
Λ_{ss}	thermal conductivity of sand and silt, J cm^{-1} C^{-1} day^{-1}
Λ_{v}	thermal conductivity of water vapor, J cm^{-1} C^{-1} day^{-1}
λ_L	longitudinal dispersivity, cm
λ_T	transversal dispersivity, cm
μ	relative change in soil hydraulic conductivity per unit pressure head, cm^{-1}
ν_c	albedo of crop
ν_s	albedo of soil
ξ	carbon supply ratio (proportion of carbon that was initially directed to the shoot but sent to roots due to water stress)
Π	precipitation (or irrigation), cm
$\pi_{R,D}$	root osmotic potential at dawn, bar
ρ_R	root mass per unit of soil volume, g cm^{-3}
$\rho_{R,T}$	threshold root mass per unit of soil volume, g cm^{-3}
ρ_s	soil bulk density, g cm^{-3}
σ	soil specific water capacity, cm^{-1}
τ_c	tortuosity factor of solute diffusion
τ_g	tortuosity factor of gas diffusion
υ	row orientation measured eastward from north, degrees
φ	local latitude, degrees
ϕ_n	finite element basis functions for node n, cm^2
ψ_L	leaf water potential, bar
ψ_R	root water potential during the day, bar
$\psi_{R,D}$	root water potential at dawn, bar
ψ_s	soil water potential, bar
ψ^{sa}	average soil water potential in cells where new roots appear, bar
$\psi_{s,D}$	soil water potential at dawn, bar
Ω_e	area of element e
a	atmospheric transmission coefficient
$\hat{a}$	coefficient of the basis function of triangular element, cm
A	area of the soil cell, cm^2
A_C	leaf area per unit soil surface area covered by crop canopy (leaf area index)
$A_{C,e}$	effective leaf area index allowing for the fact that light at low angles traverses more leaves to reach the soil
A_L	total plant leaf area, cm^2
$\hat{b}$	coefficient of the basis function of triangular element, cm
b_ε	saturation water vapor pressure change per one degree of temperature change, kPa $(^{o}C)^{-1}$
b_g	surface gas flux change per unit of gas content in soil air at the soil surface (gas transfer coefficient), cm day^{-1}
b_R	amount of carbon needed to produce one unit of root dry mass, g·g^{-1}

b_T surface heat flux change per degree of soil surface temperature (surface conductance of heat exchange), J·cm^{-2} day^{-1} C^{-1}

b_{tort} tortuosity change per unit of the air-filled porosity

$B_{R,max}$ rate at which carbon would be supplied to growing roots if all translocated carbon went to roots, g day^{-1}

$B_{R,min}$ rate at which carbon would be supplied to growing roots if all potential shoot growth had been satisfied, g day^{-1}

B_V actual rate of carbon supply to vegetative parts of the shoot and root, g per plant per day

$B_{V,max}$ maximum rate of carbon supply to vegetative parts of the shoot and root, g per plant per day

c solute concentration, g per cm^3 of the soil solution

$\hat{c}$ coefficient of the basis function of triangular element, cm

$\hat{C}$ total heat capacity of the soil solid material and water, J g^{-1}

C_{om} heat capacity of soil organic matter, J g^{-1}

C_{sm} heat capacity of soil solid mineral constituents, J g^{-1}

C_w heat capacity of water, J g^{-1}

CEC soil cation-exchange capacity, eq L^{-1}

cs Michaelis-Menten constant of denitrification, g cm^{-3}

d lateral distance from the row, cm

$d_{e,n}$ length of soil domain boundary segment which serves as border of element e and ends at node n, cm

d_{rs} row spacing, cm

d_{sc} radius of soil cylinder surrounding a root, cm

d_{sh} width of shadow cast by row crop measured perpendicular to the row, cm

d_{Tr} width of soil surface associated with transpiration, cm

$D_{0,st}$ gas molecular diffusion coefficient at standard conditions, cm^2 day^{-1}

D_g gas molecular diffusion coefficient in soil air, cm^2 day^{-1}

D_m ion or molecule diffusion coefficient in free water, cm^2 day^{-1}

D_{xx} solute dispersion coefficient reflecting dispersion in the 'x' direction caused by a concentration gradient in the 'x' direction, cm^2 day^{-1}

D_{xz} solute dispersion coefficient reflecting dispersion in the 'x' direction caused by a concentration gradient in the 'z' direction, or in the 'z' direction caused by a concentration gradient in the 'x' direction, cm^2 day^{-1}

D_{zz} solute dispersion coefficient reflecting dispersion in the 'z' direction that is caused by a concentration gradient in the 'z' direction, cm^2 day^{-1} E_c
potential transpiration rate from the crop, cm day^{-1}

$E_{c,high}$ limiting value of transpiration rate above which transpiration does not influence plant resistance to water stress, cm day^{-1}

$E_{c,low}$ limiting value of transpiration rate below which transpiration does not influence plant resistance to water stress, cm day^{-1}

E_s potential evaporation rate from soil surface, cm day^{-1}

E^a actual evaporation rate from soil surface, cm day^{-1}

fa	Fraction of the mineral nitrogen available for immobilization
f_π	factor describing ability of plant to osmoregulate when water stressed (= change in osmotic potential/change in water potential)
f_{Beer}	Beer's law correction for radiation interception
f_c	fraction of the solar radiation intercepted by the crop
f_{cl}	proportion of sky covered with cloud (1 - full cover)
f_D	proportion of total radiation that is diffuse
$f_D^{\,0}$	proportion of the diffuse radiation on cloudless days
f_{Di}	proportion of diffuse radiation intercepted by "solid" rows of plants assuming they are opaque cylinders
f_{di}	proportion of direct radiation intercepted by rows of plants
f_e	Microbial synthesis efficiency
f_h	Humification fraction
f_{ET}	correction factor to convert pan evaporation to potential evapotranspiration
f_{CPR}	proportion of carbon supply partitioned to root
f_{rg}	root growth reduction factor
f_{str}	water stress response function = proportion of potential transpiration rate that is actually used by plant
f_R	proportion of radiation not adsorbed by ozone or water vapor
$f_V^{\,c}$	correction factor for convection on hot, still days
F_L	latent heat of evaporation, J g^{-1}
g	gas content, g per cm^3 of the soil air
g_{surf}	gas content at the soil surface, g cm^{-3} of the soil air
g_{Ox}	soil oxygen content, g per cm^3 of soil air
G_g	surface gas flux component that does not depend on soil surface gas content, g cm^{-2} day^{-1}
G_T	surface heat flux component that does not depend on soil surface temperature, $J{\cdot}m^{-2}$ day^{-1}
h	soil water pressure head, cm
h_s	air-entry capillary head, cm
$h_{2,high}$	the lowest soil water pressure head at which plant can maintain the potential transpiration rate, cm
$h_{2,low}$	the highest soil water pressure head at which plant can maintain the potential transpiration rate, cm
H	soil suction, cm
H_c	height of top leaves above soil, cm
I	ionic strength of the soil solution, mol L^{-1}
I_e	effective ionic strength of the solution, mol L^{-1}
I_R	rain intensity, cm day^{-1}
J	day of the year (Julian date)
K_1	selectivity coefficient of Ca-Na cation exchange
K_2	selectivity coefficient of Mg-Na cation exchange
k	soil hydraulic conductivity, cm^3 of water per cm^2 of soil per day

$\bar{K}$	average soil hydraulic conductivity over element, cm day^{-1}
K_k	parameter of the soil hydraulic conductivity model, cm day^{-1}
K_s	saturated hydraulic conductivity of soil, cm day^{-1}
k_h	Potential mineralization rate fro the stable humus pool, day^{-1}
kL	Potential plant residue decomposition rate, day^{-1}
km	Potential rate of the organic fertilizer decomposition, day^{-1}
km	Potential rate of the organic fertilizer decomposition, day^{-1}
kn	Potential rate of nitrification, day^{-1}
L_M	density of mature roots in the soil cell, cm cm^{-3}
l_Y	length of existing mature roots in the soil cell, cm
l_Y	length of existing young roots in the soil cell, cm
m	concentration of non-associated ion or ion pair in the soil solution, mol L^{-1}
m'	total analytical concentrations of ions in soil solution, mol L^{-1}
m_R	root mass in soil cell, g
M	total contents of ions in the soil solution, soil adsorbing complex and soil solid salts expressed in mol per L of soil
M_{Calc}	content of solid calcite expressed in mol $CaCO_3$ per L of soil
M_{Gyps}	content of solid gypsum expressed in mol $CaCO_3$ per L of soil
n	parameter of the soil water retention model
nq	Ratio of the mineral nitrate amount to the mineral ammonium amount characteristic to the particular soil material
n_g	parameter of gas diffusion coefficient dependence on temperature
$n_{\Gamma,x}$	transversal component of the vector that has a unit length and is normal to the border of element
$n_{\Gamma,z}$	vertical component of the vector that has a unit length and is normal to the border of element
N	total number of observations in a data set
N_e	total number of elements
N_n	total number of nodes
N_P	total number of plants per meter of a row
$N_{S/D}$	nitrogen supply/demand ratio of the plant
P_L^0	leaf turgor pressure at the beginning of the interval, bar
P^0_{LT}	threshold leaf turgor pressure at the beginning of the time step, bar
P_{CO2}	partial pressure of CO_2 in the soil air, MPa
P_L	leaf turgor pressure, bar
P_{LT}	threshold leaf turgor pressure at the end of time step, bar
P_M	soil mechanical resistance pressure, bar
$P_{M,D}$	soil mechanical resistance pressure at dawn, bar
$P_{R,D}$	root turgor pressure at dawn, bar
$P_{R,T}$	threshold turgor pressure at which root growth starts to grow, bar
$q_{e,n}$	water flux through soil domain boundary to/from element, cm day^{-1}
q_x	volumetric water fluxes in 'x' direction, cm^3 of water per cm^2 of surface per day
q_z	volumetric water fluxes in 'z' direction, cm^3 of water per cm^2 of surface per day

Q_g	boundary gas flux, g cm^{-2} day^{-1} at the surface and g day^{-1} or g cm^{-1} day^{-1} for inner boundary nodes
$\mathrm{Q_T}$	boundary heat flux, J cm^{-2} day^{-1} at the surface and J day^{-1} or J cm^{-1} day for inner boundary nodes
r0	C/N ratio of the decomposer biomass and humification products
rL	C/N ratio of plant residues
rm	C/N ratio of the organic fertilizer
$\mathrm{r_c}$	crop surface roughness parameter
$\mathrm{r_M}$	total resistance of the water path from soil to leaf through mature roots, bar day g^{-1} cm^{-1}
r_{RM}	radial resistance of mature roots, bar day g^{-1} cm^{-1}
r_{RY}	radial resistance of young roots, bar day g^{-1} cm^{-1}
r_s	resistance of soil to water flow to roots, bar day g^{-1} cm^{-1}
r_v	root vascular resistance, bar day g^{-1} cm^{-1}
r_Y	total resistance of the water path from soil to leaf through mature roots, bar day g^{-1}cm^{-1}
R	actual radiation incindent at earth's surface, W·m^{-2}
R_n	actual radiation incindent at earth's surface at noon, W·m^{-2}
$R_{0,n}$	potential radiation incident at earth's surface at noon, W·m^{-2}
$R_{00,n}$	radiation incident at the top of the atmosphere at noon, W·m^{-2}
R_d	direct solar radiation flux at the earth's surface, W·m^{-2}
R_D	diffuse solar radiation flux at the earth's surface, W·m^{-2}
R_i	actual radiation incident at earth's surface, W·m^{-2}
R_I	daily solar radiation integral, J·m^{-2}
R_{Nc}	net radiation incident on the crop assuming complete cover, W·m^{-2}
R_{Ns}	net radiation on the soil surface assuming bare soil, W m^{-2}
R_s^e	equivalent total radiation falling on the soil, W m^{-2}
R_c^e	equivalent total radiation intercepted by the crop, W m^{-2}
R_u	net upward long wave radiation, W·m^{-2}
s_{Ca}	exchangeable calcium content expressed in mol per liter of soil
s_{Mg}	exchangeable magnesium content expressed in mol per liter of soil
s_{Na}	exchangeable sodium content expressed in mol per liter of soil
S	water extraction rate from the element (soil cell), day^{-1}
$\bar{S}$	average nodal water extraction rate from an element, day^{-1}
S'	nodal water extraction rate, day^{-1}
S_c	solute extraction rate, g cm^{-3} day^{-1}
$\bar{S}_c$	average nodal solute extraction rate, g cm^{-3} day^{-1}
S_c'	nodal solute extraction rate, g cm^{-3} day^{-1}
S_g	gas extraction rate, g cm^{-3} day^{-1}
$\bar{S}_g$	average nodal gas extraction rate, g cm^{-3} day^{-1}
S_g'	nodal gas extraction rate, g cm^{-3} day^{-1}
t	simulated time, days
t_{dn}	time of dawn, hours

t_d	daylength or photoperiod, hours
t_{dk}	time of dusk, hours
T	soil temperature,°C
t_{gr}	time counted after emergence, day
t_{maxhr}	time of maximum air temperature measured from dawn, hr
T_{min}	minimum air temperature during the day, °C
T_a	air temperature, °C
T_{dk}	air temperature at sunset, °C
T_{dry}	dry bulb temperature, °C
T_{max}	maximum air temperature during the day, °C
T_{mint}	minimum air temperature during the next day, °C
T_{surf}	temperature at the soil surface, °C
T_{wet}	wet bulb temperature, °C
T_y	air temperature at sunset of the previous day, °C
u	actual value of water uptake by roots from soil cells, cm day^{-1}
u^0	auxiliary value of water uptake by existing roots from soil cells, cm day^{-1}
U_1	total water uptake by old and new roots for the leaf water potential equal to its threshold value and satisfied shoot growth, cm day^{-1}
U_2	total water uptake by old and new roots when leaf turgor pressure equals to 2 bars and shoot does not grow, cm day^{-1}
U_B	total water uptake by old roots for the leaf water potential equal to its value at the beginning of time step, cm day^{-1}
V	wind speed at 2 m height, km hr^{-1}
W_R	average root dry weight per unit length, g·cm^{-1}
x	transversal coordinate (horizontal coordinate for planar flow and radial coordinate for the axisymmetrical flow), cm
X_{om}	volumetric fraction of an organic matter in soil, cm^3 per cm^3 of soil
X_{sm}	volume fraction of a mineral soil components
z	vertical coordinate directed upward, cm
Z	radius-vector of the Earth