Advances in modelling two-phase flow in porous media: Theory, experiments and simulations

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Original Darcy's law was proposed for **1D steady-state flow** of almost pure incompressible water in saturated homogeneous isotropic rigid sandy soil under isothermal conditions

$$q = -K \frac{\partial h}{\partial x}$$
$$h = p / \rho g + z$$

"Extended" Darcy's law is assumed to apply to **3D unsteady flow of two** or more compressible fluids, with any amount of dissolved matter, in heterogeneous anisotropic deformable porous media under non-isothermal conditions $q_i^{\alpha} = -K_{ij}^{\alpha} \quad \frac{\partial h^{\alpha}}{\partial x_i}$ $h^{\alpha} = p^{\alpha} / \rho^{\alpha} g + z$





FOR THREE-DIMENSIONAL FLOW







FOR DEFORMABLE MEDIA is assumed to be a function of **POROSITY or DEFORMATION** Univ siteit Utrecht



FOR FLOW IN UNSATURATED ZONE: is assumed to be a function of water content Universiteit Utrecht









"Extended" Darcy's Law
$$q = -K \frac{\partial h}{\partial x} \qquad \longrightarrow \qquad q_i^{\alpha} = -K \frac{\partial h^{\alpha}}{\partial x_j}$$

We have added bells and whistles to a simple formula to make it applicable to a much more complicated system!

One must follow a reverse process:

- develop a general theory for a complex system
- reduce it to a simpler form for a less complex system



Comparison of theories of Aristotle and Galileo on free fall of objects with hypothetical measurements





Standard two-phase flow equations

$$\frac{\partial \left(nS^{\alpha} \right)}{\partial t} + \nabla \bullet \mathbf{q}^{\alpha} = 0$$

$$\mathbf{q}^{\alpha} = -\frac{k^{r\alpha}}{\mu^{\alpha}} \mathbf{K} \bullet \left(\nabla P^{\alpha} - \rho^{\alpha} \mathbf{g}\right)$$

$$P^n - P^w = f\left(S^w\right) = P^c$$

$$k^{r\alpha} = k^{r\alpha} \left(S^{w} \right)$$

Effective stress in unsaturated soils

Effective stress:

$$\sigma_{ij}^{eff} = (\sigma_{ij} - P^{air}\delta_{ij}) + \chi P^c \delta_{ij}$$

 P^{air} : pore air pressure, P^c : capillary pressure, $(P_a - P_w)$, or matric suction χ : effective stress parameter;assumed equal to saturation

$$\chi = f(S^w)$$



Measurement of Capillary Pressure-Saturation Curve (SWCC)



Often it takes more than one week to get a set of wetting and drying curves



Two-phase flow dynamic experiments (PCE and Water)

Selective pressure transducers used to measure average pressure of each phase within the porous medium



Hassanizadeh, Oung, and Manthey, 2004

Two-phase flow dynamic experiments (PCE and Water)

Static Pc-S Curves



Hassanizadeh, Oung, and Manthey, 2004

Two-phase flow dynamic experiments (PCE and Water)



Hassanizadeh, Oung, and Manthey, 2004



There is no unique *p^c*-S curve.



Relative permeability-saturation curve





Relative permeability is supposed to be less than 1.

Water and oil relative permeabilities in 43 sandstone reservoirs plotted as a function of water saturation; *Berg et al. TiPM, 2008*

Standard theory does not model the development of vertical infiltration fingers in dry soil





Standard theory does not model the development of vertical infiltration fingers in dry soil



Infiltration experiments;

Rezanejad et al., 2002



Standard theory does not model the development of vertical infiltration fingers in dry soil



Experiments by Rezanejad et al., 2002

Non-monotonic distribution of saturation during infiltration into dry soil; experiments in our gamma system



Fritz et al., 2012

Non-monotonic distribution of saturation during infiltration into dry soil; experiments in our gamma system





Non-monotonic distribution of pressure during infiltration into dry soil; experiments in our gamma system



Effective stress in unsaturated soils

Effective stress:

$$\sigma_{ij}^{eff} = (\sigma_{ij} - P^{air}\delta_{ij}) + \chi P^c \delta_{ij}$$

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$$\chi = f(S^w)$$



Effective stress parameter, χ , **is a hysteretic function of saturation or suction**


Outline

Averaging-Thermodynamic approach for developing new theories of two-phase flow

New theories of two-phase flow

Experimental and computational determinations of capillary pressure under equilibrium conditions

Experimental and computational determinations of capillary pressure under non-equilibrium conditions

Truly extended Darcy's law

A new generation of micro-models for two-phase flow experiments



Flow network of micro-models created in PDMS, which is hydrophobic.

Overall dimensions: length of 35 mm and width of 5 mm; No. of pores: 2000 to 6000 pore bodies and 6000 to 24000 pore throats

Pore size: mean pore size of 40 to 70 µm and constant

depth of the same size

Liquids used: Water (dyed with ink) and Fluorinert



A new generation of micro-models for two-phase flow experiments





Visualization set-up



Visualization of interfaces in a micromodel Dynamic drainage and imbibition (Karadimitriou et al., 2012)



Averaging-Thermodynamic Approach

First, a microscale picture of the porous medium is given:
Porous solid and two fluid phases fil the space;
separated by three interfaces: solid-water, water-air, solid-air, and a water-air-solid common line.
There is mass, momentum, energy associated with each phase

and interface.





Averaging-Thermodynamic Approach

First, a microscale picture of the porous medium is given: Porous solid and two fluid phases fill the space; separated by three interfaces: solid-water, water-air, solid-air, and a water-air-solid common line.

Microscale conservation equations for mass, momentum, and energy are written for points within phases or points on interfaces and the common line.

These equations are averaged to obtain macroscale conservation equations.

No microscopic constitutive equations are assumed.

Macroscopic constitutive equations are proposed at the macroscale and restricted by 2nd Law of Thermodynamic.



Equations of conservation of mass

For each phase:
$$\frac{\partial \left(nS^{\alpha}\rho^{\alpha}\right)}{\partial t} + \nabla \bullet \left(\rho^{\alpha}\mathbf{q}^{\alpha}\right) = \sum_{\beta \neq \alpha} r^{\alpha,\alpha\beta}$$
Divide by a constant ρ and neglect mass exchange term:

$$\frac{\partial \left(nS^{\alpha}\right)}{\partial t} + \nabla \bullet \mathbf{q}^{\alpha} = 0$$
For each interface:

$$\frac{\partial \left(a^{\alpha\beta}\Gamma^{\alpha\beta}\right)}{\partial t} + \nabla \bullet \left(a^{\alpha\beta}\Gamma^{\alpha\beta}\mathbf{w}^{\alpha\beta}\right) = r^{\alpha,\alpha\beta} + r^{\beta,\alpha\beta}$$
Divide by a constant $\Gamma^{\alpha\beta}$:

$$\frac{\partial a^{\alpha\beta}}{\partial t} + \nabla \bullet \left(a^{\alpha\beta}\mathbf{w}^{\alpha\beta}\right) = E^{\alpha\beta}$$

Results from imposing the Second Law of Thermodynamics

Definition of capillary pressure

Under equilibrium conditions, we get:

$$\left(P^{g} - P^{w}\right)\Big|_{e} = -\rho^{m} \frac{\partial \psi^{m}}{\partial S^{w}}$$

Under equilibrium conditions, we get:

$$P^{g} - P^{w} = -\rho^{m} \frac{\partial \psi^{m}}{\partial S^{w}} - \tau \frac{\partial S^{w}}{\partial t} = P^{c} - \tau \frac{\partial S^{w}}{\partial t}$$
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Results from imposing the Second Law of Thermodynamics

Definition of fluid phase pressures:

$$\boldsymbol{\sigma}^{\alpha} = -\left(\rho^{\alpha}\right)^{2} \frac{\partial \psi^{\alpha}}{\partial \rho^{\alpha}} \mathbf{I} = -p^{\alpha} \mathbf{I} \qquad \alpha = w, g$$

Definition of solid phase pressure and effective stress:



Results from imposing the Second Law of Thermodynamics

Definition of solid phase pressure and effective stress:

$$\boldsymbol{\sigma}^{s} = \boldsymbol{\sigma}_{eff}^{s} - \chi P^{c} \mathbf{I}$$

$$\chi = S^w + \kappa a^{wn} / P^c$$



Extended theories of two-phase flow

Extended Darcy's law (linearized equation of motion):

$$\mathbf{q}^{\alpha} = -\rho^{\alpha}\mathbf{K}^{\alpha} \cdot \left(\nabla \mathbf{G}^{\alpha} - \mathbf{g}\right)$$

where G^{α} is the Gibbs free energy of a phase:

$$G^{\alpha} = G^{\alpha} \left(\rho^{\alpha}, a^{wn}, S^{\alpha}, T \right)$$

Extended Darcy's law :

$$\mathbf{q}^{\alpha} = -\frac{k^{r\alpha}}{\mu^{\alpha}} \mathbf{K} \cdot \left(\nabla P^{\alpha} - \rho^{\alpha} \mathbf{g} - \boldsymbol{\psi}^{\alpha \alpha} \nabla a^{wn} - \boldsymbol{\psi}^{\alpha S} \nabla S^{\alpha}\right)$$

where $\psi^{\alpha a}$ and $\psi^{\alpha S}$ are material coefficients.

Extended theories of two-phase flow

Linearized equation of motion for interfaces:

$$\mathbf{w}^{wn} = -K^{wn} a^{wn} \Gamma^{wn} (\nabla G^{wn} - \mathbf{g})$$

where G^{wn} is the Gibbs free energy of wn-interface: $G^{wn} = G^{wn} \left(\Gamma^{\alpha}, a^{wn}, S^{\alpha}, T \right)$

Simplified equation of motion for interfaces (neglecting gravity term):

$$\mathbf{w}^{wn} = -K^{wn} \left[\gamma^{wn} \nabla a^{wn} + \Omega^{wn} \nabla S^{w} \right]$$

where Ω^{wn} is a material coefficient and γ^{wn} is macroscale surface tension.

Summary of extended two-phase flow equations

$$\frac{\partial \left(nS^{\alpha}\right)}{\partial t} + \nabla \bullet \mathbf{q}^{\alpha} = 0$$
$$\mathbf{q}^{\alpha} = -\frac{1}{\mu^{\alpha}} \mathbf{K}^{\alpha} \bullet \left(\nabla P^{\alpha} - \rho^{\alpha} \mathbf{g} - \psi^{\alpha \alpha} \nabla a^{wn} - \psi^{\alpha S} \nabla S^{\alpha}\right)$$
$$\frac{\partial a^{wn}}{\partial t} + \nabla \bullet \left(a^{wn} \mathbf{w}^{wn}\right) = E^{wn} \left(a^{wn}, S^{w}\right)$$
$$\mathbf{w}^{wn} = -K^{wn} \left[\gamma^{wn} \nabla a^{wn} + \Omega^{wn} \nabla S^{w}\right]$$
$$P^{n} - P^{w} = P^{c} - \tau \frac{\partial S^{w}}{\partial t} \quad P^{c} = f\left(S^{w}, a^{wn}\right)$$

A new generation of micro-models for two-phase flow experiments





Visualization of interfaces in a micromodel Drainage Imbibition



 $S^n = 24\%$ $P^c = 4340$ Pa $A^{wn} = 18.32$ mm²

Karadimitriou et al., 2012

 $S^n = 24\%$ $P^c = 2200 Pa$ $A^{wn} = 30.56 mm^2$

Capillary pressure-saturation points





Capillary pressure-saturation curve is hysteretic

Capillary pressure-saturation data points measured in laboratory (Morrow and Harris, 1965)

Capillary pressure and saturation are two independent quantities



Macroscale capillary pressure; theoretical definition





Projection of the P^c-a^{wn}-S^w surface on the P^c-S^w plane gives the collection of all P^c-S^w curves (primary, main, scanning, etc.)

Capillary pressure-saturation-interfacial area Surface Fitted to drainage points – Micromodel experiments



Capillary pressure-saturation-interfacial area Surface Fitted to imbibition points – Micromodel experiments



Capillary pressure-saturation-interfacial area Surface

The average difference between the surface for drainage and the surface with all the data points is 9.7%.

The average difference between the surface for imbibition and the surface with all the data points is -5.77%.

$$a^{wn} = \alpha_1 S (1-S)^{\alpha_2} * P_c^{\alpha_3}$$



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Capillary Pressure-Interfacial Area-Saturation data form a (unique) surface

This has been shown by:

- Reeves and Celia (1996); Static pore-network modeling
- Held and Celia (2001); Static pore-network modeling
- Joekar-Niasar et al. (2007) Static pore-network modeling
- Joekar-Niasar and Hassanizadeh (2010, 2011) Dynamic/static pore-network modeling
- Porter et al. (2009); Column experiments and LB modeling
- Chen and Kibbey (2006); Column experiments
- Cheng et al. (2004); Micromodel experiments
- Chen et al. (2007); Micromodel experiments
- Bottero (2009); Micromodel experiments
- Karadimitriou et al. (2012); Micromodel experiments

Effective stress in unsaturated soils

Bishop (1959):

$$\sigma_{ij}' = (\sigma_{ij} - P_a \delta_{ij}) + \chi P_c \delta_{ij}$$

 P_a : pore air pressure, P_c : capillary pressure, $(P_a - P_w)$, or matric suction χ : effective stress parameter;was assumed equal to saturation

$$\chi = f(S^w)$$



Effective stress parameter, χ , is a function of saturation and water-air interfacial area

$$\sigma_{ij}' = (\sigma_{ij} - P^a \delta_{ij}) + \chi P_c \delta_{ij}$$

where: $\chi = S^w + \frac{k^{wa} a^{wa}}{P_c}$

which gives the following definition of Suction Stress:

$$SS = S^w P_c + k^{wa} a^{wa}$$



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Comparison with experimental results

 $SS = S^w P_c + k^{wa} a^{wa}$



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Fluids Pressure Difference vs Saturation at position z1 Coefficient τ can be determined from these data



Value of the damping coefficient τ as a function of saturation; local scale

Sw	$\tau[Pa.s]$
0.85	$1.587 * 10^5$
0.80	$1.451 * 10^5$
0.75	$1.361 * 10^5$
0.70	$1.375 * 10^5$
0.65	$1.404 * 10^5$
0.60	$1.402 * 10^5$
0.55	$1.461 * 10^5$



Bottero et al., 2011

Simulation of non-equilibrium primary drainage; Local pressure difference vs time; Injection pressure, 35kPa





Bottero, 2009

Summary of extended two-phase flow equations

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Horizontal redistribution of moisture in soil; a numerical example




Equilibrium moisture distribution from standard two-phase flow equations with no hysteresis





Equilibrium result from standard twophase flow equations with hystresis





Summary of extended two-phase flow equations

$$n \frac{\partial S^{\alpha}}{\partial t} + \nabla \bullet \mathbf{q}^{\alpha} = 0$$
$$\mathbf{q}^{\alpha} = -\frac{1}{\mu^{\alpha}} \mathbf{K}^{\alpha} \bullet \left(\nabla P^{\alpha} - \rho^{\alpha} \mathbf{g} - \psi^{\alpha \alpha} \nabla a^{wn} - \psi^{\alpha S} \nabla S^{\alpha}\right)$$
$$\frac{\partial a^{wn}}{\partial t} + \nabla \bullet \left(a^{wn} \mathbf{w}^{wn}\right) = E^{wn} \left(a^{wn}, S^{w}\right)$$
$$\mathbf{w}^{wn} = -K^{wn} \left[\gamma^{wn} \nabla a^{wn} + \Omega^{wn} \nabla S^{w}\right]$$
$$P^{n} - P^{w} = P^{c} - \tau \frac{\partial S^{w}}{\partial t} \quad P^{c} = f\left(S^{w}, a^{wn}\right)$$

Long-term result from extended twophase flow equations with no hystresis



awn: 400 450 500 550 600 650 700 750 800 850



Horizontal redistribution of moisture in soil



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Significance of interfacial area in mass transfer among phases

Mass transfer: kinetics depend on interfacial area!



Interphase mass transfer takes place across the fluidfluid interface

But... interfacial energy or interfacial area are not model parameters in current theories!



Remobilization of attached colloids by moving interfaces





Remobilization of attached colloids by moving interfaces



Low surface tension; reduced by dissolving salt in water



CONCLUSIONS

The driving forces in Darcy's law should be gradient of Gibbs free energy and gravity.

- Difference in fluid pressures is equal to capillary pressure but only under equilibrium conditions.
- Fluid-fluid interfacial areas should be included in multiphase flow theories.
- Hysteresis can be modelled by introducing interfacial area into the two-phase flow theory.
- Suction stress is not only a function of saturation but it depends on capillary pressure too.



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