GUIDELINES FOR MICRO- AND MESOSCALE COMPUTER MODELLING OF FLUID FLOWS IN THE SOIL-ROOT SYSTEM

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Abstract. Fluid flows in the soil, in the plant root zone, are linked with many phenomena, which may be considered in several scales. Interdisciplinary, complex knowledge explaining these phenomena in micro- and mesoscale may be effectively used in a computer model simulating the flow. The work constitutes a preliminary analysis of possibilities for implementation of this project. The researchers have pointed out promising computational methods (MD, SPH, LG), which are employed in similar problems. These methods are available in some flow-simulating applications, however they are not soil environment-oriented. Difficulties in adaptation are brought about by the number of phenomena, complicated material and geometrical structure of soil, and changes in this structure generated by flow. Model framework is planned to be based on three object groups: soil, fluids, plant roots. The model should be open, allowing to make extensions through introducing new components and modules, e.g. new soil constituents, and methods describing their behaviour in the aspect of flow.

Key words: flow, soil, computational method, computer model

Introduction

Modelling of fluid flows in the soil is one of the more difficult issues. Soil is a porous body, with pores that in majority are open, in which flows are slow, non-turbulent, and have multiphase character. They determine water-air relations in soil, and therefore affect the root feeding mechanism for plants. Fluids (soil solutions, gases) move in soil, taking part in many biological, physical and chemical processes [Dobrzański and Zawadzki 1981]. These processes modify the properties of fluids and flow medium, the latter additionally affected by root mass growth. Interactions occur mainly in more shallow layers and include washing out and micro-erosion effects, dissolving, mixing, advection, settling, conglutination, and other. As a result of fluid-channel links and the influence of external factors, soil environment is subject to continuous, although slow transformations. The flow type depends on channel diameter and bendiness, porosity of its walls, occurring cohesion forces and related phenomena making up the pF curve, pH value, and other factors. Intensity of fluid exchange process in the root-soil system depends on fluid potential, and is the highest in the small root section, the so-called hair zone. The mentioned phenomena as well as the other omitted ones, have been extensively explained in numerous scientific sources. Moreover, the researchers developed many models: mathematical, experimental, analogue, or only qualitative [Czachor and Lipiec 2005; Davita et al. 2010; Jendele 2002; Soares and Mansura 2006; Walczak 2001].

Strong soil structure diversification and its non-stationary character do not allow to consider the flows in one geometric similarity equivalence class. Using an averaged flow resistance coefficient tensor has allowed to describe flow through porous bodies in a macroscopic scale, useful for land melioration or plant growing. Darcy or Richards equations are known here, derived from the basic *Navier-Stokes* (NS) relation, based on the continuity postulates and determinations of the so-called substantial derivative, equilibrium conditions, and other. The microscopic scale is the smallest. In this scale the phenomena are observed at elementary, atomic level, and proper dependencies are provided by statistical physics. Mesoscopic, intermediate scale is defined as the one that allows to explain trajectory of flow resistance tensor values, present diversity of basic soil structure components, and determine relations between soil and fluid structure, also using the elements of macro- and micro-scale analysis. This scale allows to describe elementary exchange processes between inanimate and animate environment, e.g. in relation *water potential – cell turgor*. This is where the local mechanical properties of soil are developed, depending on the presence or absence of fluids, which are important for the plant growth and nuisance of agrotechnical operations- from hard, dried out “ceramic” structure to muddy, viscous liquid.

The purpose and scope of work

Accumulation of phenomena, especially in root area, generates high complexity problems and hence justifies considering the supporting role of informatics for phenomena modelling, and creating knowledge bases and a repository allowing to collect the research results. The purpose of this work is to identify necessary components of computational environment for flow simulations, primarily in micro- and mesoscopic scale, intended for the implementation in the soil-plant system. The area under consideration covers a not very deep, few centimetres-thick root zone with hair layer, i.e. active root feeding zone. Below the considered layer there is a ground water table (phreatic surface). This water table is an exchange surface for free (non-pressurised) flows occurring above it. It outlines the lower boundary for the environment absorbing the water flowing in from the top, and at the same time it is a source releasing water into the upper layers including hair zone via capillaries or evaporation and condensation. Figure 1 presents the zone under consideration. It is located within the reach of aeration, and pore volume is filled with numerous substances, soil solutions and gases. It is also assumed that the soil structure and root system are predetermined at process input. Soil structure may be modified by the flow, i.e. it is not determined in parallel by external factors, e.g. stresses introduced by agrotechnical operations. The system input is constituted by moderate inflow of fluids into the zone from the top, and infiltration from the bottom, and output – change in soil channel structure and flow parameters in the root zone.

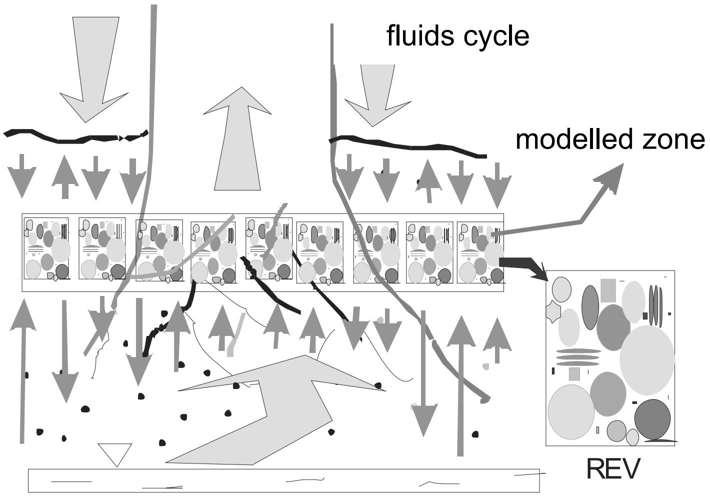

Fig. 1. Modelled zone for simulation of flows in root environment

Review of computational methods

The studies, which take up the issues involving flows modelling, in majority use Numerical Hydrodynamics and its computer support - CFD (*Computational Fluid Dynamics*). Methods including: finite difference method (FDM), finite element method (FEM), finite volume method (FVM), boundary element method (BEM), or other similar become more complicated with increasing flow medium geometrical complexity, which is substantial for soil and is visible especially in the mesoscale (pores, obstacles, gas bubbles, suspensions, etc.). Less susceptible to this complexity are: *molecular dynamics* (MD), *lattice gas* (LG) including *lattice Boltzmann gas* (LBG), and *smoothed-particle hydrodynamics* (SPH). The concept of fluid as a set of particles links them, and particle definition distinguishes them. Fluid motion is a combination of motion of particles subjected to various influences, including geometrical constraints (obstacles, channel walls, etc.) [Chen and Doolen, 1998; Roy 1995].

The CFD methods are employed in the commercial flow simulation applications (e.g. FLUID application), which may be used to solve some of the above-mentioned problems. However, we think that the phenomena extent and diversity encountered in the soil justify the consideration of a specialised computational environment. Among the CFD methods, the molecular description is particularly convenient for the flow analyses in micro- and mesoscale, and complies with the purpose of this work.

The MD method is associated with the Knudsen criterion – particle is a molecule; principles known from atomic constitution of matter are applicable. Newtonian mechanics laws are employed in the classic MD, yet unrestricted by the “three bodies” barrier. However, even if we use huge computational capacities of many processors, it is difficult to take into account number of particles (molecules) exceeding 10^9, which translates into fluid volume reaching fraction of μm^3 at most. The developed concepts and range of the MD algorithms (espe-cially the Verlet algorithm), and their utilisation went substantially beyond this method scope.

The MD scale seems to be adequate for modelling the diffusion phenomena “fluid (water, oxygen, CO_2) – root (hair, selected group of cells)”, ions motion description, values of cohesion forces between water particles and selected surfaces, especially in the aspect of the microscopic flow at walls (hygroscopic and pellicular water, water bounded in complexes), nitrification process characteristics, some bonds between the soil structure elements (sticky substances), the role of water lubricating layer in forming muddy substances and explaining some processes accompanying the advection.

Particles in the LG and SPH models have a fictitious character, they are mentally separated fluid constituents reduced to the points characterised by specific properties, e.g. mass, momentum. Modelling scale is extensive and adequate also for mesoscopic scale. The number of artificial particles in a specific volume is much smaller than the number of fluid molecules, and so, for predetermined computational capacity (boundary value was specified earlier), it is possible to assume much higher volumes than in the MD. The number of particles should be large enough for the model fluid to represent “macroscopically” the modelled fluid. The LG and SPH methods differ in the description of interactions occurring between particles.

The LG is a set of many similar methods, in general referring to the idea of a cellular automaton, while the LBG method is the leading one. Particle is a very tiny “ball” compared to flow channel volume. Particle moves along a lattice of a given type in strictly determined directions, and its motion leads to collisions with other particles. This method is not derived from the NS, but from the Boltzmann kinetic equation linking substantial derivative with the particles motion probability distribution (the so-called one-point distribution function) and collision cross-section. The collision operator has gone through some evolution, and currently the researchers use a linearised, probabilistic BGK operator (abbreviation for names Bhatnagar-Gross-Krook), which allows to obtain results in conformity with the NS equations, but in a much easier way (linearisation). It is also assumed that the LBG method is more flexible and more universal than the NS, reduces the number of computations, and is close to the Euler’s analysis, in which changes are observed in a local lattice node. The FHP type lattices in 2D or 3D version have gained recognition. Fractions of particles may represent different types of fluids in liquid or gaseous form. Due to collisions and probability distributions, this method is useful for modelling behaviours of compressible fluids (gases), but it is also applied for low viscosity liquids, primarily water.

If we take into account fluid behaviours within exchange zone around the root (“horizontal” root environment with hair layer), then – appropriate for mesoscopic scale – characteristic dimensions remain within range from a few to several dozen millimetres. This environment constitutes sort of a store and factory of products being consumed during the exchange, ensuring exchange process continuity. The following issues will be appropriate for the LBG method:

- water flow through the larger capillaries (infiltration), and its drawing by the plant,
- gravitational flow in the larger channels, taking into account positive and negative sources of fluids,
- collecting and spreading gas mixture: air, CO_2, steam,

- dissolving, percolation and repercolation, advection of various substances feeding a plant, that make up soil solutions,
- the growth of living organisms,
- change in soil channel profiles during flow (sedimentation, floating, dissolving, stratification, other).

In the SPH method, the $i^{\text{-th}}$ particle (pseudomolecule) is subject to motion laws, which are formulated on the basis of differential equation describing flow (e.g. NS), and thus the method has a numerical solution character. These laws are formulated on the grounds of estimation of the selected fluid properties for steam ($\boldsymbol{r}$, h), i.e. in environment circled with radius h for given fluid volume indicated by radius $\boldsymbol{r}$. Particle characteristics is the result of point pattern interpolation inside environment h using specially selected interpolation kernel. It becomes the carrier relocating information on local fluid properties, e.g. position, density, mass, sound wave passage velocity (through that particle), temperature (internal energy u), pressure (of particle). Their gradients may be estimated likewise, which allows to replace differential structures with discrete expressions. Particle kinetic behaviour does not result from collisions as in the LBG, but it is an outcome of external and internal interactions. The SPH is close to the MD in its concept and uses similar algorithms. Application area and modelling advantages in the SPH partially coincide with the LBG, however it is deemed that the SPH resolves better the issues involving high viscosity and density of fluids. Due to these reasons, this method is appropriate for modelling some of the already mentioned phenomena, and situations when excess water leads to the structure loosening, making soil resemble a viscous liquid, and to the occurrence of rheological phenomena manifested in mesoscale in soil structure subsidence and relocation of masses under gravity forces.

The concept of computational environment model

Suitable information environment, using the discussed computational methods, should allow to shape soil properties freely and to carry out studies on the flow effects in an interesting scale. Complexity of issues induces considering only the basic components forming a framework of this environment. This framework should be based on three fundamental groups of objects, at the same time creating the space to allow the user to determine simulation conditions, which include:

a) model structure of soil consisting of materials with various physical and chemical properties, concentrations of living organisms, in general – components diversified due to flows,
b) model fluids in liquid and gaseous forms,
c) model plant roots.

Ad a) Model soil structure is an arrangement of the basic elements. Soil characteristic repeatability in its larger volume (determined spatial correlation radius) allows to propose the method for soil modelling in two steps:

1. in the first step, the following basic elements shall be specified:

- soil structure material types, including mineral grains, organic substances, and other. They should be grouped according to common characteristics determined in the aspect of flow (e.g. components which are: wettable, floatable, soluble, hydratable, changing their volume, non-permeable for some fluids, etc.);

- bonding rules for the above-mentioned components, taking into account cohesion forces resulting from the presence of water, sticky substances, or other reasons. These rules may make cohesion forces dependent on flow conditions;
- geometrical shapes. In the likeness of ceramics, the soil forms porous structures remaining in the equilibrium not only due to cohesion forces, but as a result of sticking elements characterised by specific geometry. Hence, the initial geometrical components of constituent shapes are important, and geometrical properties of the model flow channels with different diameters and bendiness are the result of their arrangement in the soil.

2. in the second step, it is assumed to create soil component with user-defined properties, and in particular:

- a pattern (as mm^3, cm^3) consisting of elements specified as in par. a, corresponding to the REV (*representative elementary volume*), i.e. smallest volume cut out from the material where average value of a characteristic corresponds to the average for the zone under consideration. The REV would be an elementary soil structure component, and its multiple duplication with integration rules should convey "macroscopic" character of soil. Possibility to compose model soil of various patterns is not excluded, as well. It seems purposeful to establish a data bank (libraries) of different REVs corresponding to typical soil structures. This solution would evidently allow successive users to expand the model, and would reduce labour amount.

Ad b) In hydrodynamics, the term REV as the *reference element of volume* is such a small volume with attributed mean value of a characteristic, that a set of these volumes may be interpreted as a model continuous medium, and "large" enough not to notice discrete character of an atomic constitution. Therefore, fluid mean REV has local character from mesoscopic scale point of view. With reference to the LG or SPH computational methods, fluid REV may constitute the basis for defining fluid particle. Presence of fluids induces various phenomena dependent on structure of soil, in which individual methods assigned to the components – objects – individualise their behaviours. It is essential to distinguish conditions that are favourable for the exchange in the root hair zone from unfavourable conditions known from the plants physiology. The upper boundary zone surface is the exchange surface for air flowing into soil and gases released from the soil.

Ad c) In the first approximation, plant root and its part with hair is a "negative" source. Water is drawn if specific conditions related to soil structure and soil solution are met in the closest vicinity of hair. Water potential relative to the potential of hair cell fluids is important, and exchange efficiency is determined by the potential difference, which has to exceed the potential of cohesion forces between the water particles and soil matter. Oxygen assimilation mechanism is complicated as well, as in general it requires the ionisation degree to be analysed. In order to consider the role of this object in detail, the following are required: participation of a plant physiology specialist and acquisition of knowledge that is coherent with the proposed model.

Summary

In order to develop computational environment model, it is proposed to apply the following incremental procedure:

1. construction of a prototype and a basic model differentiating typical situations, susceptible to experimental verification,
2. extending the model by complementing or adding new components (roots growth, impurities, chemical changes, thermodynamic dependencies, etc.),
3. introducing the following in the model: elements of prediction, artificial intelligence and other methods for its improvement, calibration, teaching based on actual data,

system integration with other computer systems: measuring, image identifying, etc.

Gradual model functionality extension will not be ensured by simple handling of parameters, but rather by expanding it through adding new, specialised modules. This solution requires suitable knowledge in information science, or the need to use information services. It would be ideal to develop an information environment in a form of an open framework with a specified programming interface (API), where the user's interface would be determined by the network services.

Bibliography

Czachor H., Lipiec J. 2005. Próba zastosowania stopu Wood'a do oznaczeń makroporowatości gleby. Acta Agrophysica 6(1). pp. 43-52.

Davita Y., Debenesta G., Woodd B., Quintarda M. 2010. Modeling non-equilibrium mass transport in biologically reactive porous media. Advances in Water Resources Vol. 33. Issue 9. pp. 1075-1093.

Dobrzański B. (red.), **Zawadzki S.** (red.). 1981. Gleboznawstwo. PWRiL Warszawa. pp. 613.

Libor Jendele. 2002. An improved numerical solution of multiphase flow analysis in soil. Advances in Engineering Software, Vol. 33, Issues 7-10, July-October 2002, pp. 659-668. [Dostęp: 2010-10-10] Dostępny w Internecie: http://www.sciencedirect.com/ science/article/B6V1P-471VY1M-1/2/d8d5bbc66f11fe7129cd6c1a71ed85a7

Shiyi Chen, Gary D. Doolen. 1998. Lattice Boltzmann Method for fluid flows. Annu. Rev. Fluid Mech. 1998. Vol.30. pp. 329-364.

Soares D. Jr., W.J. Mansura. 2006. Dynamic analysis of fluid–soil–structure interaction problems by the boundary element method. Journal of Computational Physics. Vol. 219. Issue 2. pp. 498-512.

Roy T.M. 1995. Physically-Based Fluid Modeling using Smoothed Particle Hydrodynamics. Masters Thesis. University of Illinois at Chicago. [Dostęp: 2010-10-10]. Dostępny w Internecie: http://www.plunk.org/~trina/thesis/html/thesis_toc.html

Walczak R.T. 2001. Agrofizyka: fizyka środowiska i żywności, Materiały XXXVI Zjazdu Fizyków Polskich. Toruń. Instytut Agrofizyki PAN im. B. Dobrzańskiego. Lublin. Maszynopis.

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ZAŁOŻENIA DLA MODELOWANIA KOMPUTEROWEGO W MIKRO- I MEZOSKALI PRZEPŁYWÓW PŁYNÓW W SYSTEMIE GLEBA-KORZEŃ

Streszczenie. Przepływy płynów w glebie, w strefie przykorzennej roślin, są związane z wieloma zjawiskami, które można rozpatrywać w kilku skalach. Interdyscyplinarna, złożona wiedza objaśniająca te zjawiska w mikro- i mezoskali może być efektywnie wykorzystana w modelu komputerowym symulującym przepływ. Praca jest wstępną analizą możliwości realizacji takiego projektu. Wskazano na obiecujące metody obliczeniowe (MD, SPH, LG), które są wykorzystywane w zbliżonych zagadnieniach. Metody te udostępnia kilka programów symulujących przepływ, niemniej nie są one ukierunkowane na środowisko glebowe. Trudności adaptacji wnosi liczba zjawisk, skomplikowana struktura materialna i geometryczna gleby, oraz zmiany tej struktury na skutek przepływu. Szkielet modelu zamierza się oprzeć o trzy grupy obiektów: glebę, płyny, korzenie roślin. Model powinien posiadać charakter otwarty, pozwalający na rozszerzenia przez wprowadzanie nowych komponentów i modułów, np. nowych składników gleby jak i metod opisujących ich zachowania w aspekcie przepływu.

Słowa kluczowe: przepływ, gleba, metoda obliczeniowa, model komputerowy

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