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Estimates of conservative contaminants vertical travel time throughout vadose zone in young glacial areas

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Motivation

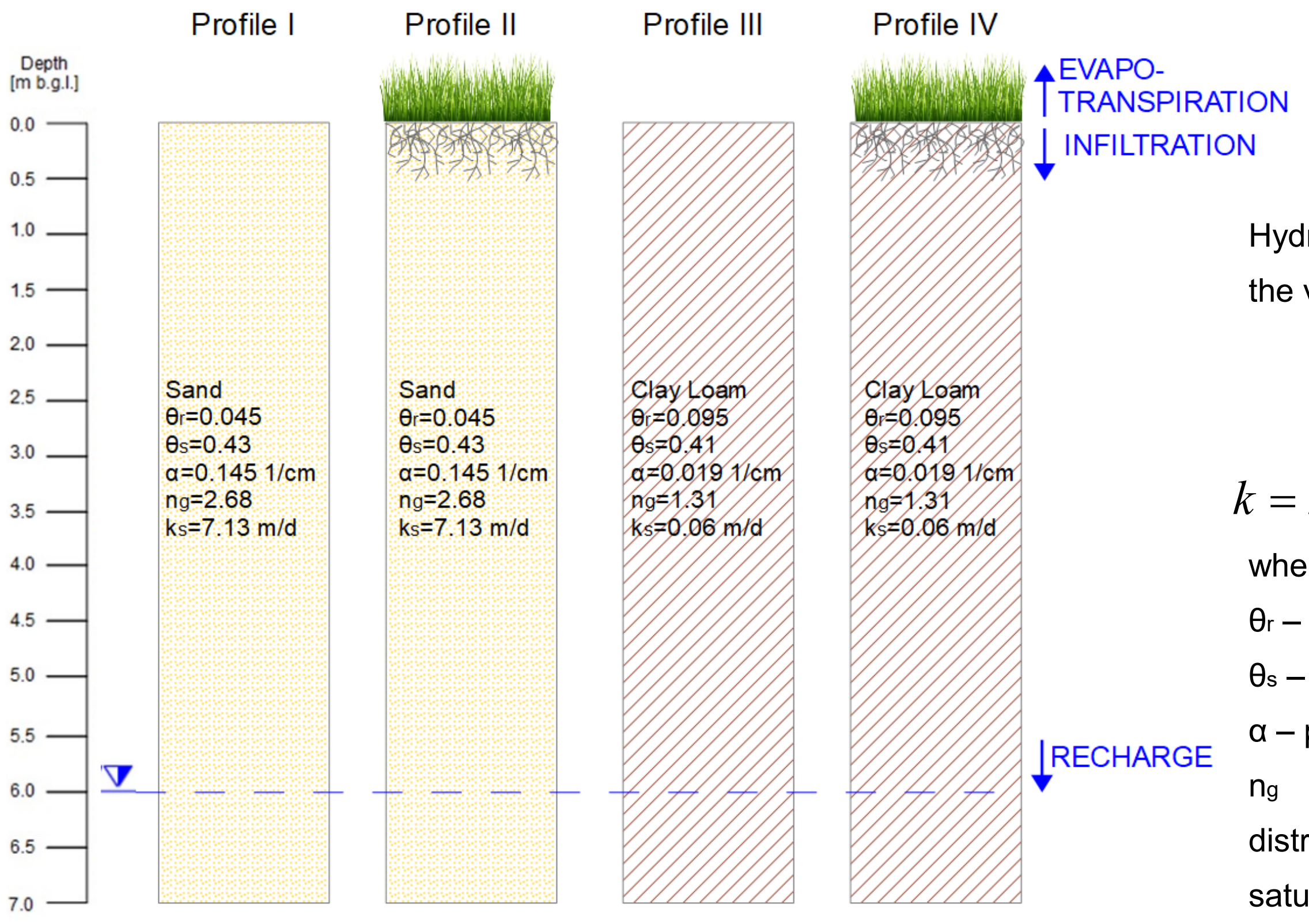
Estimation of contaminant travel time in the unsaturated zone is important for assessing aquifer vulnerability, delineating wellhead protection zones, planning monitoring and remediation, predicting the effects of land use and climate change.on groundwater quality.

Travel time can be computed using several methods of varying complexity, based on either transient or steady flow assumption, but comparative studies are limited.

Objectives

- Comparison of numerical simulations of transient flow and advective-dispersive transport with simple methods based on the assumptions of steady state flow and advective transport
- Evaluting the role of the hydrodynamic dispersion and root zone influence on conservative contamination travel time

Soil profiles



Hydraulic functions described by the van Genuchten (1980) model:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[1 + \left(\alpha |h|\right)^{n_g}\right]^{-m_g} \qquad (2)$$

$$k = k_s\, k_r = k_s \sqrt{S_e}\left[1 - \left(1 - S_e^{1/m_g}\right)^{m_g}\right]^2 \qquad (1)$$

where:

θ_r – residual water content,

θ_s – water content at fully saturated conditions,

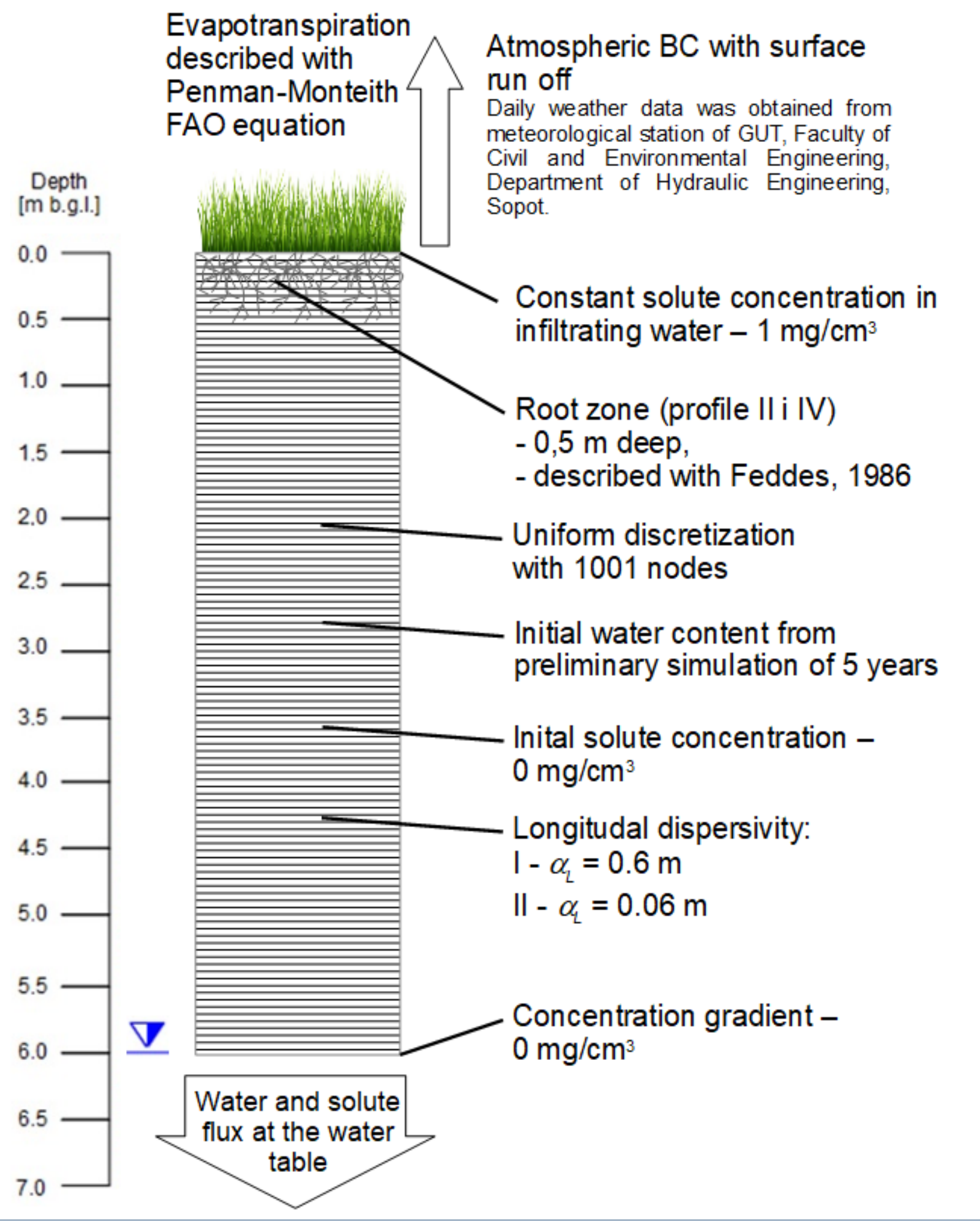
α – parameter related to the average pore size,

n_g – parameter related to the pore size distribution, ks - hydraulic conductivity at saturation.

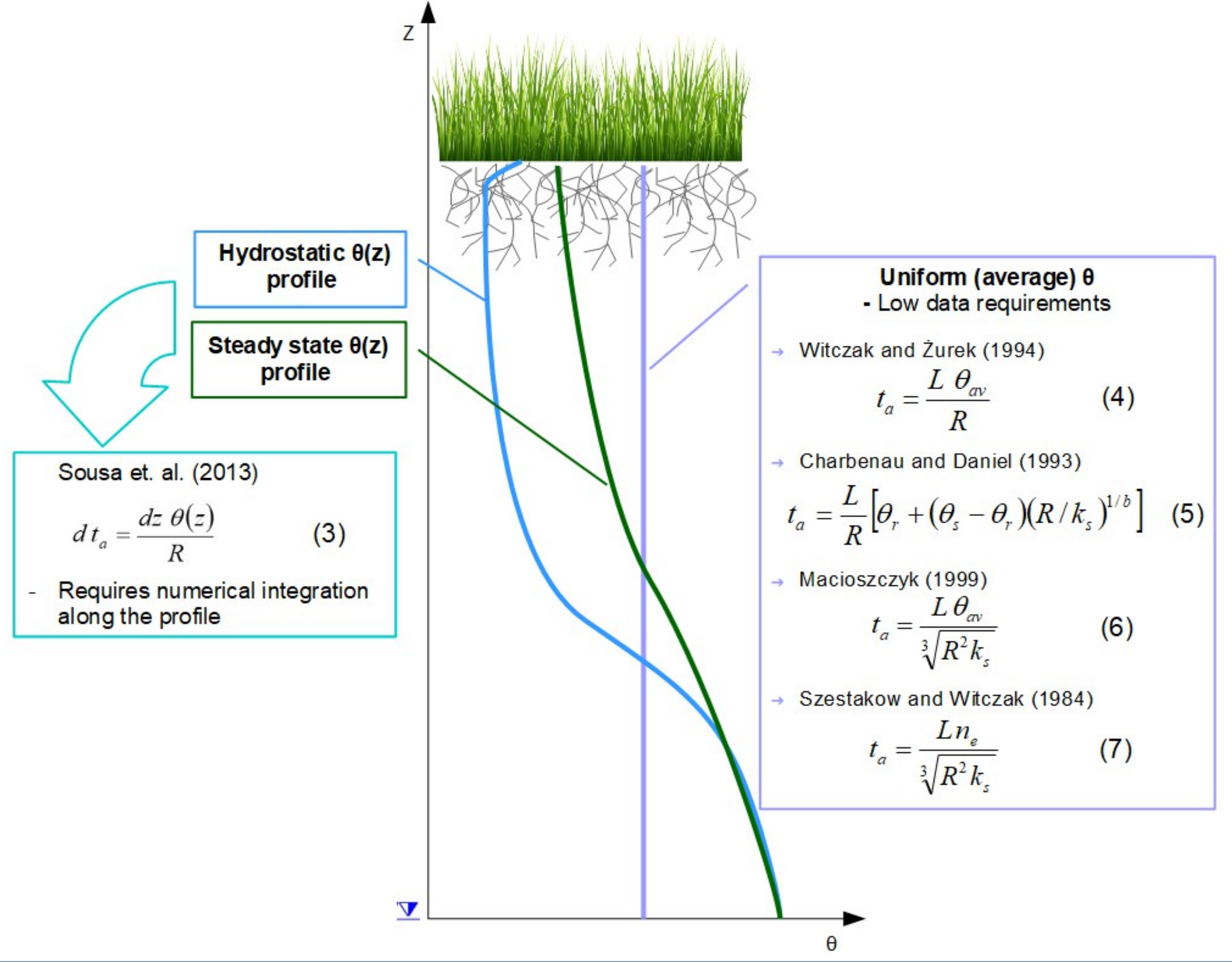
Numerical modeling of transient flow and transport

- **Implementation of Richards equation and advective-dispersive transport equation.**
- **Require a large amount of data.**
- **Significant computational effort.**
- **Both recharge flux and travel time are obtained.**

- HYDRUS-1D (Šimůnek et. al., 2008) computer program was employed to carry out the calculations.
- Simulated periods were 5 years for sand and 60 years for clay loam.
- Times of conservative contamination travel were specified for concentrations c=0.01 mg/cm³ and c=0.99 mg/cm³ appeared at the bottom boundary of model.



Analytical methods



Sousa et. al. (2013)

$$dt_a = \frac{dz\,\theta(z)}{R} \qquad (3)$$

- Requires numerical integration along the profile

Uniform (average) θ
- Low data requirements

→ Witczak and Żurek (1994)

$$t_a = \frac{L\,\theta_{av}}{R} \qquad (4)$$

→ Charbenau and Daniel (1993)

$$t_a = \frac{L}{R}\left[\theta_r + (\theta_s - \theta_r)(R/k_s)^{1/b}\right] \qquad (5)$$

→ Macioszczyk (1999)

$$t_a = \frac{L\,\theta_{av}}{\sqrt[3]{R^2 k_s}} \qquad (6)$$

→ Szestakow and Witczak (1984)

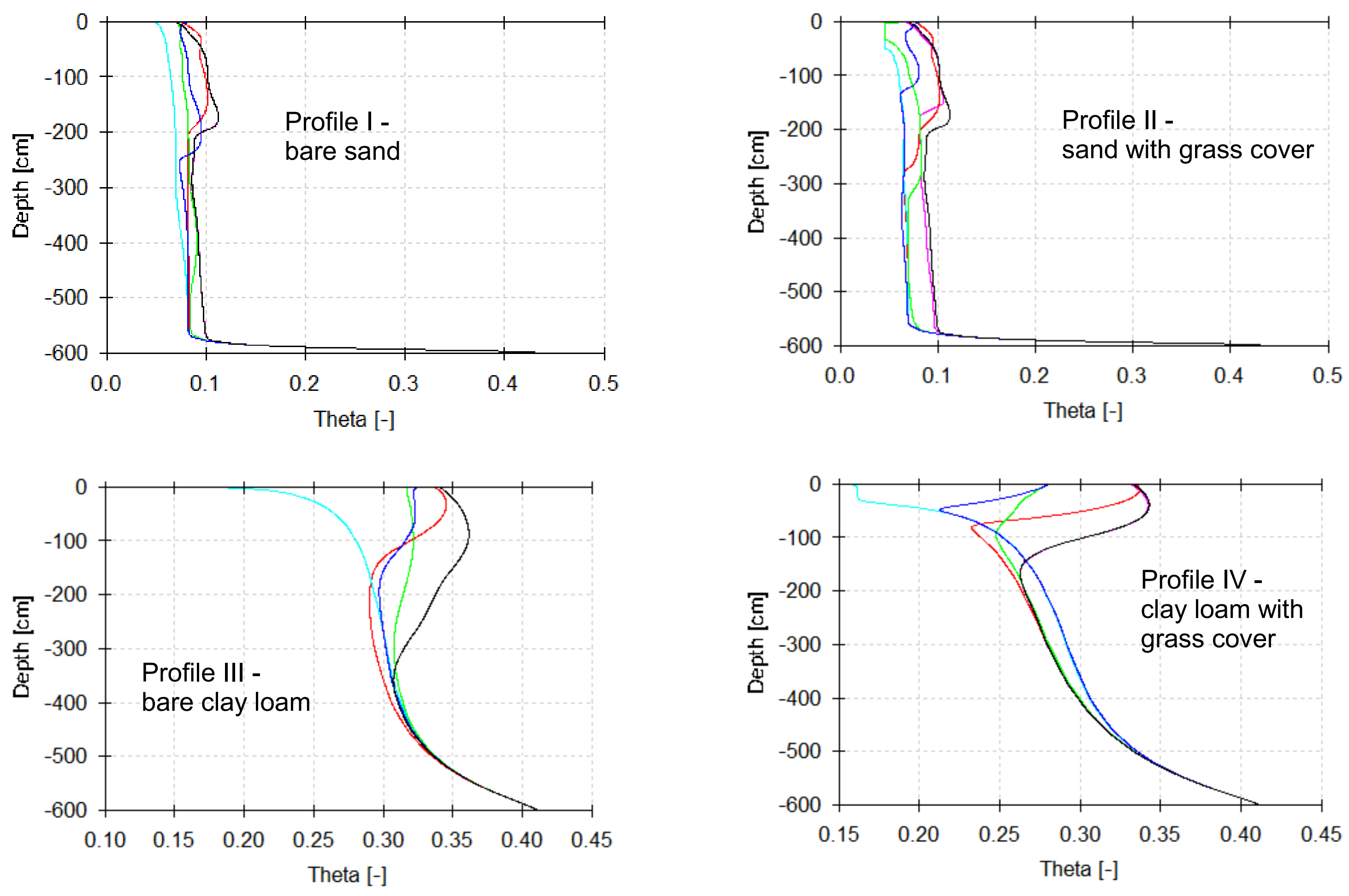
$$t_a = \frac{L n_e}{\sqrt[3]{R^2 k_s}} \qquad (7)$$

- **Transport only by advection (no dispersion).**
- **Steady downward flow.**
- **θ can be uniform or variable.**
- **Recharge (R) taken from transient simulations**
- **θ, ne and b estimations based on literature data.**

Parameters applied in numerical methods

	Sand	Clay Loam
θ	0.07-0.10	0.24-0.32
n_e	0.2-0.385	0.1-0.315
b	4.19	9.45

Results



Volumetric water content profiles obtained from HYDRUS-1D simulations for profile I (bare sand), profile II (sand with grass cover), profile III (bare clay loam)and profile IV (clay loam with grass cover).

Quantity	Sand-bare	Sand-grass	Clay loam-bare	Clay loam-grass
Mean annual recharge [mm/yr]	336	154	121	31
Rechage / precipitation ratio [-]	0.61	0.28	0.22	0.06

The average annual values of recharge (Tab. 2) computed by HYDRUS-1D show very significant influence of the vegetative cover, which reduces the recharge by a factor of about 2 for sand and about 4 for clay loam.

Parameters	Sand-bare	Sand-grass	Clay loam-bare	Clay loam-grass
$\alpha_L = 0.60$ m, $c = 0.01$ mg/cm³	81	102	1060	3898
$\alpha_L = 0.60$ m, $c = 0.99$ mg/cm³	620	803	3362	8419
$\alpha_L = 0.06$ m, $c = 0.01$ mg/cm³	398	801	2669	7864
$\alpha_L = 0.06$ m, $c = 0.99$ mg/cm³	628	846	3918	11329

The early appearance of contaminant at the water table (c = 0.01 mg/dm³) is strongly influenced by the dispersion coefficient (Tab. 3), especially in sand where the travel time is 5 to 8 times shorter for large dispersion case compared to the small dispersion case. For clay loam the differences are smaller, but still very significant, with the difference in travel time by a factor of 2. On the other hand the differences in arrival time of the high concentration (c = 0.99 mg/dm³) are much less significant and do not exceed 35%.

Profile	Sand-bare	Sand-grass	Clay loam-bare	Clay loam-grass
steady flow	590	1184	5850	21584
hydrostatic	357	779	5237	20441

The hydrostatic profile assumption results in shorter travel times (Tab. 4), however the differences are not very big. The largest relative difference between the steady flow and hydrostatic case occurs for bare sand, the smallest one for vegetated clay loam.

Equation	Sand-bare	Sand-grass	Clay loam-bare	Clay loam-grass
(4) (Witczak and Żurek 1994)	455 – 649	899 – 1285	4360 – 5813	16841 – 22455
(5) (Charbeneau and Daniel 1993)	589	1176	5011	17675
(6) (Macioszczyk 1999)	23 – 33	35 – 50	827 – 1182	1849 – 2642
(7) (Bindemann, cited in Szestakow and Witczak 1984)	66 – 127	112 – 214	319 – 999	784 – 2461

Travel times calculated with analytical methods vary greatly between the formulas (Tab. 5). For sand Eq (4) seems to be in a relatively good agreement with the results from transient simulations (small dispersion case). For clay loam the estimated travel time was significantly longer than the one obtained from HYDRUS-1D, especially in the case of vegetation. The method of Charbeneau and Daniel (1993) gave travel times within the range predicted by Eq. (4). In contrast, both Eq. (6) I Eq. (7) in all scenarios gave travel times much shorter than the ones computed from HYDRUS-1D and other methods. For sand Eq. (6) leads to the shortest travel times, because the volumetric water content is smaller than the effective porosity used in Eq. (7). For clay loam, if one uses small values of the effective porosity, as commonly reported in the literature, Eq. (7) predicts shorter time lag than Eq. (6).

Conclusions

- **Groundwater recharge flux strongly depends on the presence of root zone, for either sand or clay loam. Consequently, the travel time of pollutant also is affected by the presence of root zone.**
- **The assumed dispersion constant have significant influence on the arrival time of contaminant at the water table, which seems to be important in view of the widespread calculation of travel time based on the assumption of purely advective flow.**
- **The methods using steady flow approximation showed mixed performance, even though it was assumed that the exact value of average groundwater recharge is known for each soil profile. Care should be taken if simple analytical formulas are to be used to estimate unsaturated zone travel time. In view of the growing computer capacities and availability of simulation software and parameter data, it seems advisable that numerical simulations are used for at least partial comparisons with the analytical results.**

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