DETERMINATION AND MODELING OF SOLUTE DIFFUSION TORTUOSITY FACTORS IN UNSATURATED SOILS

Hsin-yi Chou and Laosheng Wu

Department of Environmental Sciences, University of California, Riverside

Introduction

Solute diffusion flux in soil is described by Fick's law along with a tortuosity factor to account for the tortuous and reduced diffusive pathway blocked by soil particles:

$$J = -\xi D_0 \frac{\partial C}{\partial z} = -D_s \frac{\partial C}{\partial z}$$

$$\xi = \frac{D_s}{D_0}$$

Predictive models based on empirical or conceptual relationships with other more commonly measured soil attributes have been proposed to replace the time-consuming and multifarious laboratory measurements. However, these models have not been systematically tested and evaluated with soils of different textures under comparable conditions.

Objectives

- **Evaluate the solute diffusion tortuosity factor models with soils of different textures under unsaturated conditions.**
- **Assess the effect of water retention hysteresis effect on solute diffusivity.**

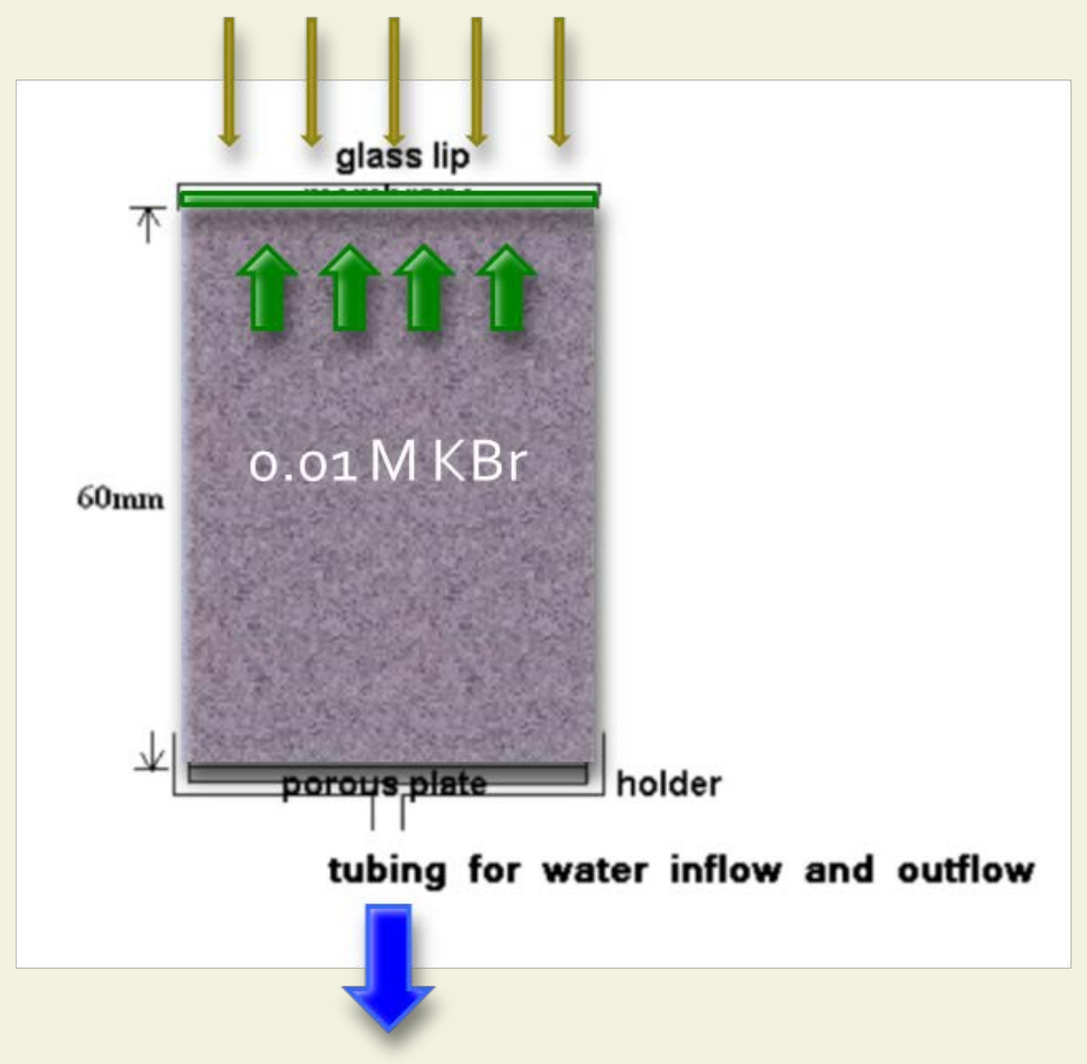
Materials

Texture	Particle size distribution (%)				Bulk density ($\mathrm{g\ cm^{-3}}$)	Porosity ($\mathrm{cm^3\ cm^{-3}}$)	Specific area ($\mathrm{m^2\ g^{-1}}$)
	Coarse sand	Fine sand	Silt	Clay			
Sand	16.1	71.2	10.6	2.1	1.60	0.40	0.61
SC loam	0.6	65.3	12.6	21.5	1.45	0.45	19.73
Clay	0.2	5.5	36.4	57.9	1.60	0.40	37.19

Methods

- **Cores (5 cm by 6 cm) packed to predetermined bulk densities.**
- **Diffusion cells saturated with 0.01 M potassium bromide, and then equilibrated to prescribed pressures.**
- **The cells were transferred to a 25 ° C, vapor saturated humidity chamber to equilibrate for 7 days for the diffusion experiments.**
- **Cl⁻ saturated polythersulfone/copolymer anion-exchange membrane (PALL, SB-6407) was placed in contact with the exposed soil surface to act as the sink for the diffusing Br⁻ [*Tinker*, 1969]**
- **Each treatment was replicated for 3 times.**

Measuring Solute Diffusion Coefficient in Soil



Results

Power functions

$\xi = c\theta^{\varepsilon}$

Papendick et al.

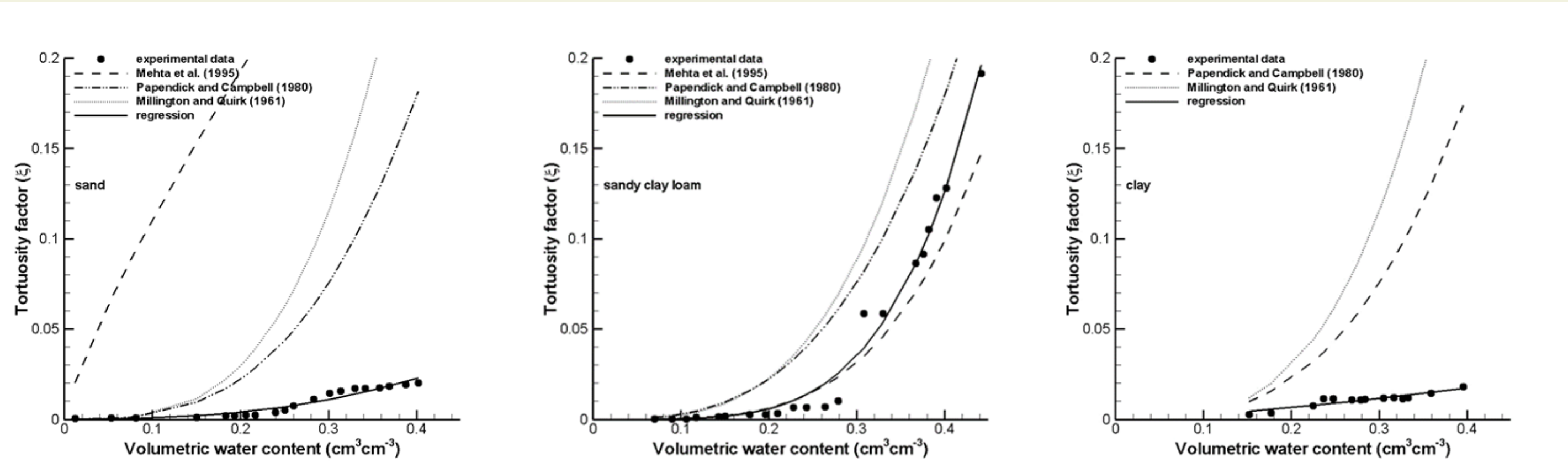
$\xi = \gamma \frac{\theta^{n}}{\phi^{m}}$

Millington and Quirk (1961)

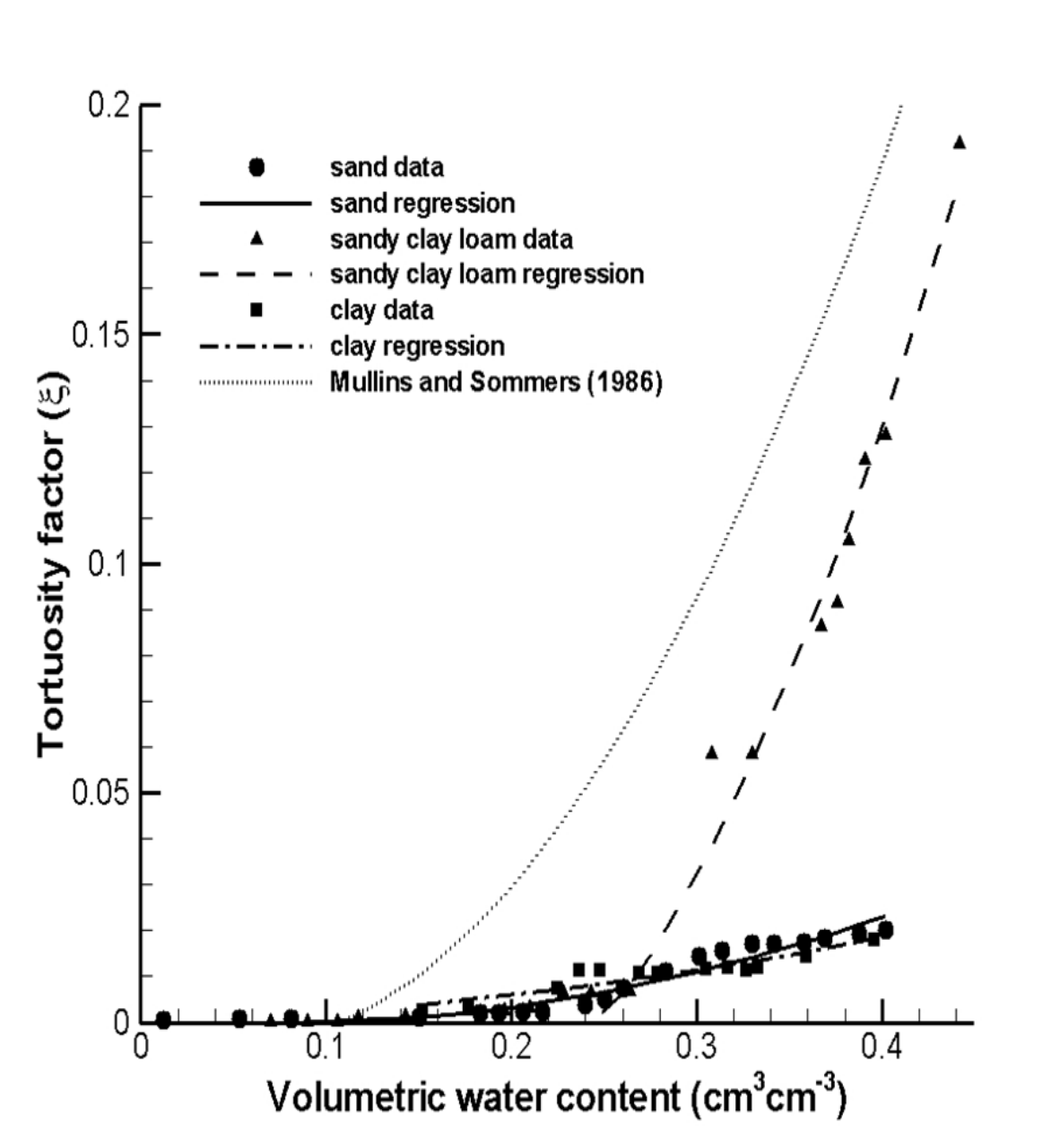
$[\xi = \theta^{10/3}/\phi^{2}]$

$\xi = \xi^{*} \cdot \theta \cdot (\frac{\theta}{\phi})^{k_1 + k_2 b}$

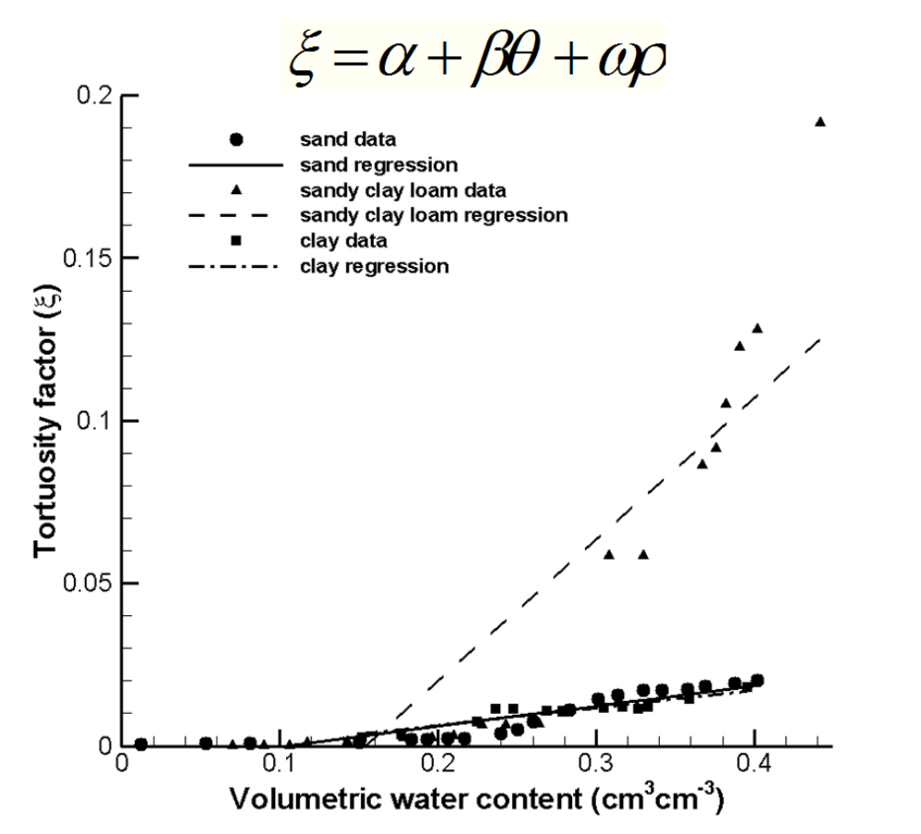
Olesen et al. (1996)



Quadratic functions: Mullins & Sommers



Linear function

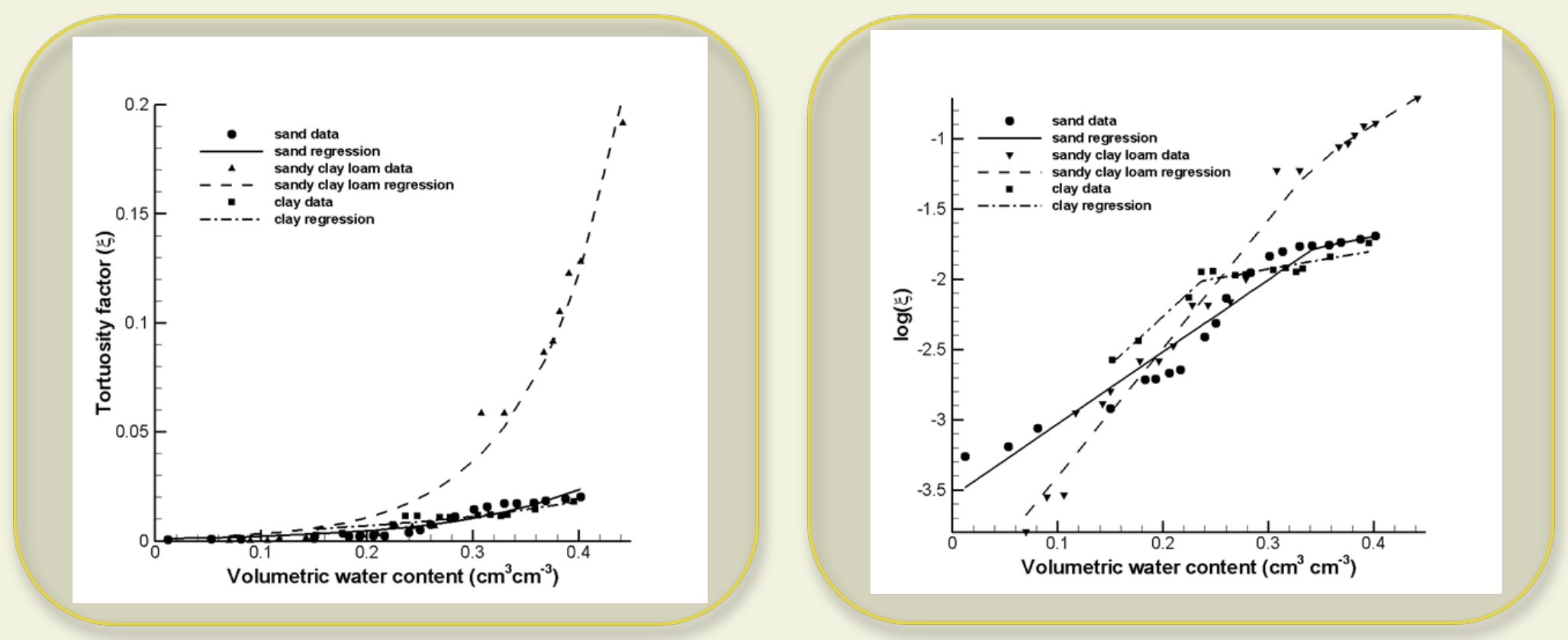


$\xi = \alpha + \beta\theta + \omega p$

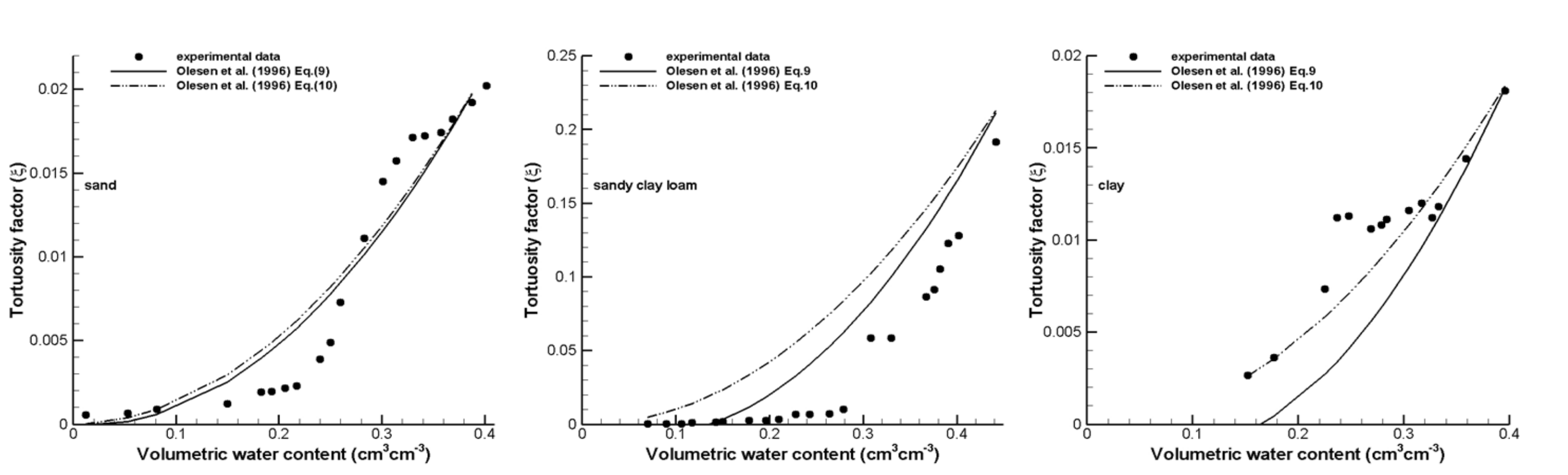
Exponential function

$\xi = \Omega \cdot \exp(\lambda\theta)$

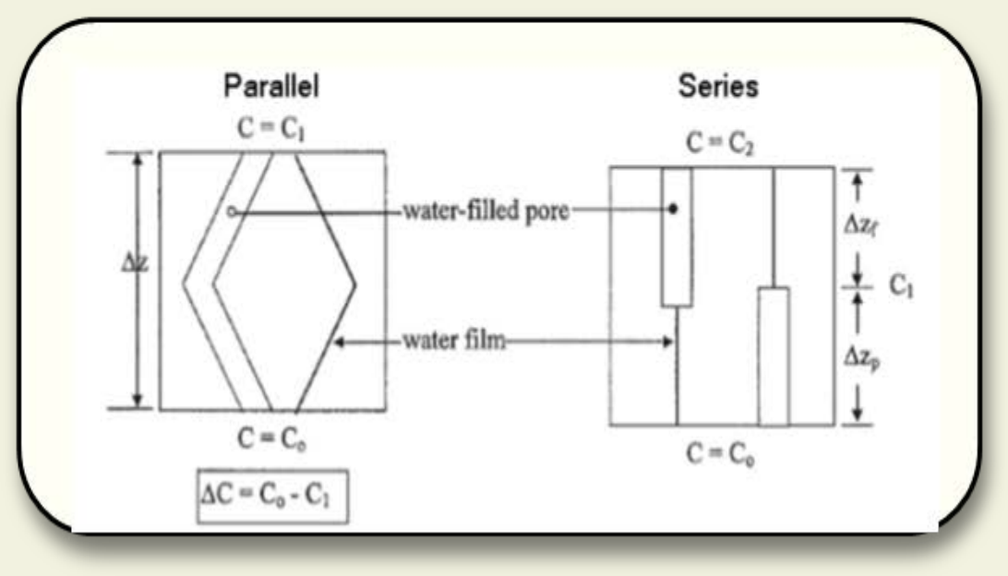
$\xi = 10^{a\theta + b}$

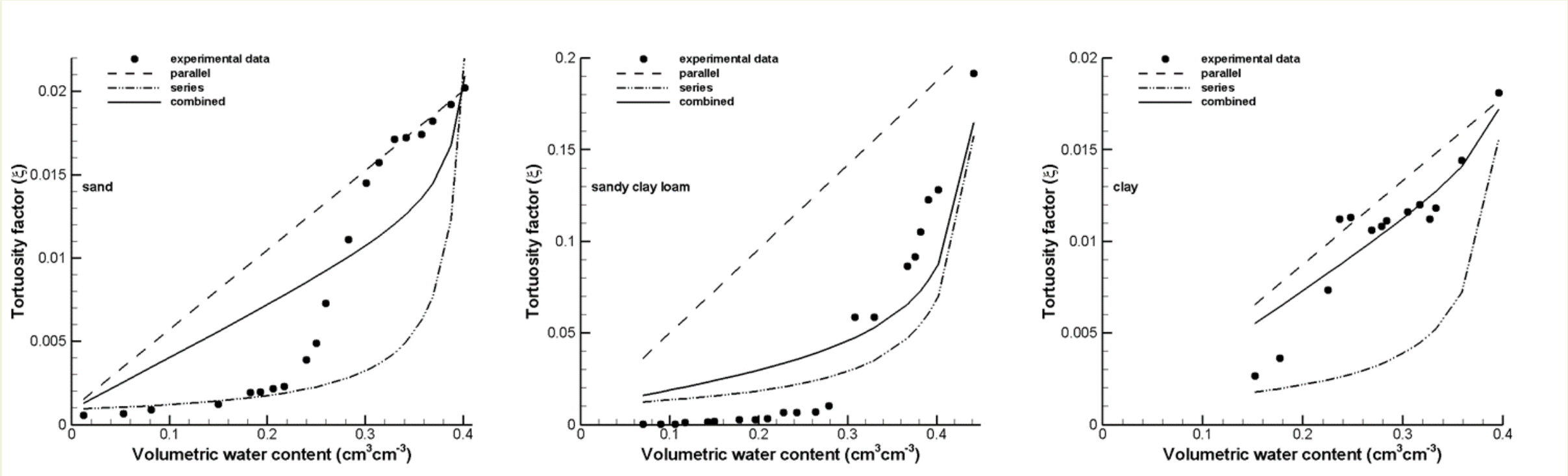


Quadratic functions: Olesen et al. (1996)



Conceptual Model





Models with Minimum Akaike information criterion (*AICc*) and largest AIC weight

Models	Parameters	*AICc*			*AIC* weights		
		sand	SCL	clay	sand	SCL	clay
Olsen and Kemper [1968] Equation (2)	Ω, λ	-233.26	-189.02	-171.49	0.0018	0.0002	0.0219
Hamamoto [2009] Equation (3)	ξ_c, s_1, s_2, θ	-239.13	-193.96	-175.65	0.0344	0.0025	0.1754
Papendick and Campbell [1980] Equation (4)	c, ξ	-241.78	-201.35	-174.44	0.1290	0.0994	0.0960
Olesen et al. [1996] Equation (6)	*c*	-242.46	-202.75	-175.73	0.1815	0.1999	0.1826
Mullins and Sommer [1986] Equation (7)	*δ, μ*	-245.02	-205.25	-172.41	0.6533	0.6981	0.0346
Moldrup et al. [2007] Equation (11)	*H*	-226.54	-165.43	-118.92	0.0001	0.0000	0.0000
So and Nye [1989] Equation (14)	α, β	-222.13	-145.14	-175.81	0.0000	0.0000	0.1902
Lim et al. [1998] Equation (18)	η	-217.9	-148.47	-176.72	0.0000	0.0000	0.2994

* The model with the lowest AICc, but highest AIC weight value is the best.

Summary

- **There is not a particular model that can fit the solute diffusion data for all the three test soils with different textures.**
- **The solute diffusion tortuosity factors of the sand and sandy clay loam soils are best described by a quadratic function, i.e., the Mullins and Sommer [1986] model. For the clay soil, the combined parallel-series conceptual model provides the best description for the change of tortuosity factor with soil water content.**
- **Currently, most simulation models use the Millington and Quirk [1961] tortuosity factor model. Our evaluation shows that this model overestimates the experimental data for all three test soils when their suggested model parameters are used.**

Reference

Chou, Hsinyi, Laosheng Wu, Lingzao Zeng, and Andrew Chang. 2012. Evaluation of solute diffusion tortuosity factor models for variously saturated soils, Water Resour. Res. 48: W10539

Contact: Laosheng.Wu@ucr.edu