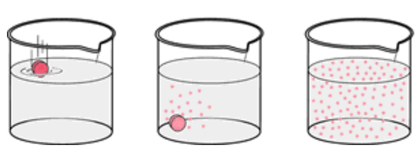
مکانیک خاک غیراشباع
انتقال جرم

Mass Transfer

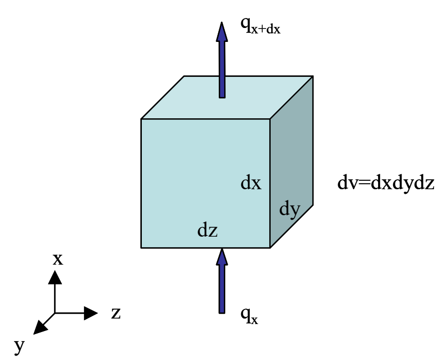
Hasan Ghasemzadeh

پخش جرم در محیط متخلخل

$$q_{diff} = -\theta \, D_{diff} \nabla C$$



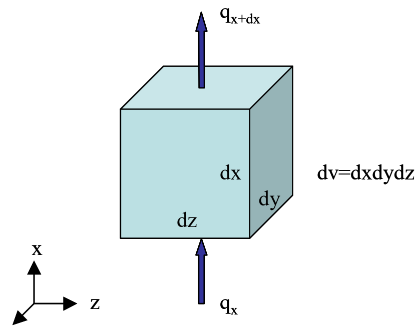
molecular diffusion coefficient



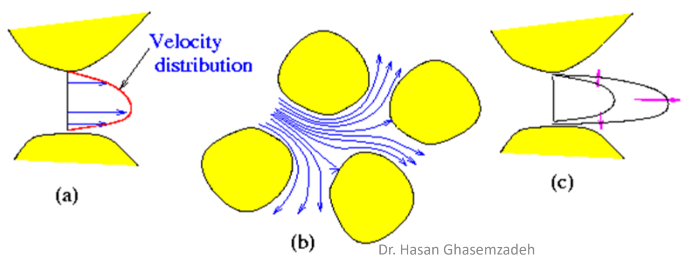
$$\theta = nS_r$$

پخش جرم در محیط متخلخل

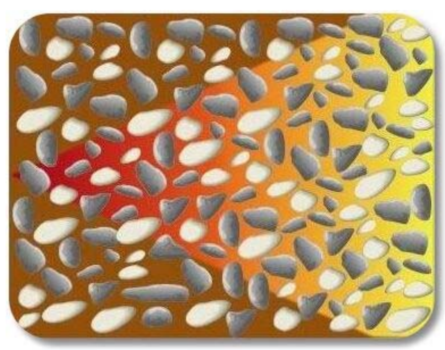
$$q_{disp} = -\theta\, D_{disp} \nabla C$$



Dispersion coefficient



پخش جرم در محیط متخلخل



$$q_{conv} = \theta v C$$

$$q_{tot} = q_{diff} + q_{disp} + q_{conv}$$

$$q_{tot} = \left(-\theta \mathrm{D} \nabla C + \left(\theta v\, C\right)\right)$$

Hydrodynamic dispersion coefficient

پخش جرم در محیط متخلخل

$$\frac{\partial(\theta C)}{\partial t} = -div(q_{tot})$$

$$\frac{\partial(\theta C)}{\partial t} = \nabla.(\theta\, \mathbf{D} \nabla C) - \nabla.(\theta v C)$$

$$\mathbf{D} = D_{disp} + D^*$$

$$D^*_{ij} = D_m T^*_{ij}$$

D_{disp} ضریب پخش مکانیکی

D^* ضریب پخش مولکولی موثر

D_m ضریب پخش مولکولی

D ضریب پخش هیدرودینامیکی

T^*_{ij} تانسور تابع خمیدگی محیط متخلخل

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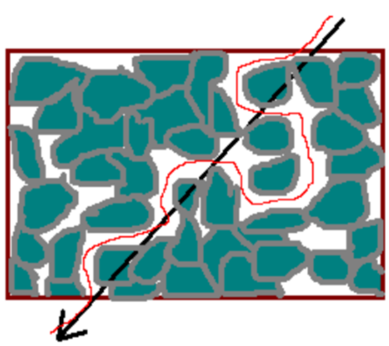
پخش جرم در محیط متخلخل

Tortuosity



D* = *effective* diffusion coefficient

D* < D because the phenomenon of *tortuosity* decreases the gradient in concentration that is driving the diffusion

D* = **T** D , where **T** < 1

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پخش جرم در محیط متخلخل

$$D^* = D_m \frac{\theta^{10/3}}{n^2}$$ Millington et Quirk (1961)

$$D^* = D_m \frac{\theta}{\tau}$$ Greenkorn et Kessler (1972)

$$D_m = \frac{K_b T}{6\pi\eta r}$$

τ, tortuosity
K_b, Boltzmann constant (1.3805 10^{-23} J/K)
T, absolute temperature (°K)
η, dynamic viscosity(cP)
r, molecular agregate radious (m).

$$D_{msel} = \frac{(z_+ + |z_-|) D_{m+} D_{m-}}{z_+ D_{m+} + |z_-| D_{m-}}$$

D_{m+} و D_{m-} ضریب پخش آنیون و کاتیون
z_+ و z_- بارهای آنیون و کاتیون

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پخش جرم در محیط متخلخل

$$D_{disp} = \begin{bmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{bmatrix}$$

ماده شیمیایی	ضریب پخشودگی در آب آزاد (10^{-9} m²/s)
H^+	9.311
OH^-	5.273
Na^+	1.334
K^+	1.957
Ca^{2+}	0.792
Pb^{2+}	0.945
Cl^-	2.032
Mg^{2+}	0.706

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پخش جرم در محیط متخلخل

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_{TH} \frac{v_y^2}{|v|} + \alpha_{TV} \frac{v_z^2}{|v|}$$

$$D_{yy} = \alpha_L \frac{v_y^2}{|v|} + \alpha_{TH} \frac{v_x^2}{|v|} + \alpha_{TV} \frac{v_z^2}{|v|}$$

$$D_{zz} = \alpha_L \frac{v_z^2}{|v|} + \alpha_{TV} \frac{v_x^2}{|v|} + \alpha_{TV} \frac{v_y^2}{|v|}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_{TH}) \frac{v_x v_y}{|v|}$$

$$D_{yz} = D_{zy} = (\alpha_L - \alpha_{TV}) \frac{v_y v_z}{|v|}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_{TV}) \frac{v_x v_z}{|v|}$$

$$|v| = \sqrt{v_x^2 + v_y^2 + v_z^2}$$

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پخش جرم در محیط متخلخل

عدد پکلت $$P_e = \frac{vd}{D^*}$$

طول مشخصه $$d = \frac{0.1484}{|h|}$$

فشار آب (cm) h

$P_e << 1$ Dispersive dominant

$P_e >> 1$ Convective dominant

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حل معادله

$$\frac{\partial (C)}{\partial t} = \frac{\partial}{\partial x} D_L \frac{\partial C}{\partial x} - v_x \frac{\partial C}{\partial x}$$

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x - v_x t}{2\sqrt{D_L t}} \right) + exp(\frac{x v_x}{D_L}) erfc\left(\frac{x + v_x t}{2\sqrt{D_L t}} \right) \right]$$

$$erfc(B) = 1 - erf(B)$$

$$erf(B) = \sqrt{1 - \exp(-4B^2 / \pi)}$$

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حل معادله

$$C_R(P_e, t_R) = 0.5\left[erfc\left((1 - t_R)\sqrt{\frac{P_e}{4t_R}} \right) + exp(P_e) erfc\left((1 + t_R)\sqrt{\frac{P_e}{4t_R}} \right) \right]$$

$$C_R(P_e, t_R) = C / C_0$$
$$t_R = v_x t / L$$
$$P_e = v_x L / D_L$$

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Heat and contaminant transport in unsaturated soil (Ghasemzadeh)

Chloride solution transport

- is validation of solute dispersion in unsaturated medium without any chemical reaction
- For this purpose, the experiments of Nützmann et al. (2002) on unsaturated glass beads were used

Properties	Unit	Values
Porosity	n(cm^3/cm^3)	0.347
Particle density	ρ(kg/dm^3)	2.57
Saturated hydraulic conductivity	K_s(cm/s)	0.0794
Volumetric water content	θ(cm^3/cm^3)	0.14
Infiltration rate	q_{in}(cm/s)	0.009867
Initial sorbent concentration	C_s (g/l)	0.06

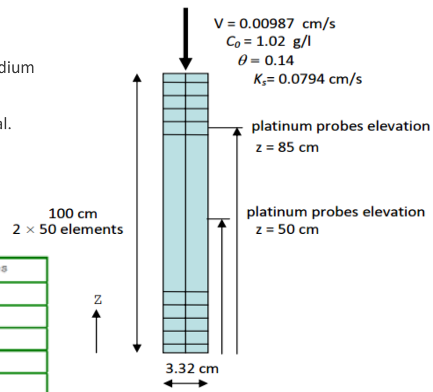

Fig. 7 Geometry of example 2

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Chloride solution transport

- The tracer was injected after steady state water flow through the column was reached; thus there is no hysteresis problem molecular
- Peclet numbers were between 40<Pemol<600, indicating that mass flux was dominated by dispersion with negligible diffusion (Pfannkuch, 1963; Van Genuchten and Wierenga, 1976). All experiments have been repeated three times
- In the numerical study, a mesh of 2 * 50 rectangular elements was used and The tracer (Nacl) with a concentration of 1.02 g/l was injected to the top

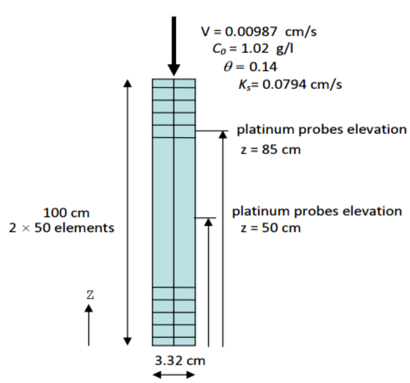

Fig. 7 Geometry of example 2

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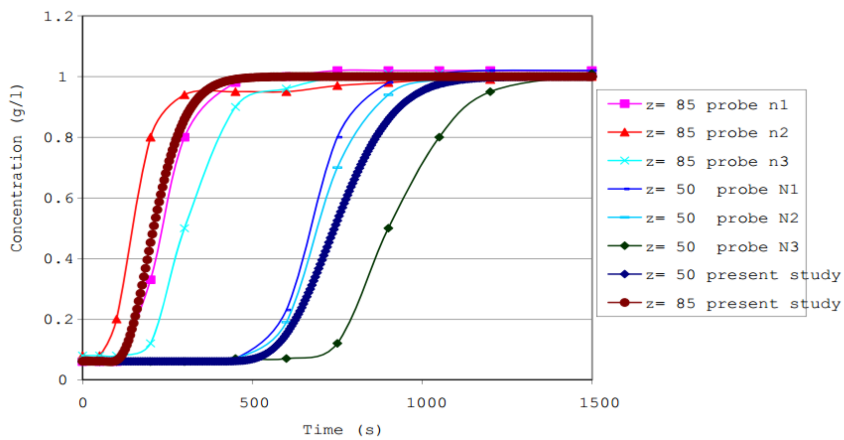

Measured tracer breakthrough curves in unsaturated glass beads for different probes from Nützmann et al. (2002) and results of present study.

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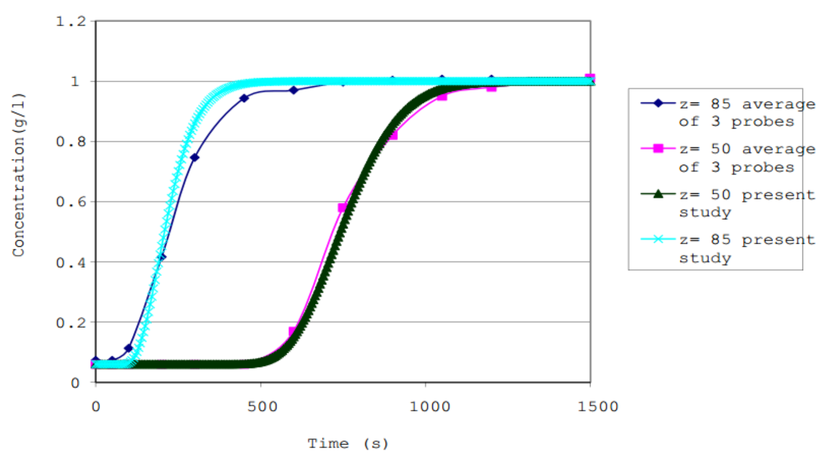

Comparison of present study results and average of measured tracer breakthrough curves in unsaturated glass beads from Nützmann et al. (2002).

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پخش جرم در محیط متخلخل

$$\frac{\partial(\theta C)}{\partial t} = \nabla.\left(\theta \mathbf{D} \nabla C\right) - \nabla.\left(\theta v C\right) + \Sigma \mathrm{R}_n$$

$$\sum R_n = -\rho_b \frac{\partial C_s}{\partial t} - \lambda_1 \theta C - \lambda_2 \rho_b C_s$$

$$C_s = ?$$

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واکنش ها

$$\frac{\partial(\theta C)}{\partial t} = \nabla.\left(\theta \mathbf{D} \nabla C\right) - \nabla.\left(\theta v C\right) + \Sigma \mathrm{R}_n$$

Isothermal linear

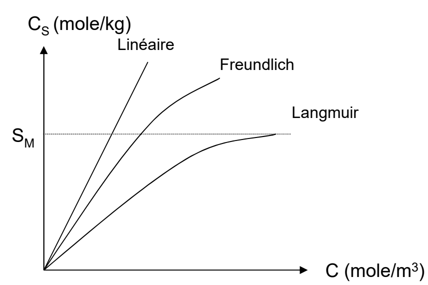
$$C_s = K_d . C$$

Freundlich

$$C_s = K_F . C^n$$

Langmuir

$$C_s = S_M . \frac{K_L . C}{1 + K_L . C}$$



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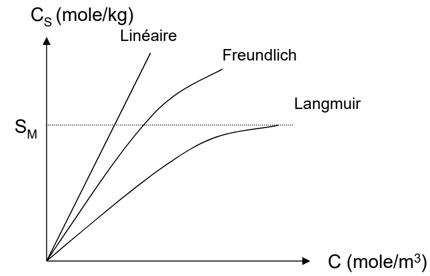
Langmuir with two surfaces

$$C_s = S_{M1} \cdot \frac{K_{L1}.C}{1+K_{L1}.C} + S_{M2} \cdot \frac{K_{L2}.C}{1+K_{L2}.C}$$

$$\frac{\partial C_s}{\partial t} = K_0.C$$



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واکنش ها

$$\frac{\partial C_s}{\partial t} = K_1.C - K_2.C_s$$

linear reversible

$$\frac{\partial C_s}{\partial t} = \gamma(K_3.C - C_s)$$

$$\frac{\partial C_s}{\partial t} = K_4.C^N - K_5.C_s$$

Non linear reversible

$$\frac{\partial C_s}{\partial t} = K_6 C.(\beta - C_s) - K_7 C_s$$

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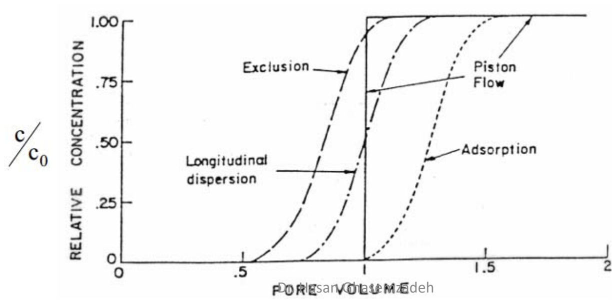
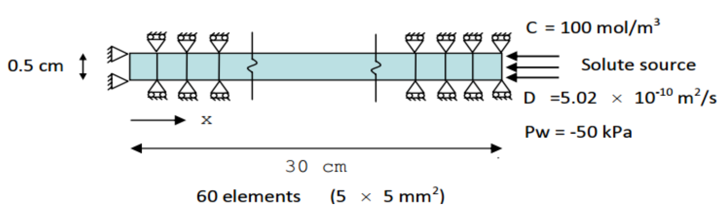
BTC's - Adsorption and Exclusion

- **Solute Exclusion and Chemical Reaction:**
  1) When R>1 (chemical adsorption) the BTC is retarded and appears at the column outlet later than for R=1.
  2) When R<1, the BTC is shifted to the left of T*=1 and applied solutes appear at the bottom of the column "earlier" than in other scenarios. This case may represent a situation of solute exclusion or the presence of immobile (stagnant) water regions which reduce the mean flow path, thereby increasing the effective velocity (v)



Heat and contaminant transport in unsaturated soil (Ghasemzadeh, 2008)

- Solute transfer and soil deformation



Properties	Unit	Values
Hydraulic Conductivity	K (m/s)	1×10^{-12}
Porosity	n(cm^3/cm^3)	0.33
Initial degree of saturation	S_r	0.60
Temperature	T(°C)	20
Solute dispersion Coefficient	D (m^2/c)	5.02×10^{-10}
Molecular mass of solute	M (gr/mol)	58.5
Bulk density	ρ (kg/dm^3)	1.5
Osmotic Efficiency	ω	0.3

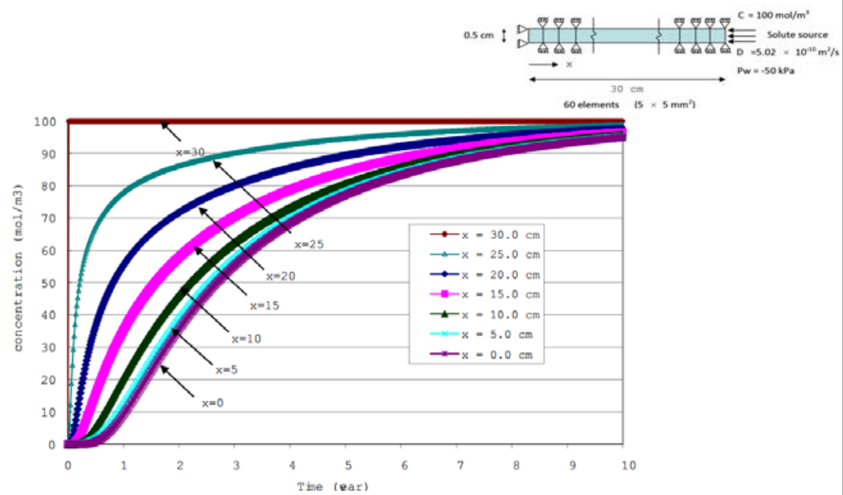


Fig. 11 Variation of solute concentration in different distances.

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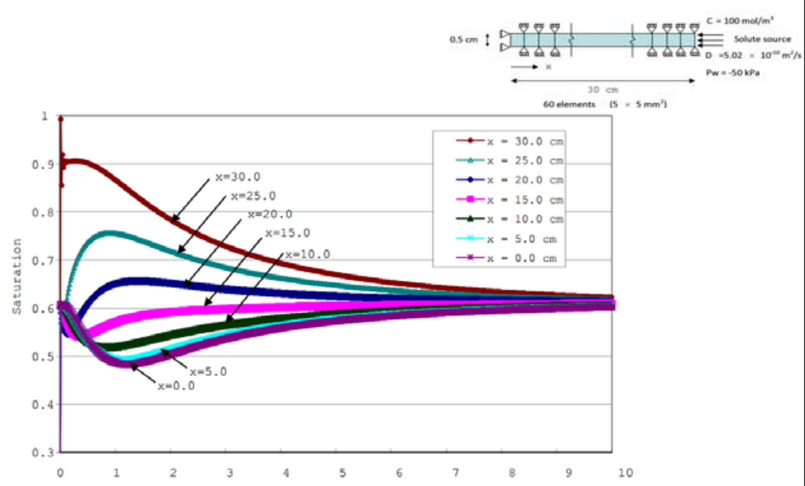

Fig. 12 Variation of saturation degree in different distances.

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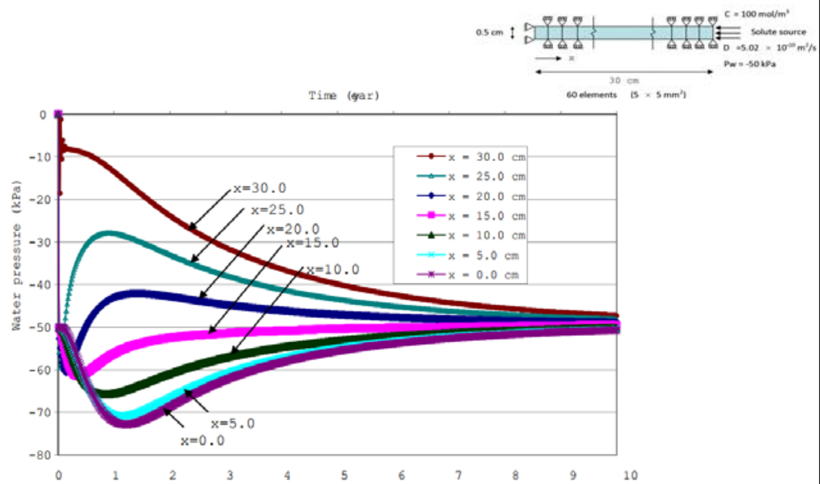

Fig. 13 Variation of water pressure in different distances.

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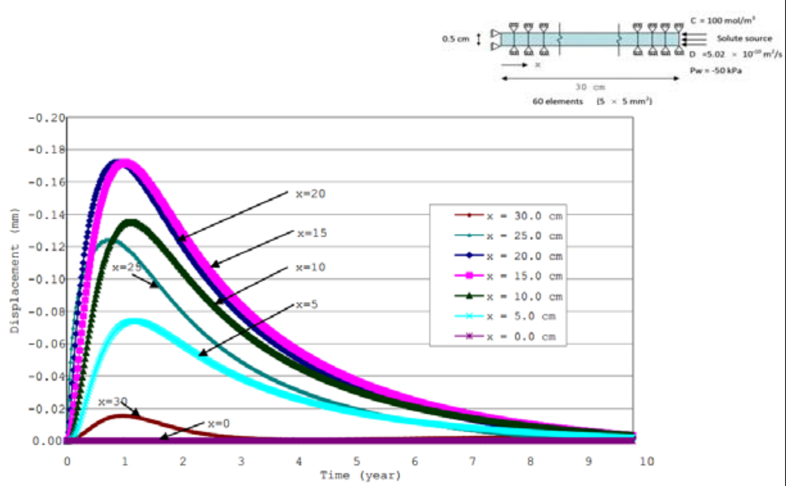

Fig. 14 Soil displacement in different nodes

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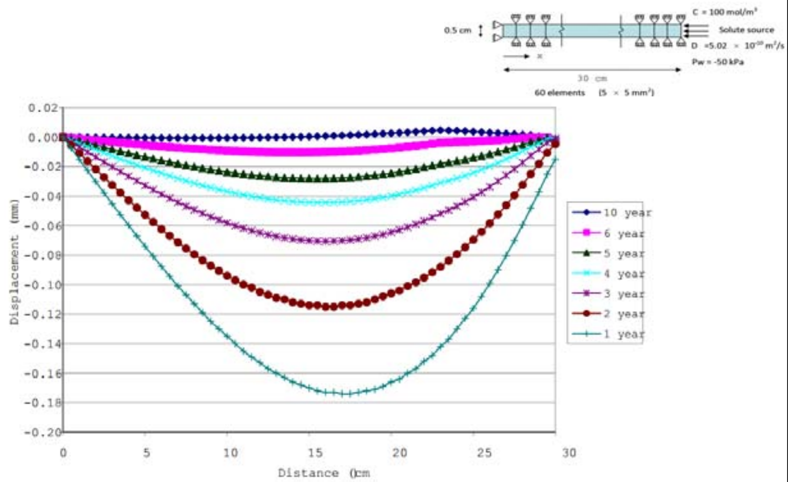
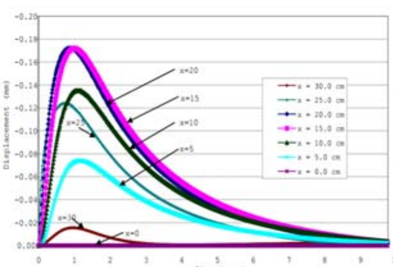
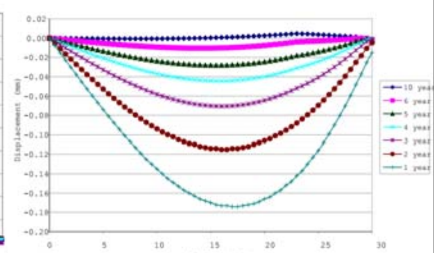


Fig. 15 Soil displacement of specimen in different times





- These results show that deformation consists of contraction and expansion in the soil sample. This deformation occurs due to change of suction in nodes. As noted in Figure 12 and Figure 13, there is movement of water toward solute source and so decreasing of water pressure or increasing of suction. This suction results in contraction in points that are far from solute source.
- On the other hand, in the region near the solute source expansion occurs because of diminution of suction due to generation of osmotic pressure in this region.

Heat and contaminant transport in unsaturated soil
H. Ghasemzadeh
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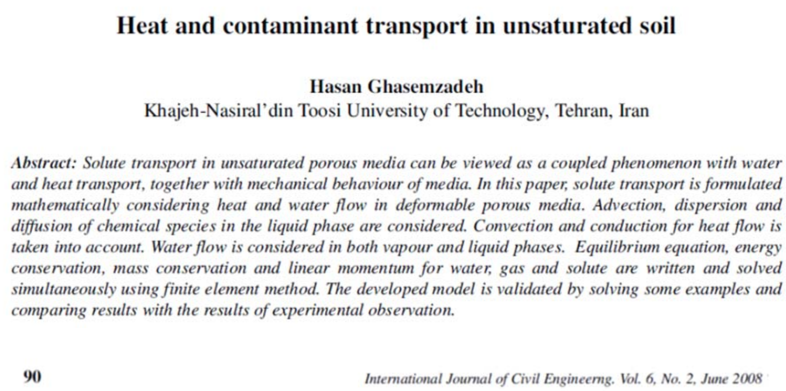

Heat and contaminant transport in unsaturated soil

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Abstract: *Solute transport in unsaturated porous media can be viewed as a coupled phenomenon with water and heat transport, together with mechanical behaviour of media. In this paper, solute transport is formulated mathematically considering heat and water flow in deformable porous media. Advection, dispersion and diffusion of chemical species in the liquid phase are considered. Convection and conduction for heat flow is taken into account. Water flow is considered in both vapour and liquid phases. Equilibrium equation, energy conservation, mass conservation and linear momentum for water, gas and solute are written and solved simultaneously using finite element method. The developed model is validated by solving some examples and comparing results with the results of experimental observation.*

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