Predicting the Soil-Gas Diffusion Coefficient: Universal Water-Induced Linear Reduction (U-WLR) Model for Repacked and Intact Soil

Per Moldrup[1*], Chamindu Deepagoda[1], Toshiko Komatsu[2], Ken Kawamoto[2], Dennis E. Rolston[3], and Lis Wollesen de Jonge[4]

[1] Department of Biotechnology, Chemistry and Environmental Engineering, Aalborg University, DENMARK (*pm@bio.aau.dk)
[3]Graduate School of Science and Engineering, Saitama University, JAPAN
[3]Dept. of Land, Air, and Water Resources, University of California, Davis, USA
[2] Dept. of Agroecology and Environment, Faculty of Agricultural Sciences, Aarhus University, DENMARK

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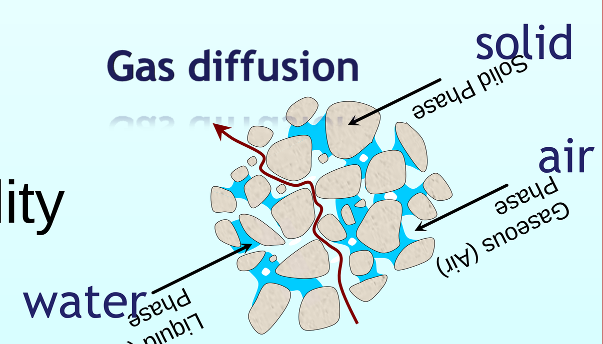
BACKGROUND

- The soil-gas diffusion coefficient (D_p) is a major control of transport, reactions, emissions, and uptake of vadose zone gases, including oxygen, greenhouse gases, applied fumigants, and spilled volatile organics.
- The D_p depends on soil moisture, texture, aggregation, compaction, and not at least, on the local-scale variability of all of these.
- This likely explains why different predictive models have been developed and used for D_p in intact and repacked soils, respectively.



MODELS

- Millington and Quirk (1961)

$$\frac{D_p}{D_o} = \frac{\varepsilon^{\frac{10}{3}}}{\Phi^2} \qquad [1]$$

D_p: Soil-gas diffusion coefficient (cm³ soil air /cm soil sec)
D_o: Soil-gas diffusion coefficient (cm²/sec)
ε : air-filled porosity (cm³ soil-air/cm³ soil)
Φ : Total porosity (cm³ void space /cm³ soil)

- WLR- Marshall Model (Moldrup et al.,2000)

$$\frac{D_p}{D_o} = \varepsilon^{1.5} \qquad [2]$$

- U-WLR Model (Moldrup et al.,2012)

$$\frac{D_p}{D_o} = \varepsilon^{(1+C_m*\Phi)*\left(\frac{\varepsilon}{\Phi}\right)} \qquad [3]$$

C_m : Media complexity factor

RESULTS AND DISCUSSION

- In this study, the model exponent of the frequently used Water-induced Linear Reduction (WLR; Moldrup et al. 2000) model for D_p was modified with a porosity term including a coefficient of local-scale (sample-scale) complexity and heterogeneity, C_m. With $C_m = 1$, the universal WLR model (U-WLR) accurately predicted gas diffusivity (D_p/D_o, where D_o is the gas diffusion coefficient in free air) in sieved, repacked soils with between 0 and 54% clay, Fig. 1.
- With $C_m = 2$, the model on the average gave excellent predictions for 280 intact soils grouped into 2 data bases, hereunder performed well for sub-groupings with respect to soil depth, texture, and compaction (density). In general, the U-WLR model outperformed similar D_p/D_o models also depending only on total and air-filled porosity, including the original WLR and the Millington and Quirk (1961) models, Fig. 2 and 3.
- Representing both repacked and intact soil conditions well and for the first time distinguishing between them, the U-WLR model is recommended instead of the commonly used WLR and Millington and Quirk type models for predicting gas transport and fate in soil, with recommended values of C_m = 1 for repacked soil and C_m = 2 for intact soil. Additionally, for risk assessment and uncertainty analyses of soil-gas transport, the U-WLR model with C_m = 0.5 and 3, respectively, represent likely upper- and lower-limit D_p/D_o predictions (window of soil-gas diffusivity) for intact soil, Fig. 4.

MODEL TESTS

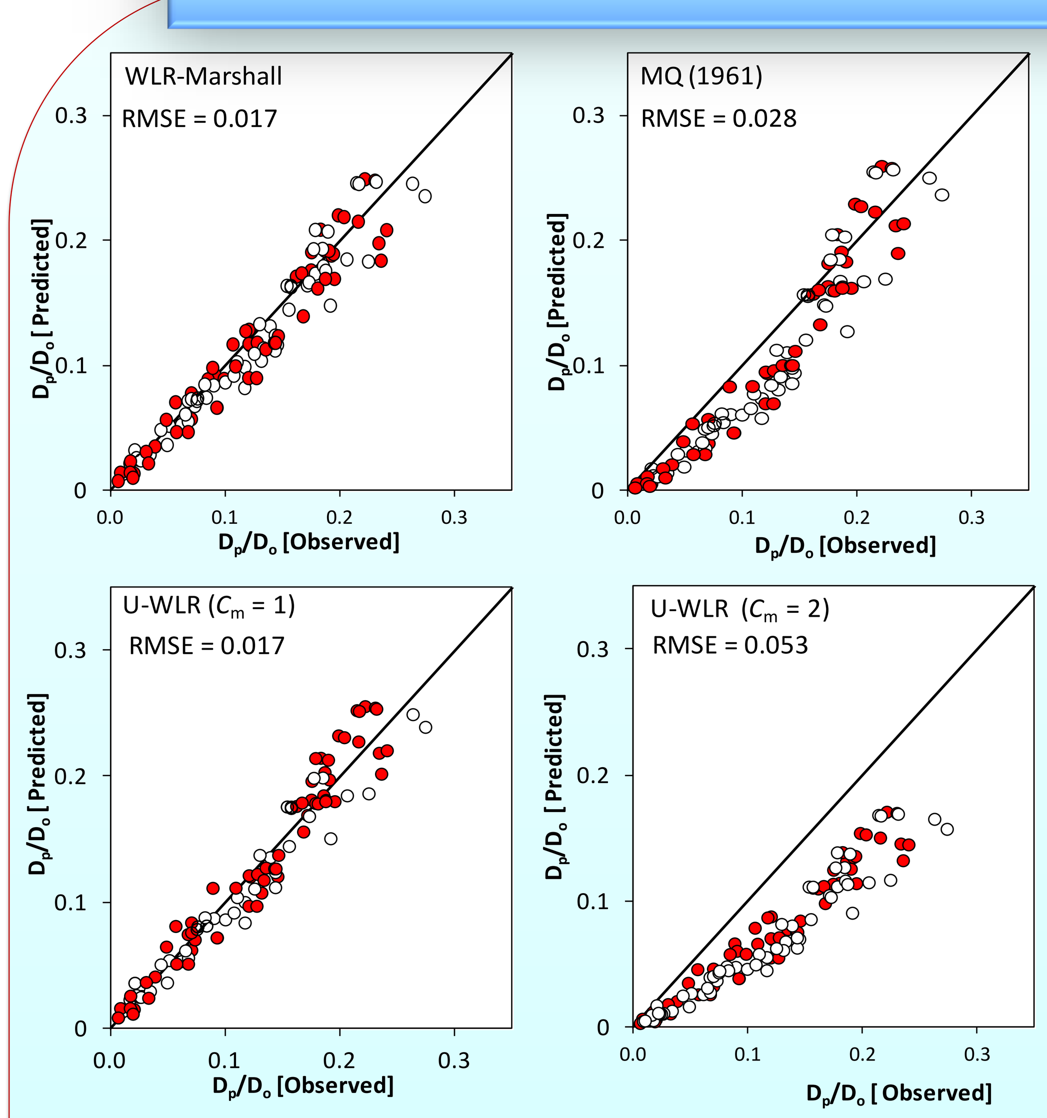


Fig 1. Test of four soil-gas diffusivity models against data for 11 repacked soils
Data: Moldrup et al., 2012

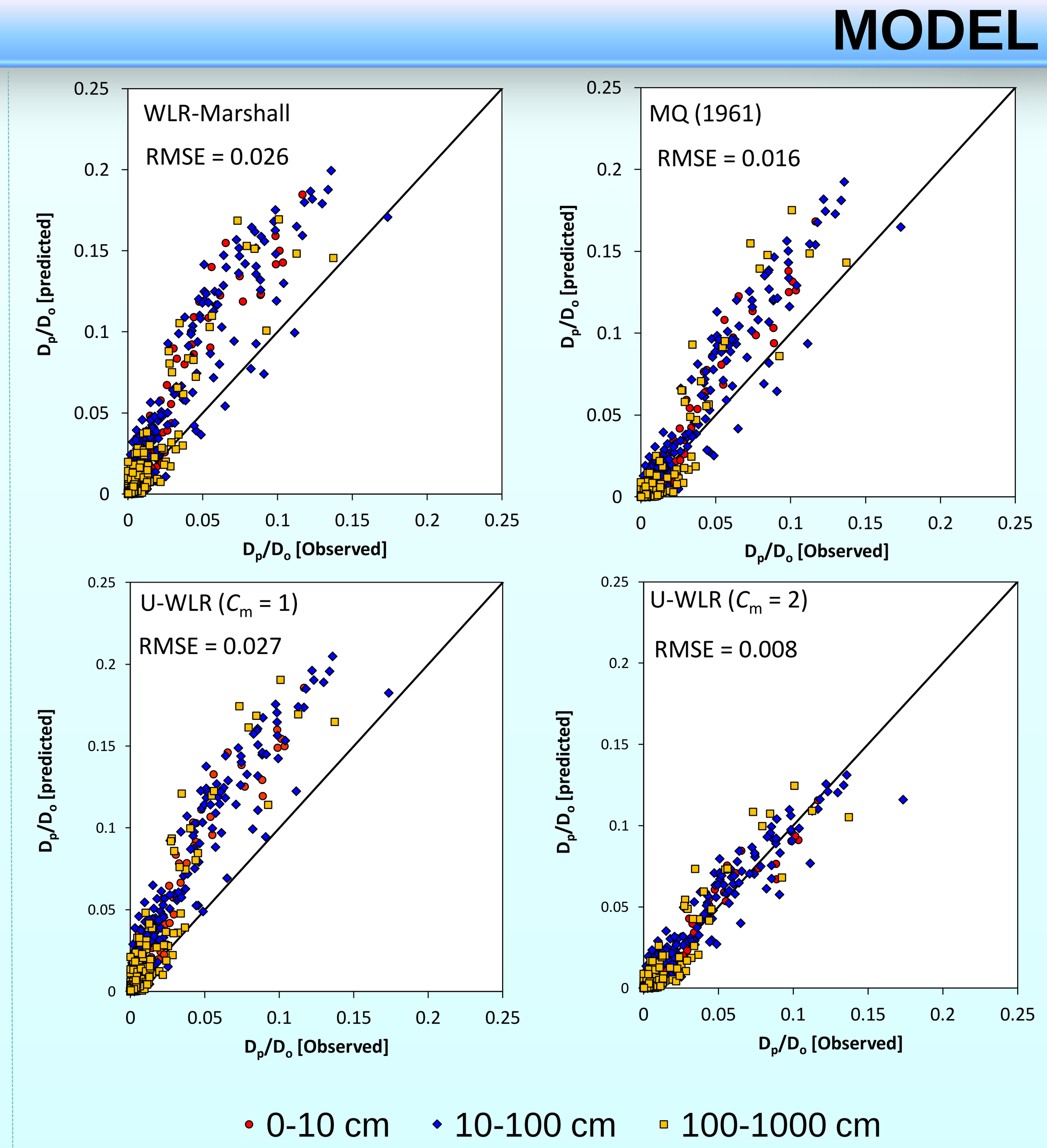


Fig 2. Test of four soil-gas diffusivity models against data for 150 intact soils
Data: Moldrup et al.,2012

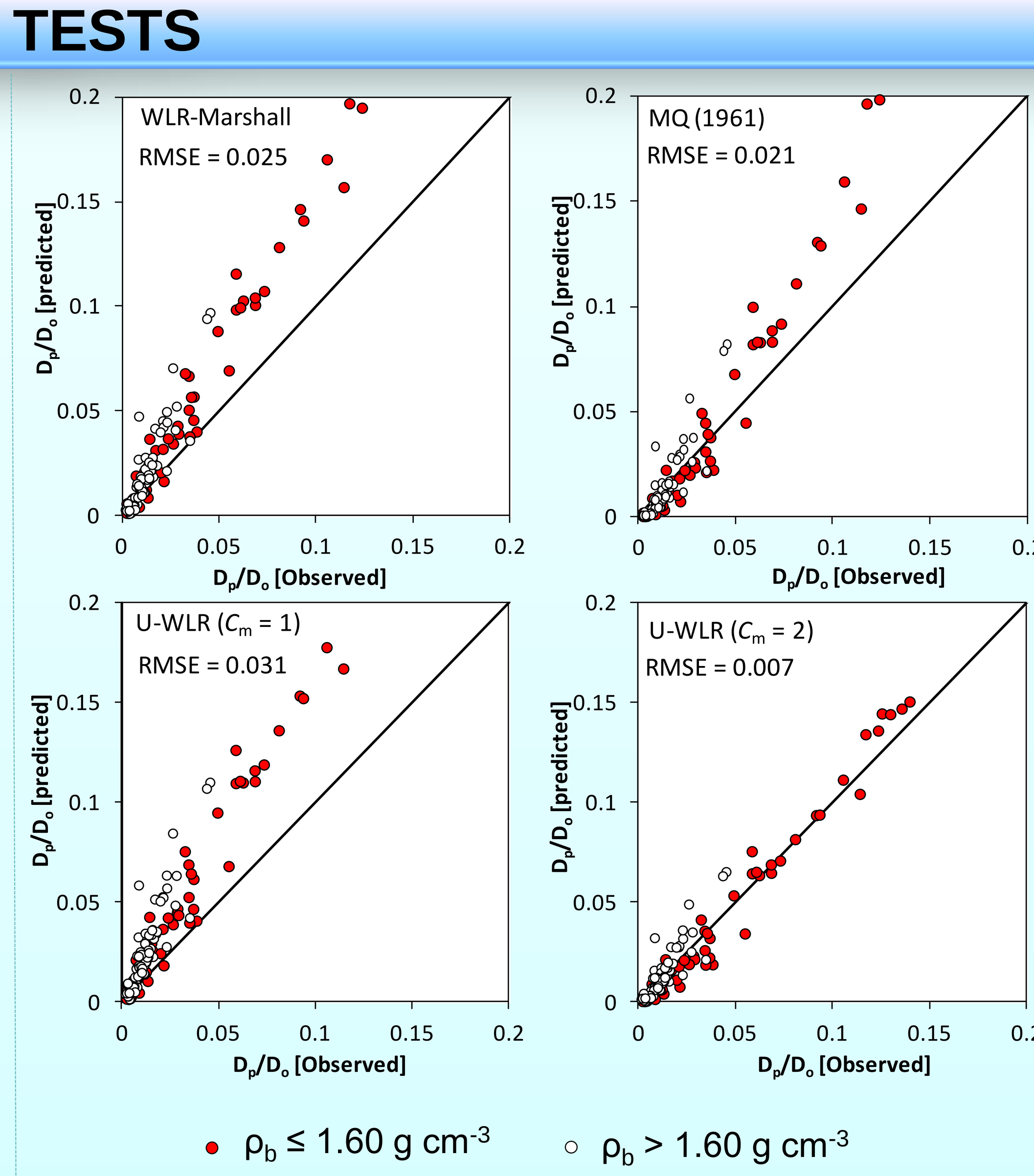


Fig 3. Test of nine soil-gas diffusivity models against data for additional 130 intact soils
Data: Moldrup et al., 2012

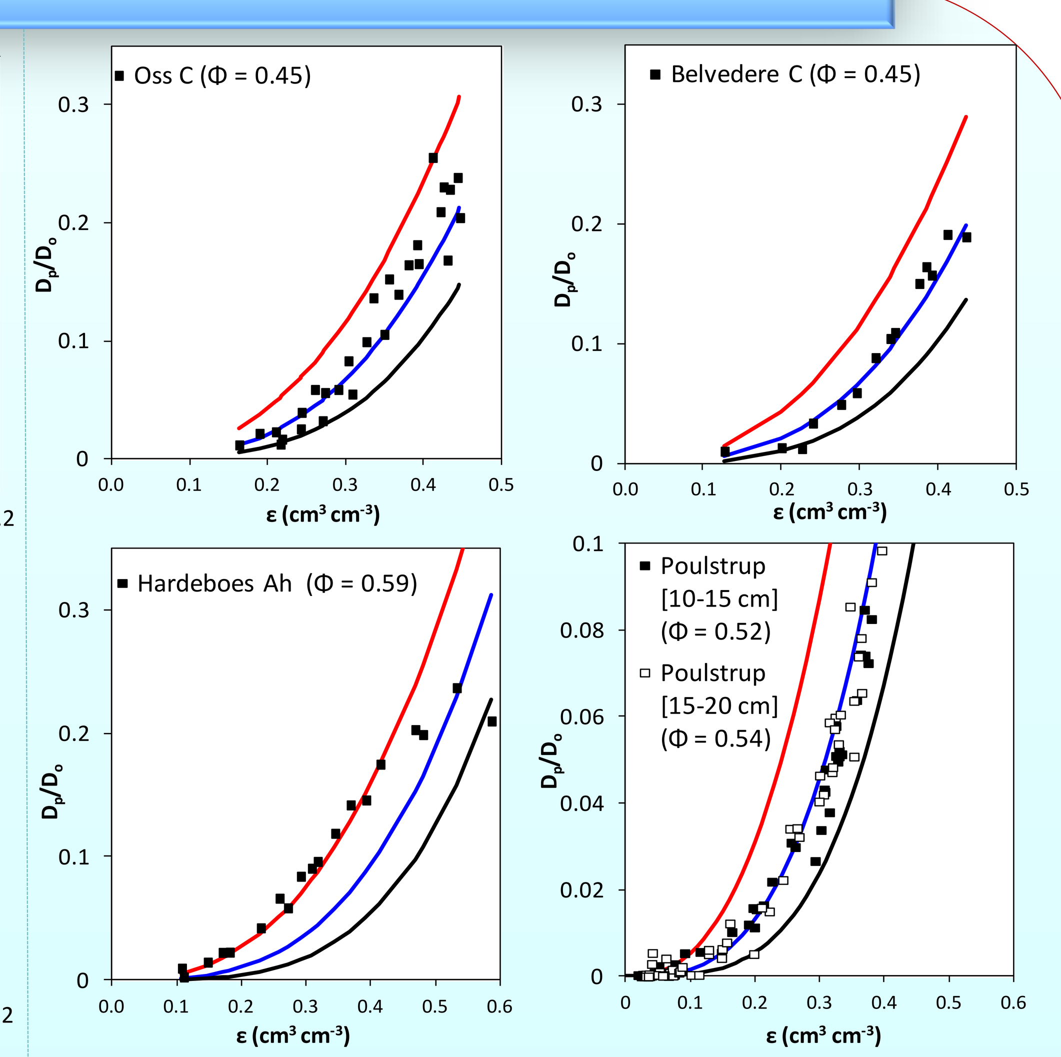


Fig 4. Windows of soil-gas diffusivity for intact "extreme" soils not included in Fig. 2 and 3. U-WLR model predictions with Cm = 0.5 (red), 2 (blue), and 3 (black) for a sandy soil (96% sand), a high-silt soil (79% silt), an aggregated high-silt soil (62% silt and 5% organic matter; data suggesting two-region behavior), and a high-organic forest soil (two layers).
Data: Freijer (1994) and Moldrup et al. (1996).

ACKNOWLEDGEMENT

This study was part of the project Gas Diffusivity in Intact Unsaturated Soil ("GADIUS") and the large framework project Soil Infrastructure, Interfaces, and Translocation Processes in Inner Space ("Soil-it-is"), both from the Danish Research Council for Technology and Production Sciences. This study was in part supported by the Japan Science and Technology Agency (JST) in the Core Research Evolutional Science and Technology (CREST) project. We also gratefully acknowledge the assistance of the Innovative Research Organization of Saitama University, Japan. Finally, S. Thomas Albert and Christian Michael are acknowledged for their coherent input, inspirational design, and strong presence at major scientific venues including the SSSA annual meetings.

REFERENCES

- Freijer, J.I. 1994. Calibration of jointed tube model for the gas diffusion coefficient in soils. Soil 7 Sci. Soc. Am. J. 58:1067-1076.
- Millington, R.J., and J.P. Quirk. 1961. Permeability of porous solids. Trans. Faraday Soc. 57:1200-1207.
- Moldrup, P., T. Olesen, J. Gamst, P. Schjønning, T. Yamaguchi, and D.E. Rolston. 2000. Predicting the gas diffusion coefficient in repacked soil: Water-induced linear reduction model. Soil Sci. Soc. Am. J. 64:1588–1594.
- Moldrup, P., T.K.K. Chamindu Deepagoda, S. Hamamoto, T.Komatsu, K. Kawamoto, D. E. Rolston, and L.W. de Jonge. 2012. Predicting the soil-gas diffusion coefficient in repacked and intact soil: A universal, water-induced linear reduction model. Soil Sci. Soc. Am. J. (under review)