

## Applications of material coordinates in the soil and plant sciences

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Received 4 May 1987; accepted 22 June 1987

*Key words:* continuum mechanics, solute transport, deformation of soils, growing tissues

### Abstract

The continuum theory of mixtures is used to show the common basis of models in three areas. In each of these areas the central problem is the description of the deformation and motion of a reference continuum and of the movement of one or more constituents relative to this reference continuum. The three applications concern the movement of solutes relative to the soil water, the movement of soil water relative to the solid phase of swelling/shrinking soils, and the movement of water, solutes, and gases relative to growing plant tissues.

### Introduction

Soils and plants are complex and their variety is great. Fortunately the physical-mathematical theories that are used to describe processes in soils and plants exhibit a remarkable coherence. Around 1960 a common basis for the energy status of water became established (Bolt & Frissel, 1960; Slatyer & Taylor, 1960). Around 1970 an analysis of simultaneous transport of water and solutes in clay pastes (Bolt & Groenevelt, 1969) stimulated the development of a similar model for plant roots (Dalton et al., 1975).

This paper deals with the application of certain concepts from the theory of mixtures (Truesdell & Toupin, 1960; Truesdell, 1984, Ch. 5) in three areas, namely:

- (1) the deformation, motion, and root uptake of soil water, and the transport of soil solutes relative to soil water,
- (2) the deformation, motion, and decay of soil solid material, and the transport of soil water relative to soil solid material,
- (3) the deformation, motion, and growth/cell division in plant tissues, and the transport of water, solutes, and gases relative to plant tissues.

**Kinematics of a reference continuum**

The material description of deformation and motion gives for any parcel  $X$  of reference continuum  $r$  the places  $x$  occupied in the course of time  $t$ :

$$x = x [X, t]. \tag{1}$$

Differentiation of this functional relationship gives the two key concepts for describing the deformation and motion of continuum  $r$ , namely the deformation gradient tensor  $F$ , and the velocity vector  $v$ :

$$F = \partial x / \partial X|_r, \tag{2.1}$$

$$v = \partial x / \partial t|_x. \tag{2.2}$$

The local properties of the deformation from a reference configuration at time  $t_0$  to a configuration at time  $t$  are described by  $F$ . If, from any configuration actually occupied, the reference configuration can be reached by a continuous motion, then  $J = \det F > 0$  and then the polar decomposition theorem gives two unique, multiplicative decompositions of  $F$ :

$$F = R U = V R, \tag{3}$$

where the rotation tensor  $R$  is orthogonal ( $R R^T = I$ , where the superscript T denotes the transpose and  $I$  is the identity tensor), and the right and left hand stretch tensors  $U$  and  $V$  are symmetric ( $U = U^T, V = V^T$ ). The geometric interpretation of Eq. 3 is very simple: the deformation corresponding locally to  $F$  may be regarded as resulting from pure stretches along three suitable, mutually orthogonal directions, followed by a rigid rotation of those directions, or from the same rotation followed by the same stretches along the appropriate directions. Numerous alternative measures of deformation can be derived from  $F$ .

The velocity  $v$  defined by Eq. 2 can be used to relate the spatial time derivative  $\partial./\partial t|_x$  and the material time derivative  $\partial./\partial t|_X$ :

$$\partial f / \partial t|_x = \partial f / \partial t|_X + v \cdot \partial f / \partial x. \tag{4}$$

where  $f$  may be any variable in the continuum  $r$  varying continuously with position and time.

The velocity gradient tensor  $\partial v / \partial x$  compares the current velocities of neighbouring parcels of continuum  $r$ . The tensor  $\partial v / \partial x$  can be additively decomposed in a symmetric part and a skew-symmetric part:

$$\partial v / \partial x = 1/2 (\partial v / \partial x + \partial v / \partial x^T) + 1/2 (\partial v / \partial x - \partial v / \partial x^T). \tag{5}$$

The geometric interpretation of the decomposition (Eq. 5) is very simple: the sym-

metric part  $\frac{1}{2} (\partial v/\partial x + \partial v/\partial x^T)$  describes the rate of stretch, the skew-symmetric part  $\frac{1}{2} (\partial v/\partial x - \partial v/\partial x^T)$  describes the rate of rotation of a parcel.

Differentiating Eq. 2.1, with respect to  $t$  for fixed  $X$  or Eq. 2.2 with respect to  $X$  for fixed  $t$ , it can be shown that the tensors  $F$  and  $\partial v/\partial x$  are related by

$$\partial F/\partial t_x = (\partial v/\partial x)F. \tag{6}$$

According to Eq. 6 the material derivative of  $F$  is equal to the product of  $\partial v/\partial x$  and  $F$  itself. Generally, solving this material, tensorial partial differential equation (Eq. 6) to obtain the deformation gradient tensor from one configuration of another configuration will be difficult, since the components of  $\partial v/\partial x$  at a particular parcel will generally be a function of time. In this paper, of main interest is the material, scalar partial differential equation resulting from taking the trace of Eq. 6:

$$J^{-1} \partial J/\partial t_x = \nabla \cdot v. \tag{7}$$

Integration of Eq. 7 from some past time  $t_0$  to the current time  $t$  gives

$$J = J_0 \exp \int_{t_0}^t \nabla \cdot v dt. \tag{8}$$

The determinant  $J$  of the deformation gradient tensor is a measure of the volume of a parcel of continuum  $r$ , and Eq. 8 describes the volumetric growth of such a parcel.

Consider the spatial mass balance equation associated with continuum  $r$ :

$$\partial \rho/\partial t_x = -\nabla \cdot (\rho v) + \lambda, \tag{9}$$

where  $\rho$  is the mass density and  $\lambda$  is the source strength. Adding  $v \cdot \nabla \rho$  to both sides of Eq. 9 and using Eq. 4 and Eq. 7 gives

$$(\rho J)^{-1} \partial (\rho J)/\partial t_x = \lambda/\rho. \tag{10}$$

According to Eq. 10 the relative rate of change of  $\rho J$  is equal to  $\lambda/\rho$ , the source strength per unit mass of  $r$ . In Eq. 10,  $J$  transforms the density  $\rho$  to the configuration of the reference body  $r$  at reference time  $t_0$ . Integration of Eq. 10 gives

$$\rho = \rho_0 J^{-1} \exp \int_{t_0}^t \lambda/\rho dt. \tag{11}$$

Note that since the configuration at time  $t_0$  is taken to be the reference configuration,  $J_0 = 1$ . It is important to recall that Eq. 10 and Eq. 11 apply at a parcel  $X$ , not at fixed points in space. According to Eq. 11 the mass density at a parcel  $X$  at the current time  $t$  is the product of the initial density  $\rho_0$ , a factor  $J^{-1}$  describing the effect of the deformation, and a factor describing the effect of the source strength.

For one-dimensional deformations  $F$  and  $J$  reduce to:

$$F = \begin{vmatrix} \partial x/\partial X & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}; \quad J = \partial x/\partial X. \quad (12)$$

The derivative  $J = \partial x/\partial X$  can be followed with markers. Using Eq. 12 in Eq. 11 gives:

$$\varrho = \varrho_0 \frac{\partial X}{\partial x} \exp \int_{t_0}^t (\lambda/\varrho) dt. \quad (13)$$

If the time course of  $\partial X/\partial x$  (with markers) and of  $\varrho/\varrho_0$  (with preferably some in situ technique) are followed, then the time course of the source strength  $\lambda/\varrho$  can be deduced. If  $\lambda = 0$ , then  $\varrho/\varrho_0$  can be deduced from the time course of  $\partial X/\partial x$  and vice versa.

**Transport relative to a reference continuum**

Consider some scalar entity  $\psi$  with density  $\varrho_\psi$ , velocity  $\mathbf{v}_\psi$ , and source strength  $\lambda_\psi$ . The spatial balance equation for  $\psi$  can be written as

$$\partial \varrho_\psi / \partial t_{|x} = -\nabla \cdot (\varrho_\psi \mathbf{v}_\psi) + \lambda_\psi. \quad (14)$$

Adding  $\mathbf{v} \cdot \nabla \varrho_\psi$  to both sides of Eq. 14, using Eq. 4 on the left-hand side and the product rule for differentiation on the right-hand side, multiplying both sides by  $J$ , substituting Eq. 7, combining the two terms with the time derivatives, transforming from spatial to material derivatives, and using the fact that  $\partial(JF^{-1})/\partial X = 0$  (cf. Truesdell & Toupin, 1960, section 18), gives:

$$\partial(\varrho_\psi J) / \partial t_{|X} = -\partial\{\varrho_\psi J F^{-1}(\mathbf{v}_\psi - \mathbf{v})\} / \partial X + (\lambda_\psi / \varrho_\psi) \varrho_\psi J. \quad (15)$$

In Eq. 15 continuum  $r$  serves as a reference in several respects:

1. All derivatives involve the material coordinates  $X$ ;
2.  $J$  transforms the density  $\varrho_\psi$  to the configuration of the reference body  $r$  at reference time  $t_0$ ;
3.  $F$  does the same for the relative velocity  $(\mathbf{v}_\psi - \mathbf{v})$ .

With Eq. 10, Eq. 15 can be transformed into

$$\partial(\varrho_\psi / \varrho) \partial t_{|X} = -(\varrho J)^{-1} \partial\{(\varrho_\psi / \varrho)(\varrho J) F^{-1}(\mathbf{v}_\psi - \mathbf{v})\} / \partial X + (\varrho_\psi / \varrho)(\lambda_\psi / \varrho_\psi - \lambda / \varrho). \quad (16)$$

Expressions for the mass flux  $(\varrho_\psi / \varrho)(\mathbf{v}_\psi - \mathbf{v})$  of entity  $\psi$  relative to continuum  $r$  require special constitutive assumptions for specific cases. If entity  $\psi$  is convected with continuum  $r$  so that  $\mathbf{v}_\psi = \mathbf{v}$ , then Eq. 16 reduces to

$$(\varrho_\psi / \varrho)^{-1} \partial(\varrho_\psi / \varrho) / \partial t_{|X} = \lambda_\psi / \varrho_\psi - \lambda / \varrho. \quad (17)$$

According to Eq. 17 the relative rate of change of the mass density ratio  $\rho_\psi/\rho$  is equal to the difference between the source strengths per unit mass of  $\psi$  and  $r$ . Integration of Eq. 17 gives:

$$\rho_\psi/\rho = (\rho_{\psi 0}/\rho_0) \exp \int_{t_0}^t (\lambda_\psi/\rho_\psi - \lambda/\rho) dt. \tag{18}$$

**Soil water as a reference continuum**

Richards (1931) organized scattered knowledge about water in unsaturated soils into a coherent theory. That theory is consistent with regarding soil water as a continuous medium (Raats, 1984). Thus all concepts introduced so far can be applied to soil water. The interpretations of  $F$  and  $\partial v/\partial x$  in this context are illuminating. Eq. 7 relates the expansion of the water on the left-hand side to the divergence of the velocity field on the right-hand side. For one-dimensional flows  $J$  can be determined by one or more tracers. If the density  $d$  of the water is constant, the mass density in Eqs. 9 to 11 can be easily replaced by the volume fraction of the water  $\theta = \rho/d$ . The term  $\lambda$  in these equations can represent the rate of uptake by plant roots. Eq. 11 shows that, for a given parcel of water, the water content  $\rho$  is the product of (1) the water content  $\rho_0$  at time  $t_0$ ; (2) a factor  $J^{-1}$  accounting for expansion/contraction; and (3) a factor accounting for cumulative uptake of water in the time interval  $t_0$  to  $t$ .

If the entity  $\psi$  introduced in Eq. 14 represents a solute, then Eq. 15 and Eq. 16 describe the movement of this solute  $\psi$  relative to the soil solution. The density ratio  $\rho_\psi/\rho$  in Eqs. 16 to 18 is then the concentration of the solute in the soil solution. The flux  $\rho_\psi(v_\psi - v)$  can be assumed to be given by:

$$\rho_\psi(v_\psi - v) = -D \partial(\rho_\psi/\rho)/\partial x, \tag{19}$$

where  $D$  is the diffusion/dispersion tensor. Introducing Eq. 19 in Eq. 16, setting  $\rho_\psi/\rho = c$ , and transforming  $\partial/\partial x$  to  $\partial/\partial X$  gives:

$$\partial c/\partial t_x = -(\rho J)^{-1} \partial \{ (J F^{-1} (F^T)^{-1} D \partial c/\partial X) \} / \partial X + c (\lambda_\psi/\rho_\psi - \lambda/\rho). \tag{20}$$

If the transport is one-dimensional and in the absence of uptake by plant roots ( $\lambda_\psi = 0$  and  $\lambda = 0$ ), Eq. 20 reduces to a form used in numerous recent papers (see Raats, 1982 for some early examples). If diffusion/dispersion is neglected, then Eq. 20 reduces to Eq. 17, integration giving Eq. 18, of course with  $\rho_\psi/\rho = c$  and  $\rho_{\psi 0}/\rho_0 = c_0$ . Eq. 18 then describes the time course of the solute concentration of a parcel of water as a result of selective uptake of water and solute. Such an expression is also relevant for the nutrient solution in soilless cultures (Raats, 1980). If the solute is not taken up ( $\lambda_\psi = 0$ ), then Eq. 18 reduces to a form relevant to certain aspects of salinization of root zones (Raats, 1981).

### Soil solid phase as a reference continuum

The deformation of the solid phase is often observed by establishing some type of markers of the solid phase. The markers can be some compositional or textural features of the solid phase or they can be purposely inserted objects or materials. If the time course of the density  $\varrho$  is also determined, then the source strength  $\lambda$  can in principle be determined from Eq. 10 or Eq. 11. In case of decomposition of the solid phase of an organic soil,  $\lambda$  will, of course, be negative.

In applications the one-dimensional equations 12 and 13 have been used most often. To determine the relationship between  $x$  and  $X$ , Schothorst (1977; 1980, in particular Fig. 85) used metal plates consisting of two discs connected by a bar. After placing the unit horizontally at the bottom of an auger hole, the plates were turned outwards. The auger holes were cased with tubes. A metal rod was used to locate the bar connecting the two plates, thus giving the curves relating  $x$  and  $X$ . The deformation gradients  $\partial x/\partial X$  are slopes of such curves. Related techniques were used earlier by Woodruff, and by Aitchison & Holmes (Raats, in preparation).

If all constituents of the solid phase are non-reactive, then Eq. 13 reduces to

$$\partial x/\partial X = \varrho_0/\varrho. \quad (21)$$

Integration of Eq. 21 gives

$$\int_0^X \varrho_0 dX = \int_0^x \varrho dx. \quad (22)$$

According to Eq. 22 the current location of a parcel  $X$  of the solid phase can be determined from the equality of the cumulative total mass of solid between 0 and  $X$  in the reference configuration and the cumulative total mass of solid between 0 and  $x$  in the current configuration. As far as I know, this technique was first used by Hissink (1935) and has since been used widely in the Netherlands in studies of settlement of sediments and muds of former lake bottoms and marine forelands, and also dredging materials. Hissink (1935) determined the profiles of the density  $\varrho$  in 9 polders ranging in ages from 6 to approximately 400 years. They all were reclaimed from the Dollard, an estuary formed in 1277. Hissink used marine foreland (salt marsh) with a similar textural profile as a hypothetical reference configuration. The motivation for studying historical records of subsidence of old polders was to enable a forecast of subsidence of new polders with similar texture.

In a study of decay and subsidence of peat soils, Schothorst (1977) distinguishes a conglomerate of non-reactive, mineral constituents and a conglomerate of decaying (reactive), organic constituents. As a reference configuration he chooses a uniform profile with bulk densities of the constituents identical to those found currently below the water table. He measures density profiles of the mineral and organic conglomerates. The density profile for the mineral conglomerate is used in Eq. 21 and Eq. 22 to determine  $\partial X/\partial x$ . Subsequently this result and the density profile for the organic conglomerate are used in Eq. 13 to determine the degree of decay of the organic conglomerate.

If the entity  $\psi$  introduced in Eq. 14 represents water, then Eq. 15 and Eq. 16 describe the movement of this water relative to the solid phase. The special version of this equation for one-dimensional deformation of the solid phase and flow of the water, and without source/sink terms ( $\lambda_\psi = 0, \lambda = 0$ ), has been used in numerous papers over the past two decades (Raats & Klute, 1969; Stroosnijder, 1976; Philip & Smiles, 1982; Raats, 1984). The flux  $\rho_\psi(\mathbf{v}_\psi - \mathbf{v})$  of water relative to the solid phase is the sum of two components, one due to the gradient of the pressure  $P_\psi$  of the fluid and one due to gravity (see Raats, 1984 for details). To complete the theory the pressure  $P_\psi$  must be related to the density ratio  $\rho_\psi/\rho$  and the total stress in the soil (cf. Bolt, 1974).

**Plant tissue as a reference continuum**

The kinematics of continuous media can be used to compare the same tissue at different instants and also to describe the gradual change of a tissue (Raats, 1986b). The parcels  $X$  correspond to pieces of tissue. They can be identified by specifically applied markings or by recognizable, lasting anatomical features. For example, Bensink (1971) marked young leaves of lettuce with 5-mm squares of Indian ink to observe growth patterns at different light intensities. The deformation gradient tensor  $F$ , the rotation tensor  $R$ , and the stretch tensors  $U$  and  $V$  can be used to compare configurations of a piece of tissue at different times. The rate of stretch tensor  $\frac{1}{2}(\partial\mathbf{v}/\partial\mathbf{x} + \partial\mathbf{v}/\partial\mathbf{x}^T)$  and the rate of rotation tensor  $\frac{1}{2}(\partial\mathbf{v}/\partial\mathbf{x} - \partial\mathbf{v}/\partial\mathbf{x}^T)$  can be used to describe the rate of change of the configuration. While Eq. 6 links  $F$  and  $\partial\mathbf{v}/\partial\mathbf{x}$  in general, in the literature on plant morphology attention has been focussed on mainly 1- and 2-dimensional analogs of Eq. 6, giving expressions for, respectively, the length and area of a piece of tissue (Silk, 1984).

For a tissue not only the distribution in space, but also the formation, growth, and ultimate fate of cells has been receiving much attention. Balance equations of the forms of Eq. 14 and Eq. 15 apply for cells of all sizes:

$$\partial n/\partial t_{|x} = -\nabla \cdot (\mathbf{v}n) + \gamma n, \tag{23}$$

$$\partial(Jn)/\partial t_{|x} = \gamma Jn, \tag{24}$$

where  $n$  is the total number of cells per unit volume,  $\mathbf{v}$  is the velocity of the tissue, and  $\gamma$  is the number of divisions per cell per unit time.

For a more detailed description the size structure of the cells needs to be taken into account. Again, balance equations of the forms of Eq. 14 and Eq. 15 apply for cells of size  $\sigma$ :

$$\partial n_\sigma/\partial t_{|x} = -\nabla \cdot (\mathbf{v}n_\sigma) + \gamma_\sigma n_\sigma, \tag{25}$$

$$\partial(Jn_\sigma)/\partial t_{|x} = \gamma_\sigma Jn_\sigma, \tag{26}$$

where the source strength per unit volume  $\gamma_\sigma n_\sigma$  is the sum of two parts,  $\gamma_\sigma^g n_\sigma$  related to growth and  $\gamma_\sigma^f n_\sigma$  related to fission:

$$\gamma_\sigma^g n_\sigma = - \frac{\partial}{\partial \sigma} g[t, X, \sigma] n_\sigma, \tag{27}$$

$$\gamma_\sigma^f n_\sigma = \left\{ -b[t, X, \sigma] + 4b[t, X, \sigma] \frac{n_\sigma[t, X, 2\sigma]}{n_\sigma[t, X, \sigma]} \right\} n_\sigma, \tag{28}$$

where  $g$  is the growth rate and  $b$  is the fission rate. In Eq. 23,  $vn$  is the flux of cells per unit area per unit time. Similarly, in Eq. 27  $gn_\sigma$  can be interpreted as the flux of cells past the size  $\sigma$ . The factor 4 in Eq. 28 reflects the fact that division of a cell in the range  $2\sigma + 2\Delta\sigma$  produces 2 cells in the range  $\sigma + \Delta\sigma$ .

Integration of Eq. 25 and Eq. 26 over all sizes gives the balance equations 23 and 24 for cells of all sizes. Integration of Eq. 25 over a region V chosen large enough so that the flux  $n_\sigma$  is zero at the boundary or Eq. 26 over a set of pieces of tissue comprising an entire tissue E gives:

$$\frac{\partial}{\partial t} N_\sigma[t, \sigma] = - \frac{\partial}{\partial \sigma} \bar{g}[t, \sigma] N_\sigma[t, \sigma] + \bar{\gamma}_\sigma^f[t, \sigma] N_\sigma[t, \sigma], \tag{29}$$

where the total number of cells  $N_\sigma$  per unit size, the average growth rate  $\bar{g}$  and the average net source strength  $\bar{\gamma}_\sigma^f$  per cell per unit time are defined by

$$N_\sigma = \int_V n_\sigma dx = \int_E J n_\sigma dX, \tag{30}$$

$$\bar{g} = \frac{\int_V g n_\sigma dx}{N_\sigma} = \frac{\int_E g J n_\sigma dX}{N_\sigma}, \tag{31}$$

$$\bar{\gamma}_\sigma^f = \frac{\int_V \gamma_\sigma^f n_\sigma dx}{N_\sigma} = \frac{\int_E \gamma_\sigma^f J n_\sigma dX}{N_\sigma}. \tag{32}$$

The balance equation 29 for cells of size  $\sigma$  in the entire tissue is of the same form as the balance equation for a population subject to fission reproduction derived by Bell & Anderson in 1967 (see Metz & Diekmann, 1986). (An equation of the form of Eq. 29 with  $\sigma$  representing age and  $\bar{\gamma}_\sigma^f$  the age specific mortality rate was used by van Straalen (1982) in a population study on *Collembola*.)

The theory outlined above can be specialized to describe growth and cell division in (lineal) roots (Raats, 1986b), (curved) hypocotyls of emerging seedlings (Raats, 1986a), and (2-dimensional, planar or curved) leaves.

As a prerequisite to understanding the dynamics of growth of tissues, it is necessary to describe the distribution and transport of materials, such as water, respiratory gases, nutrients, and osmotica. Eqs. 14 to 18 can be used for this purpose. Specifically it can be shown that the models of Silk & Wagner (1980), Silk, Walker & Labavitch (1984), and McCoy & Boersma (1984) fit in such framework.

### Concluding remarks

It has been shown that models used in three areas share a common basis. Researchers and teachers operating at and across disciplinary boundaries should welcome the emergence of common concepts, terminologies, and symbols for the separate disciplines.

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