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Jiří Šimůnek
USDA-ARS

Donald L. Suarez
USDA-ARS, donald.suarez@ars.usda.gov

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Modeling of Carbon Dioxide Transport and Production in Soil

1. Model Development

JIRÍ ŠIMŮNEK¹ AND DONALD L. SUAREZ

U.S. Salinity Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Riverside, California

Knowledge of the CO₂ concentration in the unsaturated zone is essential for prediction of solution chemistry in the vadose zone and groundwater recharge as well as for quantifying carbon source/sink terms as part of the global CO₂ mass balance. In this paper we present a predictive simulation model, SOILCO₂, based on process-oriented relationships. The model includes one-dimensional water flow and multiphase transport of CO₂ utilizing the Richards and the convection-dispersion equations, respectively, as well as heat flow and a CO₂ production model. The transport of CO₂ in the unsaturated zone can occur in both the liquid and gas phases. The gas transport equation accounts for production of CO₂ and uptake of CO₂ by plant roots associated with root water uptake. The CO₂ production model considers both microbial and root respiration which is dependent on water content, temperature, growth, salinity and plant and soil characteristics. Heat flow is included, since some gas transport parameters, partitioning coefficients and production parameters are strongly temperature dependent. The resulting set of partial differential equations is solved numerically using the finite element and finite difference methods.

1. INTRODUCTION

The presence of CO₂ exerts a major control on biological and chemical systems in the soil. Elevated CO₂ concentrations in the soil relative to the atmosphere have a direct effect on solution chemistry of the entire subsurface, since almost all groundwaters are recharged through a biologically active soil zone. Elevated CO₂ gas concentrations result in production of carbonic acid and subsequent dissociation of the weak acid which lowers pH. Therefore, prediction of the pH of nonacidic soil-water systems is not possible unless the CO₂ pressure is specified. Carbon dioxide concentrations are thus required for proper modeling of adsorption, precipitation-dissolution reactions (especially carbonate minerals) and transport of solutes to groundwater. Since CO₂ production is the result of respiration or oxidation processes, CO₂ partial pressures greater than 15–18 kPa are associated with anoxic conditions. These conditions have a dominant effect on the chemistry of redox sensitive elements such as Fe, Mn, As and Se (which in turn affect trace metals such as Cu, Zn and Pb), as well as an adverse effect on plant growth.

Due to the biological nature of the processes and the importance of soil aeration to plant growth, it is not surprising that most studies on soil CO₂ production and distribution have been reported by plant scientists. Because these measurements of CO₂ concentrations in soil have been related to agricultural concerns, primarily proper soil aeration, the measurements were usually taken only during the growing season [e.g., Witkamp and Frank, 1969; de Jong and Schapert, 1972; Edwards, 1975; Robbins, 1986; Buyanovsky and Wagner, 1983; Buyanovsky et al., 1986]. Several studies of hydrochemical interest consider data from an entire annual cycle [Rightmire, 1978; Reardon et al., 1979; Solomon and Cerling, 1987]. These chemical studies have primarily exam-

ined the seasonal variations in CO₂ concentration with the intent of relating these changes to solute composition.

Modeling of CO₂ spatial distribution or fluxes has been limited and has been attempted mostly by statistical correlation with specific parameters. For example, Buyanovsky and Wagner [1983] and Buyanovsky et al. [1986] measured CO₂ concentrations in the soil over several years and then evaluated the influence of air temperature, soil temperature and soil water content on the concentration of CO₂ using regression analysis. Brook et al. [1983] and Kiefer [1990] developed a regression model to predict the average CO₂ concentrations in soil using actual evapotranspiration, which was considered to reflect a variety of climate factors, such as temperature, radiation, precipitation, and soil water storage. These models are likely site specific or limited to the conditions encountered during the investigation. We anticipate that the limiting conditions for CO₂ production vary from one ecosystem to another and may depend on soil water content, temperature or nutrient status under different environmental conditions.

The existing nonempirical models are mostly based on the assumption that the principal transport mechanism for CO₂ is molecular diffusion [van Bavel, 1951; de Jong and Schapert, 1972; Solomon and Cerling, 1987] and do not consider other transport mechanisms nor the influence of water flow and airflow. Analytical solutions for oxygen transport based on Fick's second law of diffusion have been developed by Papendick and Runkles [1965, 1966] and Kowalik et al. [1979]. Solomon and Cerling [1987] developed a numerical model of CO₂ transport and applied this model for soil-air and for snow-air layers. Their model provides a good simulation of the effect of snowpack on soil CO₂ but does not meet all of our objectives for a predictive model since CO₂ production and the effective diffusion coefficient (which depend on soil water content) are not generated by the model, but fitted to the experimental data. Patwardhan et al. [1988] proposed the framework for a physically based model capable of describing the dynamic status in the root zone of not only CO₂, but also water, air, and oxygen.

In the last decade there has been much interest in the

¹On leave from Research Institute for Soil Reclamation and Protection, Prague, Czechoslovakia.

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development of theory to describe the transport of volatile organic chemicals [Jury *et al.*, 1983; Corapcioglu and Baehr, 1987; Baehr and Corapcioglu, 1987; Baehr, 1987; Sleep and Sykes, 1989; Mendoza and Frind, 1990]. This theory, developed for the transport of volatile organics, can be modified and applied to the modeling of CO₂ transport.

Our objective is to develop a process-based model suitable to predict the production, transport and spatial distribution of CO₂ in soil. We consider one-dimensional water flow in partially saturated porous media and multiphase transport of CO₂. The transport of CO₂ in the unsaturated zone can occur in both the liquid and gas phases. In addition to diffusion of CO₂ in the gas phase, which is generally recognized as the primary mechanism of CO₂ transport, other transport phenomena also need to be considered, such as convection and dispersion in the liquid phase and convection in the gas phase. The gas transport model requires a term for uptake of CO₂ by plant roots associated with root water uptake. An important requirement of the model is a CO₂ production submodel which considers microbial and root respiration, both strongly dependent on water content, temperature, CO₂ concentration, depth and time. The heat flow problem must be solved to account for the effect of soil temperature on the equation governing CO₂ transport, since some gas transport parameters, partitioning coefficients and the production parameters are strongly temperature dependent. The effect of temperature on water flow within the temperature range encountered in soils is relatively small in comparison with the effect of soil variability and uncertainty in the hydraulic parameters and therefore is not included in the model.

In this paper we develop a mathematical model, SOILCO₂, and discuss its numerical solution. The organization of the paper is as follows. In section 2 the governing equation for the water flow in the unsaturated zone is described together with initial and boundary conditions. The hydraulic characteristics and detailed description of the root growth model and water uptake by plant roots are also given in this section. In section 3 we derive the governing equation for the CO₂ transport in soil and discuss the boundary conditions and importance of individual transport mechanisms. Section 4 describes the production term of the CO₂ transport equation. It also contains a description of individual processes which influence the total CO₂ production in the soil profile. The description of heat transport is given in section 5. Section 6 deals with the numerical solution of the resulting system of equations for water flow, and CO₂ and heat transport.

2. WATER FLOW

The one-dimensional water movement in a partially saturated rigid porous medium is described by a modified form of the Richards equation under the assumptions that the air phase plays an insignificant role in the liquid flow process and that water flow due to a thermal gradient can be neglected:

$$\frac{\partial \theta_w}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial h}{\partial z} - 1 \right) \right] - Q \quad (1)$$

where h is the water pressure head [L] (terms expressed within brackets represent dimensions of the variable), θ_w is

the volumetric water content [$L^3 L^{-3}$], K is the unsaturated hydraulic conductivity function [LT^{-1}], t is time [T], z is the spatial coordinate [L] (positive downward) and Q is the sink/source term [$L^3 L^{-3} T^{-1}$], which encompasses the water uptake by plant roots. The assumptions and limitations of this prevalent approach have been discussed in detail by others [e.g., Nielsen *et al.*, 1986].

The unsaturated hydraulic properties of the porous medium are expressed by the hydraulic characteristics $K(h)$ and $\theta_w(h)$. The soil water retention, $\theta_w(h)$, and hydraulic conductivity, $K(h)$, functions are described with *van Genuchten's* [1980] closed form approach, based on the capillary model of *Mualem* [1976]:

$$\theta_w(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \quad (2)$$

and

$$K(h) = K_s S_e^{1/2} [1 - (1 - S_e^{1/m})^m]^2 \quad (3)$$

respectively, where

$$S_e = \frac{\theta_w - \theta_r}{\theta_s - \theta_r} \quad m = 1 - 1/n \quad n > 1 \quad (4)$$

and where θ_r and θ_s denote the residual and saturated water contents [$L^3 L^{-3}$], respectively, K_s is the saturated hydraulic conductivity [LT^{-1}], K_r is the relative hydraulic conductivity [dimensionless], S_e is relative saturation [dimensionless], and m , n , and α are the parameters of the hydraulic characteristics without any specific physical meaning. Both hydraulic characteristics are determined by a set of five parameters, θ_r , θ_s , α , n , and K_s .

The sink term, Q , is defined as the volume of water removed from a unit volume of soil per unit time due to plant water uptake. A detailed review of different expressions for the root water uptake can be found in the work by *Molz* [1981]. In the present model we use the expression proposed by *Feddes et al.* [1978], modified to include osmotic stress:

$$Q(h) = \alpha_\phi(h_\phi) \alpha_s(h) S_p \quad (5)$$

where S_p is the potential water uptake rate [$L^3 L^{-3} T^{-1}$] in the root zone, $\alpha_\phi(h_\phi)$ is the osmotic stress response function [dimensionless], h_ϕ is the osmotic head [L], and the water stress response function $\alpha_s(h)$ is a prescribed dimensionless function of the soil water pressure head ($0 \leq \alpha_s \leq 1$) [*van Genuchten*, 1987]:

$$\alpha_s(h) = \frac{1}{1 + (h/h_{50})^b} \quad (6)$$

where h_{50} [L] and b [dimensionless] are empirical constants. The parameter h_{50} represents the pressure head at which the water extraction rate is reduced by 50%. Note that this formulation of the water stress response function, $\alpha_s(h)$, in contrast to the expression of *Feddes et al.* [1978], does not consider the transpiration reduction near saturation. *Van Genuchten* [1987] indicates that this simplification is justified for relatively short periods of time at or near saturation. The osmotic stress response function, $\alpha_\phi(h_\phi)$, can also be represented by an expression analogous to (6), where both h parameters are replaced by corresponding osmotic heads. The potential water uptake rate in the root zone is expressed

as the product of the potential transpiration rate, T_p [LT^{-1}], and the normalized water uptake distribution function, $\beta(z)$ [L^{-1}], which describes the spatial variation of the potential water uptake rate, S_p , over the root zone:

$$S_p = \beta(z)T_p \quad (7)$$

There are many ways to express the function $\beta(z)$: constant with depth, linear [Feddes et al., 1978], exponential with a maximum at the soil surface [Raats, 1974], etc. Van Genuchten [1987] suggested the following depth-dependent root distribution function $\beta(z)$:

$$\begin{aligned} \beta(z) &= \frac{5}{3L_r} & z \leq 0.2L_r \\ \beta(z) &= \frac{25}{12L_r} \left(1 - \frac{z}{L_r}\right) & 0.2L_r < z \leq L_r \\ \beta(z) &= 0 & z > L_r \end{aligned} \quad (8)$$

where L_r is the root depth [L]. The actual transpiration rate, T_a , is obtained by integrating the root water uptake rate over the root zone as follows:

$$T_a = \int_0^{L_r} Q(h, z) dz = T_p \int_0^{L_r} \alpha_s(h) \alpha_\phi(h_\phi) \beta(z) dz \quad (9)$$

The root depth, L_r , can be either constant or variable during the simulation. For annual vegetation a growth model is required to simulate the change in rooting depth with time. In this model we consider the root depth to be the product of the maximum rooting depth, L_m [L], and the root growth coefficient, $f_r(t)$ [dimensionless]:

$$L_r(t) = L_m f_r(t) \quad (10)$$

To calculate the root growth coefficient, $f_r(t)$, we combined the classical Verhulst-Pearl logistic growth function with the growth degree day (GDD) or heat unit concept [Gilmore and Rogers, 1958]. The logistic growth function is used to describe the biological growth at constant temperature, whereas the heat unit model is utilized for determining the time between planting and maturity of the plant. The heat unit model cannot be used directly to predict biomass during the growth stage since it would predict a linear growth with time at constant temperature. By combining the heat unit concept with the classical logistic growth function, we incorporate both time and temperature dependence on growth.

For the growth degree day function we used a modified version of the relation developed by Logan and Boyland [1983], who assumed that this function is fully defined by the temperature, T [K], which can be expressed by a sine function to approximate the behavior of temperature during the day, and by the three temperature limits, T_1 , T_2 , and T_3 [K]. When the actual temperature is below the base value T_1 , plants register little or no effective growth. The plant growth reaches its maximum level at temperature T_2 and remains unchanged for some interval up to a maximum temperature T_3 , above which increased temperature has a negative effect on growth. From this consideration, we propose the following dimensionless growth function:

$$g(t) = 0 \quad t \leq t_p; t \geq t_h \quad (11a)$$

$$g(t) = \frac{1}{T_{Bas}} \left[\int \delta(T - T_1) dt - \int \delta(T - T_2) dt - \int \delta(T - T_3) dt \right] \quad t \in (t_p, t_m) \quad (11b)$$

$$g(t) = 1 \quad t \in (t_m, t_h) \quad (11c)$$

where T_{Bas} are the heat units [KT] necessary for the plant to mature and the roots to reach the maximum rooting depth, t_p , t_m , and t_h represent time of planting, time at which the maximum rooting depth is reached and time of harvesting, respectively; and parameter δ [dimensionless] introduces into the heat unit concept the reduction due to the water and osmotic stress. The expression inside the brackets of (11) reaches value T_{Bas} at time t_m when roots reach the maximum rooting depth. The individual integrals in (11) are evaluated only when the particular arguments are positive. Parameter δ is defined as the ratio of the actual to potential transpiration rates:

$$\delta = T_a/T_p \quad (12)$$

Gallagher and Biscoe [1979] have indicated that barley plant growth was better related to soil temperature at the 10 mm depth than the commonly utilized air temperature in the early part of the growing season. However, air temperature provides a better relation for the majority of plant development and the GDD data base for crops is almost exclusively available only with air temperature.

Biomass or root development during the growth stage can also be expressed by the classical Verhulst-Pearl logistic growth function,

$$f_r(t) = \frac{L_0}{L_0 + (L_m - L_0)e^{-rt}} \quad (13)$$

where L_0 is the initial value of the rooting depth at the beginning of the growth period [L] and r is the growth rate [T^{-1}].

Both growth functions (11) and (13) can be used directly to model the root growth. However, to avoid the drawbacks of both concepts, as discussed above, we combine (11) and (13) by substituting the growth function calculated from the heat unit concept (11) for the time factor in the logistic growth function (13):

$$t = t_m g(t) \quad (14)$$

where t_m is the time when GDD reaches the required value for the specific plant species (T_{Bas}). This value is not known a priori; only the product rt_m must be known and that can be selected, for example, so that $f_r(t)$ equals 0.99 for $g(t) = 1$.

The initial condition for the soil water pressure head is given by

$$h(z, 0) = h_i(z) \quad (15)$$

where h_i [L] is a prescribed function of z .

One of the following boundary conditions must be specified at the soil surface or at the bottom of the soil profile:

$$h(z, t) = h_0(t) \quad z = 0; z = L \quad (16a)$$

$$-K \frac{\partial h}{\partial z} + K = q_{w0}(t) \quad z = 0; z = L \quad (16b)$$

$$\frac{\partial h}{\partial z} = 0 \quad z = L \quad (16c)$$

where h_0 [L] and q_{w0} [LT^{-1}] are the prescribed pressure head and soil water flux at the boundary, respectively, and L is the depth of the soil profile.

In addition to the system-independent boundary conditions given by (16), we consider one system-dependent boundary condition which cannot be defined a priori. Since the soil surface is exposed to the atmosphere, the potential flux is controlled by external conditions, while the actual flux depends on the antecedent soil water conditions. The boundary condition at the soil surface changes from prescribed flux to prescribed head, when the pressure head at the soil surface reaches either of the limiting points of the interval (h_A , h_B). The values h_A and h_B [L] specify the minimum and maximum pressure heads allowed under the prevailing soil conditions, respectively. The value h_A is determined from the equilibrium conditions between soil water and atmospheric water vapor [Feddes *et al.*, 1978], whereas h_B is usually set to zero and, if positive, it represents a small layer of water ponded at the soil surface which can form during heavy rains before initiation of runoff.

3. TRANSPORT OF CARBON DIOXIDE

Gas transport in the unsaturated zone is a complex physical process that includes three general transport mechanisms [Massmann and Farrier, 1992]: Knudsen diffusion, multicomponent molecular diffusion and viscous flow. Thorstenson and Pollock [1989] presented the equations that describe these transport mechanisms in a multicomponent gas mixture, as well as the Stefan-Maxwell approximation of these equations, where Knudsen diffusion and viscous flow are neglected. The original equations, as well as the Stefan-Maxwell approximation, are fully coupled and generally highly nonlinear. However, Massmann and Farrier [1992] showed that gas fluxes in the unsaturated zone can be simulated using the single-component transport equation if the gas permeability of the porous media is greater than about 10^{-10} cm². For these conditions the effects of Knudsen diffusion can be neglected. They also showed that overestimation of the gas fluxes using the single-component advection-diffusion equation becomes quite large for permeabilities of the order of 10^{-12} to 10^{-13} cm². Since permeabilities smaller than 10^{-12} cm² occur only for very fine grained materials or for soils close to saturation, use of the transport equation based on Fick's law to represent diffusive flux seems to be justified and adequate.

We assume that the CO₂ transport in the unsaturated zone can occur in both the liquid and gas phases. Furthermore, we consider that the CO₂ concentration in the soil is governed by two transport mechanisms [Patwardhan *et al.*, 1988], convective transport and diffusive transport in both gas and aqueous phases, and by CO₂ production and/or removal. Thus the one-dimensional CO₂ transport is described by the following mass balance equation:

$$\frac{\partial c_T}{\partial t} = -\frac{\partial}{\partial z} (J_{da} + J_{dw} + J_{ca} + J_{cw}) - Qc_w + S \quad (17)$$

where J_{da} describes the CO₂ flux caused by diffusion in the gas phase [LT^{-1}]; J_{dw} , the CO₂ flux caused by dispersion in the dissolved phase [LT^{-1}]; J_{ca} , the CO₂ flux caused by convection in the gas phase [LT^{-1}]; and J_{cw} , the CO₂ flux caused by convection in the dissolved phase [LT^{-1}]. The term c_T is the total volumetric concentration of CO₂ [L^3L^{-3}] and S is the CO₂ production/sink term [$L^3L^{-3}T^{-1}$]. The term Qc_w represents the dissolved CO₂ removed from the soil by root water uptake. This assumes that when plants take up water the dissolved CO₂ is also removed from the soil-water system. The individual terms in (17) can be defined [Patwardhan *et al.*, 1988] as

$$J_{da} = -\theta_a D_a \frac{\partial c_a}{\partial z} \quad (18)$$

$$J_{dw} = -\theta_w D_w \frac{\partial c_w}{\partial z} \quad (19)$$

$$J_{ca} = q_a c_a \quad (20)$$

$$J_{cw} = q_w c_w \quad (21)$$

where c_w and c_a are the volumetric concentrations of CO₂ in the dissolved phase and gas phase [L^3L^{-3}], respectively, D_a is the effective soil matrix diffusion coefficient of CO₂ in the gas phase [L^2T^{-1}], D_w is the effective soil matrix dispersion coefficient of CO₂ in the dissolved phase [L^2T^{-1}], q_a is the soil air flux [LT^{-1}], q_w is the soil water flux [LT^{-1}] and θ_a is the volumetric air content [L^3L^{-3}].

The total CO₂ concentration, c_T [L^3L^{-3}], is defined as the sum of CO₂ in the gas and dissolved phases:

$$c_T = c_a \theta_a + c_w \theta_w \quad (22)$$

After substituting (18)–(22) into (17) we obtain

$$\frac{\partial(c_a \theta_a + c_w \theta_w)}{\partial t} = \frac{\partial}{\partial z} \theta_a D_a \frac{\partial c_a}{\partial z} + \frac{\partial}{\partial z} \theta_w D_w \frac{\partial c_w}{\partial z} - \frac{\partial}{\partial z} q_a c_a - \frac{\partial}{\partial z} q_w c_w - Qc_w + S \quad (23)$$

The total aqueous phase CO₂, c_w , is defined as the sum of CO₂(aq) and H₂CO₃, and is related to the CO₂ concentration in the gas phase by [Stumm and Morgan, 1981]

$$c_w = K_H R T c_a \quad (24)$$

where K_H is the Henry's law constant [$nT^2M^{-1}L^{-2}$], R is the universal gas constant [$ML^2T^{-2}K^{-1}n^{-1}$] (8.314 kg m² s⁻² K⁻¹ mol⁻¹) and T is the absolute temperature [K]. The value of K_H as a function of temperature is taken from Harned and Davis [1943]. We do not consider the interaction of dissolved CO₂ with the solid phase at this time, as this requires a coupled, multicomponent chemical speciation model. Also, the quantity of CO₂ added or removed by mineral dissolution/precipitation reactions is relatively small compared to the production and flux values in most instances.

We define the dispersion coefficients, D_w , and the diffusion coefficient, D_a , as

$$D_w = D_{ws}\tau_w + \lambda_w \left| \frac{q_w}{\theta_w} \right| = D_{ws} \frac{\theta_w^{7/3}}{p^2} + \lambda_w \left| \frac{q_w}{\theta_w} \right| \quad (25)$$

$$D_a = D_{as}\tau_a = D_{as} \frac{\theta_a^{7/3}}{p^2} \quad (26)$$

where D_{as} and D_{ws} are the diffusion coefficients [L^2T^{-1}] of CO₂ in the gas and dissolved phase, respectively, τ_a and τ_w are tortuosity factors [LL^{-1}] in both phases, p is porosity [L^3L^{-3}], and λ_w is the dispersivity in the water phase [L]. The tortuosity factors τ_a and τ_w include not only the tortuosity of the flow paths but also the amount of air and liquid space available for diffusion, respectively. The tortuosity factors in both phases are defined in a manner similar to that used by *Millington and Quirk* [1961]. The first term in (25) represents the diffusion component and the second term the hydrodynamic component of the dispersion coefficient. We did not consider the mechanical dispersion in the gas phase since diffusion is the dominant process of CO₂ transport in this phase unless the air velocity is very high. The diffusion coefficients D_{as} and D_{ws} , as functions of temperature, are taken from *Glinski and Stepniewski* [1985].

Substituting (24) into (23) gives

$$\frac{\partial \theta_a R_f c_a}{\partial t} = \frac{\partial}{\partial z} D_E \frac{\partial c_a}{\partial z} - \frac{\partial}{\partial z} q_E c_a - Q^* c_a + S \quad (27)$$

where R_f is the retardation factor [dimensionless], D_E is the effective dispersion coefficient in the soil matrix [L^2T^{-1}], q_E is the effective velocity of CO₂ [LT^{-1}], Q^* is the CO₂ uptake rate [T^{-1}] associated with root water uptake and θ_a is the volumetric air content [L^3L^{-3}]. These parameters are defined as

$$R_f = 1 + \frac{K_H RT \theta_w}{\theta_a} \quad (28)$$

$$D_E = \theta_a D_a + K_H RT \theta_w D_w \quad (29)$$

$$q_E = q_a + K_H RT q_w \quad (30)$$

$$\theta_a = p - \theta_w \quad (31)$$

$$Q^* = Q K_H RT \quad (32)$$

Equation (27) is a nonlinear partial differential equation where, except for c_a and q_a , all parameters are either known or are obtained from solution of the water flow equation. The nonlinearity of (27) is caused by the term S which is dependent on CO₂ concentration, c_a . Since we do not consider coupled water and air movement, the flux of air, q_a , is unknown and thus it is necessary to make some additional assumptions. One possibility is to assume that the advection of CO₂ in response to the total pressure gradient is not important compared to CO₂ diffusion, and therefore to assume a stagnant gas phase and consider only diffusion transport with the gas phase ($q_a = 0$). Another possibility is to consider that because of the much lower viscosity of air in comparison to water, significant gas flow can be caused by a relatively small pressure gradient. Thus, only rarely will the gas phase not be at atmospheric pressure throughout the unsaturated zone. Therefore under most conditions the compressibility of the air can be neglected. Then with the

assumption that the air flux is zero at the lower soil boundary and that the water volume changes in the soil profile caused by the water flow must be immediately matched by the corresponding changes in the gas volume, we obtain the following equation:

$$q_a(z) = q_w(L) - q_w(z) + \int_z^{L_r} Q(z) dz \quad (33)$$

This latter assumption seems to be reasonable, since when water leaves the soil system due to evaporation and root water uptake, air enters the soil at the surface and, vice versa, when water enters the soil during precipitation and irrigation events, soil air is escaping. Only in the case of saturation (typically at the soil surface) does the condition arise that air cannot escape and is compressed under the wetting front.

The initial condition for the CO₂ concentration in the gas phase is given by

$$c_a(z, 0) = c_{ai}(z) \quad (34)$$

where $c_{ai}(z)$ is a prescribed function of z [L^3L^{-3}].

The first-type or the third-type boundary conditions may be specified at the surface (or at the bottom) of the soil profile:

$$c_a(0, t) = c_{a0} \quad (35)$$

$$-D_E \frac{\partial c_a}{\partial z} + q_E c_a = q_{E0} c_{a0} \quad (36)$$

where q_{E0} is a prescribed CO₂ effective total flux [LT^{-1}] and c_{a0} is the concentration [L^3L^{-3}] associated with this flux or prescribed at the boundary.

At the soil surface, c_{a0} represents the equilibrium concentration of CO₂ in the atmosphere (0.035%). In this case the first-type boundary condition (35) allows the maximum CO₂ flux into the atmosphere. It is difficult to apply the third-type boundary condition (36), since the parameter q_E includes both the soil air and soil water fluxes, which are not known a priori and are results obtained from solution of the water flow equation. In this model we use the boundary condition (36) only for $q_{E0} > 0$ and then we assume that the concentration c_{a0} is equal to the equilibrium CO₂ concentration in the atmosphere. For $q_{E0} \leq 0$ we use the boundary condition (35), where c_{a0} is again equal to the equilibrium CO₂ concentration in the atmosphere. Another option is to neglect the convective fluxes and to assume that there is a stagnant boundary layer of thickness d [L] at the soil surface through which the transport of a gas occurs by vapor diffusion only [*Jury et al.*, 1983, 1990; *Sleep and Sykes*, 1989], which leads to the following equation

$$-D_E \frac{\partial c_a}{\partial z} + q_E c_a = \frac{D_{as}}{d} (c_{as} - c_{atm}) \quad (37)$$

where c_{as} is the concentration in the soil gas at the soil surface [L^3L^{-3}] and c_{atm} is the concentration at the top of the stagnant boundary layer [L^3L^{-3}]. *Jury et al.* [1983] referred to D_{as}/d as the boundary transfer coefficient [LT^{-1}] and discussed ways of estimating this coefficient.

At the bottom of the soil profile either a continuous concentration profile is assumed,

$$\frac{\partial c_a}{\partial z}(L, t) = 0 \quad (38)$$

or the third-type boundary condition (36) may be used, in which case the convective fluxes q_{a0} and q_a are equal to zero as discussed above. Boundary condition (38) implies that the dispersive flux is equal to zero and that the flux through the boundary is only due to convection. A discussion of the applicability of different types of boundary conditions is given by, among others, *Baehr* [1987] and *Patwardhan et al.* [1988].

The existing nonempirical models are mostly based on the assumption that the principal transport mechanism for CO₂ is molecular diffusion [*van Bavel*, 1951; *de Jong and Schapert*, 1972; *Solomon and Cerling*, 1987] and do not consider other transport mechanisms nor the influence of water flow and airflow. In the companion paper [*Suarez and Šimůnek*, this issue] we show that water flow can have a significant effect on the soil CO₂ concentration profiles by redistributing CO₂ in the direction of flow. Thus downward flow increases the CO₂ concentrations in the lower horizons and upward flow decreases the concentration of CO₂ in the lower horizons. Diffusion in the liquid phase is usually neglected because the diffusion coefficient of CO₂ in the gas phase, D_{as} , is about 10,000 times higher than the diffusion coefficient in the liquid phase, D_{ws} . Therefore the diffusion in the gas phase is dominant within almost the entire range of water contents observed in the field. However, it can be shown that near saturation, due to the combined effect of tortuosity in both phases, the contribution of liquid phase diffusion to the effective diffusion coefficient in the soil matrix, D_E , is higher than the contribution by gas phase diffusion. Both contributions are equal when the volumetric air content, θ_a , is about 6% of the total porosity, as can be calculated from the following expression derived from (25), (26) and (29) for stagnant soil water:

$$\frac{\theta_a}{p} = \left[\left(\frac{D_{as}}{K_H R T D_{ws}} \right)^{3/10} + 1 \right]^{-1} \quad (39)$$

A similar expression can be derived for the minimum value of the effective diffusion coefficient, D_E , only the exponent 3/10 must be replaced by 3/7. This minimum is reached when only about 2% of the total porosity is occupied by air. At this point the effective diffusion coefficient, D_E , is about 5 orders of magnitude smaller than the maximum possible effective diffusion coefficient for completely dry soil. Nevertheless, diffusion continues, even if only at a very diminished rate.

4. PRODUCTION OF CARBON DIOXIDE

The mechanism of production/decay of CO₂ is a complex process that includes not only biological processes, such as the production of CO₂ by soil microbes and plant roots, but also chemical reactions with mineral and organic components, respiration of soil microfauna, etc. Since processes other than the biological ones are generally of relatively minor importance for the CO₂ balance in the soil, we do not include them in our present model for CO₂ production. The production of CO₂ is influenced by many environmental factors, the most important ones being water content and temperature. The changes in CO₂ concentration and corresponding changes in oxygen concentration in the soil atmo-

sphere may affect the CO₂ production rate. Other important factors affecting the CO₂ production are, for example, soil depth, nutrient status of the soil, and agricultural practices, such as plowing or application of fertilizers, etc. An overview of the rather extensive literature on the processes influencing the production of CO₂ is provided by *Singh and Gupta* [1977] and *Glinski and Stepniewski* [1985].

We assume that the individual CO₂ production processes are additive (equation (40)) and that it is possible to superpose individual mechanisms which reduce production from the optimal value (equation (41)). The production of CO₂ is then considered as the sum of the production by the soil microorganisms, γ_s [$L^3 L^{-3} T^{-1}$], and the production by plant roots, γ_p [$L^3 L^{-3} T^{-1}$]:

$$S = \gamma_s + \gamma_p \quad (40)$$

$$\gamma_s = \gamma_{s0} \prod_i f_{si} \quad \gamma_p = \gamma_{p0} \prod_i f_{pi} \quad (41)$$

$$\prod_i f_i = f(z)f(h)f(T)f(c_a)f(h_\phi)f(t) \quad (42)$$

where the subscript s refers to soil microorganisms and the subscript p refers to plant roots, and the various reduction coefficients are represented by $f(z)$ for that dependent on the depth [L^{-1}], $f(T)$ for that dependent on the temperature [dimensionless], $f(h)$ for that dependent on the pressure head (the soil water content) [dimensionless], $f(c_a)$ for that dependent on the CO₂ concentration [dimensionless], $f(h_\phi)$ for that dependent on the osmotic head [dimensionless], and $f(t)$ for that dependent on time [dimensionless]. The parameters γ_{s0} and γ_{p0} represent the optimal CO₂ production by the soil microorganisms or plant roots for the whole soil profile at 20°C under optimal water, solute and CO₂ concentration conditions [$L^3 L^{-2} T^{-1}$], respectively. An expression similar to (41) was used by *Hansen and Aslyng* [1984] to represent nitrogen mineralization.

The CO₂ production decreases sharply with depth as a result of a decrease in root mass and readily decomposable organic matter. *Glinski and Stepniewski* [1985] stated that over 90% of soil respiration activity is concentrated in the humus horizon of the soil. There are many possible expressions to relate the dependence of the production term $f_s(z)$ on soil depth. One example is an expression similar to the normalized distribution function $\beta(z)$ given by *van Genuchten* [1987] for the root water uptake. Another possibility is to use the exponential distribution with depth [*Raats*, 1974],

$$f_s(z) = ae^{-az} \quad (43)$$

where a is an empirical constant [L^{-1}]. The exponential function is multiplied by a constant a in order to insure that the integral from the soil surface to infinite depth of the function $f_s(z)$ is equal to unity. However, since the depth of the soil profile or the root depth is finite, the distribution function $f_s(z)$ must always be normalized. We assume that the dependence of the CO₂ production by plant roots corresponds to the root growth function $L_r(t)$ and the distribution function $\beta(z)$ used for the water uptake by plant roots.

The dependence of CO₂ production on water content has been studied by many researchers [e.g., *Miller and Johnson*, 1964; *Ekpete and Cornfield*, 1965; *Rixon*, 1968; *Williams et al.*, 1972; *Bridge and Rixon*, 1976]. With respect to the water

requirement of microbes, there is a reduction in the respiration rate at low as well as at high water contents. Low accessibility of soil water causes a reduction in CO₂ production at high pressure heads [Ektepe and Cornfield, 1965; Wilson and Griffin, 1975]. The observed reduction of the respiration rate at low pressure heads is explained by the unavailability of oxygen because of the high water content and, therefore, its low diffusion rate through the soil. On the basis of the foregoing discussion and in view of the experimental data of Williams *et al.* [1972] and Rixon [1968], the CO₂ reduction coefficient $f_s(h)$ as a function of the soil water content for soil microorganisms is expressed as

$$f_s(h) = \frac{\log |h| - \log |h_1|}{\log |h_2| - \log |h_1|} \quad h \in (h_2, h_1) \quad (44a)$$

$$f_s(h) = \frac{\log |h| - \log |h_3|}{\log |h_2| - \log |h_3|} \quad h \in (h_3, h_2) \quad (44b)$$

$$f_s(h) = 0 \quad h \in (-\infty, h_3) \cup (h_1, +\infty) \quad (44c)$$

where h_2 is the pressure head when CO₂ production is optimal [L] and h_3 is the pressure head when production ceases [L]. Note that the pressure head reduction function is assumed to be zero close to saturation for water pressure heads higher than h_1 [L]. The similar "anaerobiosis point" is defined in the dimensionless water stress response function for the root water uptake by Feddes *et al.* [1978]. Glinski and Stepniewski [1985] stated that the maximum soil microbial respiration rate is usually within a soil water pressure head interval of 0.01–1 MPa. The dependence of the reduction terms $f_p(h)$ and $f_p(h_\phi)$ on soil water pressure head and osmotic head, respectively, are represented by expressions similar to the reduction functions $\alpha_s(h)$ and $\alpha_\phi(h_\phi)$ described by (6).

The influence of temperature on chemical processes is described by the Arrhenius equation [Stumm and Morgan, 1981]

$$\ln q = -(E/RT) + a \quad (45)$$

where T is absolute temperature [K], E the activation energy of the reaction [$ML^2T^{-2}n^{-1}$] and q is the reaction rate constant. In our application q represents the rate of CO₂ production. This equation together with the Van't Hoff equation was successfully used by many authors to represent the influence of temperature on soil and root CO₂ production [Carey and Berry, 1978; Howard and Howard, 1979; Ross and Cairns, 1978]. Assuming that $f(T) = 1$ for the temperature $T_{20} = 293.15$ K (20°C), then the temperature reduction coefficient can be expressed as

$$f(T) = \exp \left[\frac{E(T - T_{20})}{RTT_{20}} \right] \quad (46)$$

The use of the term "reduction" coefficient with $f(T)$ may seem inappropriate since this coefficient is higher than 1 for temperatures greater than 20°C. We use the term to characterize the change in production with temperature, with values greater than 1 above 20°C and less than 1 below 20°C.

The dependence of CO₂ production on its own concentration (actually O₂ deficiency) can be expressed with the Michaelis-Menton equation [Glinski and Stepniewski, 1985],

$$q = \frac{q_{\max}}{1 + (K_M/c_{O_2})} \quad (47)$$

where K_M is the Michaelis constant [L^3L^{-3}], i.e., the oxygen concentration c_{O_2} , at which the oxygen uptake is equal to $1/2 q_{\max}$, and where q is oxygen uptake rate and q_{\max} is the maximum oxygen uptake rate [$L^3L^{-3}T^{-1}$]. Assuming that the respiratory quotient is equal to unity, then the Michaelis constant for the CO₂ concentration, $K_M^* = 0.21 - K_M$, and $c_a = 0.21 - c_{O_2}$; the reduction coefficient is then given by

$$f(c_a) = \frac{c_{O_2}}{c_{O_2} + K_M} = \frac{0.21 - c_a}{0.42 - c_a - K_M^*} \quad (48)$$

The disadvantage of this expression is that if $c_a = 0$ the value for $f(c_a)$ is not equal to one. Therefore, the values of the optimal production γ_{p0} and γ_{s0} must be adjusted accordingly.

The coefficient $f(t)$ introduces a time dependence into the production term. This coefficient should describe the diurnal and seasonal dynamics of soil and plant respiration. We assume that the diurnal dynamics for both soil and plant respiration is reflected by the temperature-dependent coefficient $f(T)$ and that the seasonal dynamics of soil production of CO₂ is sufficiently described by other reduction coefficients. Therefore, we use this coefficient only for the description of the changes in CO₂ production caused by the different growth stages of plants. For example, we use the same approach for annual vegetation as we used for root growth ((11)–(14)). The coefficient $f(t)$ can be described either in the same way as coefficient $g(t)$ when the GDD concept is used (equation (11)), possibly with different constants, or in combination with the classical Verhulst-Pearl logistic function (equation (13)). In this case, the maximum and initial values of the root depth should be replaced by the corresponding values of CO₂ production by plant roots.

Finally, the actual CO₂ production rate, S_T [$L^3L^{-2}T^{-1}$], is obtained by integrating the CO₂ production throughout the whole soil profile as follows:

$$\begin{aligned} S_T &= \int_0^L S \, dz \\ &= \gamma_{s0} f_s(t) \int_0^L f_s(z) f_s(h) f_s(T) f_s(c_a) f_s(h_\phi) \, dz \\ &+ \gamma_{p0} f_p(t) \int_0^{L_r} f_p(z) f_p(h) f_p(T) f_p(c_a) f_p(h_\phi) \, dz \quad (49) \end{aligned}$$

5. HEAT TRANSPORT

Neglecting the effect of water vapor diffusion on transport, one-dimensional heat transport can be described as [Sophocleous, 1979]

$$C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[\lambda(\theta_w) \frac{\partial T}{\partial z} \right] - C_w \frac{\partial q_w T}{\partial z} \quad (50)$$

where $\lambda(\theta_w)$ is the coefficient of the apparent thermal conductivity of the soil [$WL^{-1}K^{-1}$] and C and C_w are the

volumetric heat capacities [$JL^{-3}K^{-1}$] of the porous medium and the liquid phase, respectively. Volumetric heat capacity is defined as the product of the bulk density and gravimetric heat capacity. The first term on the right-hand side of (50) represents the heat flow due to conduction and the second term the heat transported by the flowing water. We do not consider the transfer of latent heat by vapor movement. According to *de Vries* [1963] the volumetric heat capacity can be expressed as

$$C = C_n\theta_n + C_o\theta_o + C_w\theta_w + C_a\theta_a \approx (1.92\theta_n + 2.51\theta_o + 4.18\theta_w)10^6 \quad (J m^{-3} \text{ }^\circ\text{C}^{-1}) \quad (51)$$

where θ is the volumetric fraction [L^3L^{-3}] and subscripts n , o , a , and w represent solid phase, organic matter, gas phase and liquid phase, respectively. The coefficient of apparent thermal conductivity $\lambda(\theta)$ combines the thermal conductivity $\lambda_0(\theta)$ of the porous medium (solid plus water) in the absence of flow and the macrodispersivity, which is a linear function of the velocity [*de Marsily*, 1986]:

$$\lambda(\theta) = \lambda_0(\theta) + \beta_t C_w |q_w| \quad (52)$$

where β_t is thermal dispersivity [L]. Thermal conductivity is described by *Chung and Horton* [1987] with the equation

$$\lambda_0(\theta) = b_1 + b_2\theta_w + b_3\theta_w^{0.5} \quad (53)$$

where b_1 , b_2 and b_3 are empirical parameters.

The upper boundary condition for soil temperature is determined by a sine function as follows [*Kirkham and Powers*, 1972]:

$$T = T_0 + A \sin \left(\frac{2\pi t^*}{p_t} - \frac{7\pi}{12} \right) \quad (54)$$

where p_t is a period of time [T] necessary to complete one cycle of the sine wave (taken to be 1 day), T_0 is the average temperature at the soil surface [K] during the period p_t , A is the amplitude of the sine wave [K] and t^* is the local time [T] within the period p_t . The second part of the sine term is included to allow the highest temperature to occur at $t^* = 1$ P.M. The lower boundary condition is assumed to be either a constant temperature measured in the soil profile or a zero gradient at the bottom of the soil profile.

6. NUMERICAL SOLUTION OF THE GOVERNING EQUATIONS

The method of finite differences is used for both the space and time discretization of the Richards equation (1). The fully implicit scheme is employed for the time discretization. The "mass-conservative" method proposed by *Celia et al.* [1990] is used for the time derivative term of (1). The partial differential equations describing the CO₂ (equation (27)) and heat transport (equation (50)) are both solved using the standard Galerkin finite element method for the space discretization and the method of finite differences for the time discretization. The Crank-Nicholson scheme is used for both transport equations. The development of the discrete equations will not be presented here since standard formulations are used, details of which can be found elsewhere [e.g., *Pinder and Gray*, 1977; *Huyakorn and Pinder*, 1983].

The solution procedure for each time step can be de-

scribed as follows. The water flow, heat and CO₂ transport equations are solved sequentially. A Picard iterative process is used first to solve the nonlinear water flow equation (1). For each iteration a system of linearized algebraic equations is derived and solved using Gaussian elimination. The coefficients are then reevaluated using the first solution, and the new equations are solved again. The iterative process continues until a satisfactory degree of convergence is obtained. After achieving convergence, the solution of the heat transport equation is implemented. This is done by first determining the nodal values of the fluid flux from nodal values of the pressure head applying Darcy's law. Values for the water content, known directly from the solution of the water flow equation, and the fluid fluxes are subsequently used as input to the heat transport equation (50), which leads again to a system of linear algebraic equations. Since (50) is linear, an iterative procedure is not necessary. The nodal values of water content, velocity and temperature, obtained from the solution of the water flow and heat transport equations, are then used to evaluate the coefficients in the discretized CO₂ transport equation (27). The CO₂ transport equation (27) is not linear because the production term S is dependent on the CO₂ concentration. To avoid the necessity to iterate, we evaluate this term with the CO₂ concentration from the earlier time step. Both sets of linear equations, obtained by discretizing the two transport equations, are also solved by Gaussian elimination. Since the water flow is considered to be invariant with respect to temperature and CO₂ transport, and similarly heat transport is considered to be invariant with respect to CO₂ transport, it is not necessary to solve all the equations simultaneously, and one may proceed directly to the next time step once the transport equations are solved for the current time step.

7. SUMMARY AND CONCLUSIONS

In this paper we developed the SOILCO₂ model, suitable to predict the production, transport and distribution of CO₂ in soil, based on process-oriented relationships. We considered one-dimensional water flow in partially saturated porous media and multiphase transport of CO₂, utilizing the Richards and convection-dispersion equations, respectively. It is assumed that the changes in the total pressure of the air phase do not affect the water movement. We developed a new model for root growth based on a combination of the heat unit concept and the classical logistic growth function. Since CO₂ transport in the unsaturated zone can occur both in the liquid and gas phases, the transport phenomena considered were convection and dispersion in the liquid phase and convection and diffusion in the gas phase. Dispersion was assumed to be the sum of molecular diffusion and hydrodynamic dispersion. The gas transport equation accounts for production of CO₂ and uptake of CO₂ by plant roots in connection with root water uptake. Either the gas phase was considered to be stagnant, or a simplified model was proposed for convection. The CO₂ production model considered both microbial and root respiration. The effects of water content, depth, temperature, CO₂ concentration, osmotic potential and time on the CO₂ production term were introduced through reduction coefficients. The water content, osmotic stress and depth reduction coefficients for plant root respiration were considered to be the same as the reduction coefficients for root water uptake. The tempera-

ture dependence of both productions was expressed with the Arrhenius equation. Since some gas transport parameters, partitioning coefficients and production parameters are strongly temperature dependent, heat flow was also calculated and soil temperature was considered in solving equations governing CO₂ transport.

In paper 2 [Suarez and Šimůnek, this issue] we show that the inclusion of water flow into the CO₂ transport model is necessary because predicted CO₂ concentrations are highly dependent on soil water content. In paper 2 we provide an evaluation of the sensitivity of the SOILCO₂ model to various parameters. We also demonstrate the predictive capabilities of the model by comparison of model simulations to published field data.

NOTATION

a	parameter in the exponential depth reduction function [L^{-1}].	h_1, h_3	pressure head when CO ₂ production ceases [L].
A	temperature amplitude of the sine wave [K].	h_{50}	empirical constant in the water stress response function [L].
b	empirical constant in the water stress response function [dimensionless].	J_{ca}, J_{cw}	CO ₂ fluxes caused by convection in the gas and liquid phase, respectively [LT^{-1}].
b_1, b_2, b_3	parameters of the thermal conductivity function [$WL^{-1}K^{-1}$].	J_{da}, J_{dw}	CO ₂ fluxes caused by diffusion in the gas and liquid phase, respectively [LT^{-1}].
c_a, c_w	CO ₂ concentrations in the gas and liquid phase, respectively [L^3L^{-3}].	K	unsaturated hydraulic conductivity function [LT^{-1}].
c_{ai}	initial condition of CO ₂ concentration in the gas phase [L^3L^{-3}].	K_H	Henry's law constant [$nT^2M^{-1}L^{-2}$].
c_{as}	CO ₂ concentration in the soil gas at the soil surface [L^3L^{-3}].	K_M, K_M^*	Michaelis constants for O ₂ and CO ₂ concentrations, respectively [L^3L^{-3}].
c_{atm}	CO ₂ concentration at the top of the stagnant boundary layer [L^3L^{-3}].	K_r	relative hydraulic conductivity [LT^{-1}].
c_{a0}	boundary condition for CO ₂ concentration in the gas phase [L^3L^{-3}].	K_S	saturated hydraulic conductivity [LT^{-1}].
C_a, C_n, C_o, C_w	volumetric heat capacities of the gas phase, solid phase, organic matter and liquid phase, respectively [$JL^{-3}K^{-1}$].	L	depth of the soil profile [L].
c_T	total volumetric CO ₂ concentration [L^3L^{-3}].	L_0	initial value of the rooting depth at the beginning of the growth period [L].
d	thickness of stagnant boundary layer [L].	L_m	maximum rooting depth [L].
D_a, D_w	effective soil matrix diffusion coefficients of CO ₂ in the gas and liquid phase, respectively [L^2T^{-1}].	L_r	root depth [L].
D_{as}, D_{ws}	diffusion coefficients of CO ₂ in the gas and liquid phase, respectively [L^2T^{-1}].	m, n	parameters of the retention curve [dimensionless].
D_E	effective dispersion coefficient in the soil matrix [L^2T^{-1}].	p	porosity [L^3L^{-3}].
E	activation energy of the reaction [$ML^2T^{-2}mol^{-1}$].	p_t	period of time necessary to complete one temperature cycle (1 day) [T].
f_p, f_s	reduction functions for CO ₂ production by plant roots and by soil microorganisms, respectively [dimensionless].	Q	sink/source term, root water uptake [$L^3L^{-3}T^{-1}$].
f_r	root growth coefficient [dimensionless].	Q^*	CO ₂ uptake rate associated with root water uptake [T^{-1}].
g	dimensionless coefficient calculated from degree day concept [dimensionless].	q	oxygen uptake rate [$L^3L^{-3}T^{-1}$].
h	water pressure head [L].	q_a, q_w	soil air and soil water fluxes, respectively [LT^{-1}].
h_A, h_B	minimum and maximum pressure heads allowed at the soil surface, respectively [L].	q_E	CO ₂ effective velocity [LT^{-1}].
h_i	water pressure head initial condition [L].	q_{E0}	prescribed CO ₂ effective boundary flux [LT^{-1}].
h_ϕ	osmotic head [L].	q_{max}	maximum oxygen uptake rate [$L^3L^{-3}T^{-1}$].
h_0	water pressure head boundary condition [L].	q_{w0}	water flux boundary condition [LT^{-1}].
h_2	pressure head when CO ₂ production is optimal [L].	R	universal gas constant [$ML^2T^{-2}K^{-1}n^{-1}$].
		R_f	retardation factor [dimensionless].
		r	growth rate [T^{-1}].
		S	production/sink term for CO ₂ [$L^3L^{-3}T^{-1}$].
		S_e	relative saturation [dimensionless].
		S_p	potential water uptake rate in the root zone [$L^3L^{-3}T^{-1}$].
		S_T	actual CO ₂ production rate [$L^3L^{-2}T^{-1}$].
		T	temperature [K].
		t	time [T].
		t^*	local time within the period p_t [T].
		t_p, t_m, t_h	time of planting, time at which maximum rooting depth is reached and time of harvesting, respectively [T].
		T_a, T_p	actual and potential transpiration rates, respectively [LT^{-1}].
		T_{Bas}	heat units necessary for the plant to mature and roots to reach the maximum rooting depth [KT].
		T_0	average temperature at the soil surface during the period p_t [K].
		T_1	minimum temperature below which plant growth stops [K].
		T_2	temperature above which plant growth remains at maximum and unchanged for some interval up to a maximum temperature [K].

- T_3 maximum temperature above which increased temperature has a negative effect on growth [K].
- z spatial coordinate (positive downward) [L].
- α parameter of retention curve [L^{-1}].
- α_s, α_ϕ dimensionless water and osmotic stress response functions, respectively [dimensionless].
- β normalized water uptake distribution function [L^{-1}].
- β_t thermal dispersivity [L].
- γ_p, γ_s actual production by plant roots and soil microorganisms, respectively [$L^3 L^{-3} T^{-1}$].
- γ_{p0}, γ_{s0} optimal production by plant roots and soil microorganisms, respectively [$L^3 L^{-2} T^{-1}$].
- δ reduction coefficient in the heat units concept [dimensionless].
- θ_a, θ_w volumetric air and water contents, respectively [$L^3 L^{-3}$].
- θ_n, θ_o volumetric fractions of solid phase and organic matter, respectively [$L^3 L^{-3}$].
- θ_r, θ_s residual and saturated volumetric water contents, respectively [$L^3 L^{-3}$].
- λ coefficient of the apparent thermal conductivity of the soil [$WL^{-1} K^{-1}$].
- λ_w dispersivity in the water phase [L].
- λ_0 thermal conductivity of the soil [$WL^{-1} K^{-1}$].
- τ_a, τ_w tortuosity factors in gas and liquid phase, respectively [LL^{-1}].

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J. Šimůnek and D. L. Suarez, U.S. Salinity Laboratory, Agricultural Research Service, U.S. Department of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501.

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