SOIL-GAS DIFFUSIVITY IN PASTURE TOPSOIL

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Abstract: Soil-gas diffusivity plays a fundamental role on diffusion-controlled migration of gases which is important in relation to soil aeration and climate gas emissions. Gas diffusivity is a function of soil type and soil structure (e.g., density) and therefore typically shows a depth-dependent behaviour. This study investigated the gas diffusivity in repacked soils taken from past literature studies. The soils were pre-characterized for particle-size distribution, organic matter content, dry density and particle density. Soil-gas diffusivity and soil-water characteristic were measured using one-chamber diffusion apparatus and sandbox, respectively. The measured diffusivity of selected repacked soil data from literature were tested against the existing predictive gas diffusivity models. A descriptive parametric two-region model was developed considering scaling factors and shape factors representing two-region behaviour of each selected soil. This two-region model performed statistically better than other predictive models for all the repacked soils.

Keywords: Diffusion; Gas diffusivity; Bimodal soils; Two-region; Tortuosity

1. Introduction

Pasture sites are predominant sources of greenhouse gases such as methane, (CH_4), and nitrous oxide (N_2O) which inevitably affect the climate resulting in global warming and climate shifts. For example, N_2O has 298 times global warming potential than that of CO_2 over a 100-year time frame (Myhre et al., 2013). Extensive applications of nitrogen fertilizer and increased stocking rates are the main factors contributing to enhanced pastoral emissions of N_2O. Primarily, N_2O is produced through nitrification and denitrification mechanisms as a result of microbial processes in the presence of anaerobic regions in the soil.

The migration of N_2O in pastoral topsoil (10-15 cm), and its emission to the atmosphere is predominantly diffusion-controlled. In addition, the soil textural and structural properties, as well as soil moisture status, play a significant role on N_2O emissions. Mitigation measures, therefore, are highly dependent on how well the diffusion-controlled gas transport processes in soil is understood.

Gas diffusion in soil is commonly described by soil-gas diffusivity, D_p/D_o where D_p (m^3 soil air m^{-1} soil s^{-1}) and D_o (m^2 air s^{-1}) are the soil-gas diffusion coefficients in soil and in free air, respectively. Measuring D_p/D_o is, however, experimentally intensive and instrumentally challenging and hence predictive gas diffusivity models are widely used to predict soil-gas diffusivity from easily-measurable properties such as air-filled porosity (ε) and total porosity (Φ).

Generally, the pasture soils are considered to be well-structured aggregated soils, having both inter-aggregate pores (i.e., pores between the aggregates) and intra-aggregate pores (i.e., pores within the aggregates), resulting in a bimodal pore structure. However, compaction of soil due to animal treading and mechanical implements on pasture sites may alter soil pore structure (Jayarathne et al., 2019). Compaction essentially reduces the macropore domains and increase the micropore domains of soil, thus shifting the bimodal nature of soil. Although there are currently available predictive models to predict gas diffusivity in non-aggregated soils, these models cannot be used directly for aggregated soils as they may result in biased results due to the presence of two distinct pore regions (Jayarathne et al., 2019). Therefore, various models have been modified and developed to predict the soil-gas diffusivity in well-structured aggregated soils.

In this study, a series of literature measurements on D_p/D_o were used to characterize gas transport behaviour on pasture topsoil (0-5 cm). The selected soils include a wide geographic origin including Sri Lankan, Japanese and New Zealand soils. An ensemble of soil-gas diffusivity models was tested against diffusivity data and a new descriptive gas diffusivity model was introduced to better characterize the pasture soils.

2. Materials and Methods

2.1 Soils and data

The important physical properties of the repacked pasture topsoil selected from the literature are given in Table 1. The soils will be referred hereafter from their corresponding sampling locations.

Table 1: Soils and data from literature and their physical properties

<table>
<tr><th rowspan="2">Soil</th><th rowspan="2">Sampling depth (cm)</th><th rowspan="2">Soil Type</th><th colspan="3">Soil Texture</th><th rowspan="2">Bulk density (mg m^{-3})</th><th rowspan="2">Organic matter (kg kg^{-1})</th><th rowspan="2">Total porosity (cm^3 cm^{-3})</th><th rowspan="2">Reference</th></tr>
<tr><th>Sand (%)</th><th>Silt (%)</th><th>Clay (%)</th></tr>
<tr><td>Wakanui, NZ (NZ-WK)</td><td>0-5</td><td>Sandy loam</td><td>70.6</td><td>25.4</td><td>4.0</td><td>0.95 (0.07)</td><td>0.09</td><td>0.64</td><td rowspan="3">Deepagoda et al. (2019)</td></tr>
<tr><td>Temuka, NZ (NZ-TE)</td><td>0-5</td><td>Sandy loam</td><td>64.4</td><td>32.3</td><td>3.3</td><td>1.14 (0.05)</td><td>0.10</td><td>0.57</td></tr>
<tr><td>Templeton, NZ (NZ-TmS)</td><td>0-5</td><td>Loamy sand</td><td>80.1</td><td>18.4</td><td>1.4</td><td>1.19 (0.18)</td><td>0.09</td><td>0.55</td></tr>
<tr><td>Peradeniya-1, SL (PD-P)</td><td>0-10</td><td>Sandy loam</td><td>72.1</td><td>25.1</td><td>2.8</td><td>1.10 (0.05)</td><td>0.10</td><td>0.57</td><td>Jayarathne et al. (2019)</td></tr>
<tr><td>Peradeniya-2, SL (PD-P)</td><td>0-10</td><td>Sandy loam</td><td>72.1</td><td>25.1</td><td>2.8</td><td>1.30 (0.05)</td><td>0.10</td><td>0.57</td><td>Jayarathne et al. (2019)</td></tr>
<tr><td>Nishi-Tokyo, JP (NT-P)</td><td>0-5</td><td>Silt loam</td><td>NA$^{\pm}$</td><td>NA</td><td>NA</td><td>0.62 (0.05)</td><td>NA</td><td>0.74</td><td>Deepagoda et al. (2011)</td></tr>
</table>

SL: Sri Lanka; NZ: New Zealand; UK: United Kingdom; JP: Japan; $^{\pm}$ NA: Not available

2.2 Measurement methods

The measurements on D_p/D_o were carried out in the literature following a common method as outlined below. Initially, the collected samples using 100 cm^3 annular cores were saturated for 72 hours and sequentially drained to nine intended moisture levels by stepwise evaporation. The samples were then kept closed for a sufficient time to reach the hydraulic equilibrium before diffusivity measurements.

Gas diffusivity was measured following the one chamber method introduced by Taylor (1949) and developed by Schjønning (1985). The drained samples were then mounted on top of the diffusion chamber through an airtight joint. Then, the chamber was flushed with 99.99% N_2 gas to remove all the O_2 inside the chamber. The sample was then opened to the atmosphere by allowing the atmospheric O_2 to diffuse through the sample into the chamber. The increase of O_2 concentration inside the chamber was monitored continually with an O_2 sensor attached to the chamber wall. Calculation of D_p/D_o was performed following both Currie (1960) and Taylor (1949) methods.

2.3 Soil-gas diffusivity modelling

Selected descriptive/predictive models

Table 2 shows the selected models for the study to compare with the developed descriptive model.

Table 2: Selected descriptive/predictive models

D_p/D_o Model	Equation
Buckingham (1904)	$\frac{D_p}{D_o} = \varepsilon^2$
Penman (1940)	$\frac{D_p}{D_o} = 0.66\varepsilon$
Marshal (1959)	$\frac{D_p}{D_o} = \varepsilon^{3/2}$
Millington (1959)	$\frac{D_p}{D_o} = \varepsilon^{4/3}$
MQ (1960)	$\frac{D_p}{D_o} = \frac{\varepsilon^2}{\emptyset^{2/3}}$
MQ (1961)	$\frac{D_p}{D_o} = \frac{\varepsilon^{10/3}}{\emptyset^2}$
WLR-Marshall	$\frac{D_p}{D_o} = \varepsilon^{1.5}\left(\frac{\varepsilon}{\emptyset}\right)$
SWLR	$\frac{D_p}{D_o} = \varepsilon^{(1+C_m\emptyset)}\left(\frac{\varepsilon}{\emptyset}\right)$

SWLR, Structure-dependent Water-induced Linear Reduction; WLR, water-induced linear reduction; MQ, Millington and Quirk.

Importantly, none of the above models has been developed for, and hence can be particularly applicable to, aggregated soils. Therefore, in this study, we developed a descriptive two-region model which takes the form of:

$$\frac{D_p}{D_o} = A(\mathcal{E} - \mathcal{E}_o)^B + C(\mathcal{E} - \emptyset_i) \qquad (1)$$

where A is model scale factor, B is model shape factor $\mathcal{E}_o$ is threshold air content below which gas diffusion ceases due to water blockage, $\emptyset_i$ is inter-aggregate porosity, C is gradient in the intra-aggregate region (assuming a linear increase).

Tortuosity calculations

The geometric tortuosity is defined as the ratio of the distance traversed by a gas molecule between two known points in the soil to the shortest (Euclidian) distance between the two points.

The tortuosity of the gaseous phase was calculated from measured D_p/D_o and air-filled porosity data using the following equation.

$$\tau = \sqrt{(\varepsilon/(D_p/D_o))} \tag{2}$$

Statistical Analysis

The analysis was done by means of two statistical indices; Root mean square error (RMSE) and Bias. From that, performance of the selected models for gas diffusivity was compared. The RMSE evaluates the overall model fit to the measured data.

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(d_i)^2} \tag{3}$$

The bias evaluates whether a model over estimated (positive bias) or under-estimated (negative bias) the observations.

$$\mathrm{Bias} = \frac{1}{n}\sum_{i=1}^{n}(d_i) \tag{4}$$

where, d_i is difference between the predicted and observed values and n is number of diffusivity measurements in a data set.

3. Results and Discussion

Pasture soils are often structurally aggregated and characterized by two distinct pore regions: the inter-aggregate pore region and the intra-aggregate pore region. As a result, typical D_p/D_o in pasture soils are expected to show non-linear behavior with two distinct pore regions.

Figure 1 shows the gas diffusivity against air-filled porosity for six repacked soils: Two Peradeniya soils, one Nishi-Tokyo soil and three New Zealand soils. Among them, Peradeniya soil (Figure 1(a) and 1(b)) and Nishi-Tokyo soil (Figure 1(c)) showed distinct two-region behaviour, but other soils showed a linear variation. This is mostly due to the compacted behaviour of the soil due to frequent compaction by machinery and animal treading and trampling which has apparently resulted in altered structural arrangement.

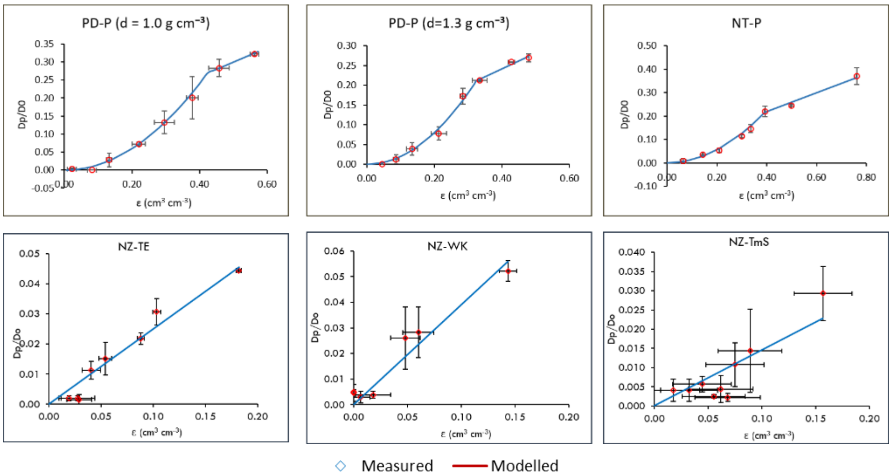

Figure 1: Variation of air-filled porosity vs gas diffusivity for two-region model for repacked soils

To reveal the behaviour of the two-region model, its performance was compared with the classical and newly developed gas diffusivity models using scatterplot comparisons as shown in Figure 2.

The performance of the selected models and newly developed two-region model against the measured gas diffusivity data for repacked soils expressed in terms of RMSE and Bias are shown in Table 3.

Table 3: Measured D_P/D_o data expressed in terms of RMSE and Bias for Repacked soils

D_p/D_o Model	Peradeniya-1, SL d = 1.0 g cm^{-3}		Peradeniya-2, SL d = 1.3 g cm^{-3}		Nishi-Tokyo, JP		Temuka, NZ		Wakanui, NZ		Templeton, NZ	
	RMSE	Bias	RMSE	Bias	RMSE	Bias	RMSE	Bias	RMSE	Bias	RMSE	Bias
Buckingham (1904)	0.0437	-0.0290	0.0594	-0.0468	0.0804	0.0083	0.0110	-0.0088	0.0179	-0.0137	0.00384	-0.00270
Penman (1940)	0.0534	0.0462	0.0418	0.0365	0.0815	0.0749	0.0351	0.0288	0.0173	0.0085	0.03979	0.03550
Marshal (1959)	0.0454	0.0324	0.0293	0.0127	0.1160	0.0751	0.0121	0.0052	0.0083	-0.0057	0.01424	0.01064
Millington (1959)	0.0738	0.0615	0.0522	0.0421	0.1401	0.1063	0.0230	0.0149	0.0098	-0.0001	0.02517	0.02033
MQ (1960)	0.0569	0.0244	0.0392	-0.0014	0.1228	0.0431	0.0085	-0.0058	0.0155	-0.0122	0.00352	-0.00001
MQ (1961)	0.0755	-0.0133	0.0697	-0.0468	0.1489	-0.0122	0.0189	-0.0146	0.0234	-0.0169	0.00997	-0.00761
WLR-Marshall	0.0504	-0.0072	0.0525	-0.0337	0.1195	0.0072	0.0145	-0.0116	0.0206	-0.0154	0.00650	-0.00524
SWLR	0.0499	-0.0122	0.0545	-0.0367	0.1127	-0.0123	0.0156	-0.0124	0.0214	-0.0158	0.00715	-0.00572
Two Region	0.0165	0.0023	0.0115	0.0010	0.0168	0.0036	0.0034	0.0009	0.0046	-0.0021	0.00419	0.00108

SL: Sri Lanka; NZ: New Zealand; JP: Japan

As demonstrated by the table, Buckingham (1904), MQ (1960), MQ (1961), WLR-Marshall and SWLR models underestimated the results while Marshal (1959) and Millington (1959) models overestimated the results. The developed two-region model gave more accurate results for all the repacked soils (Figure 2(i)).

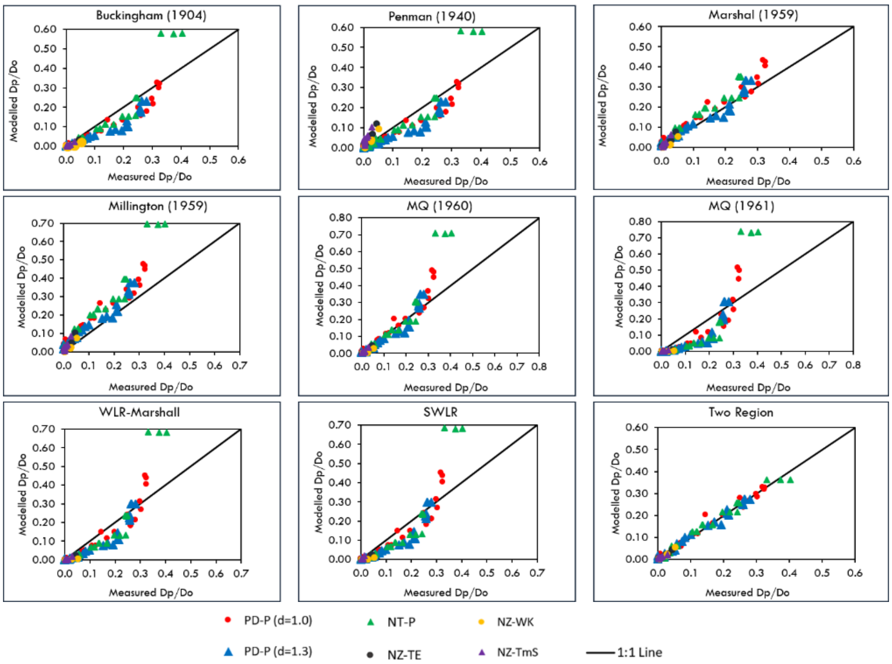

Figure 2: Measured D_p/D_o vs modelled D_p/D_o for repacked soils

Figure 3 shows scatterplot comparisons of modelled and measured soil-gas diffusivities (D_p/D_o) for six repacked soils in a log-transformed scales to make better illustration of the wet-region measurements which are more challenging to predict using nine predictive models with the newly-developed descriptive model as mentioned earlier.

According to the Figure 3, the new descriptive two-region model shows more accurate results than the other models for each soil in wet region. AlthoughWLR-Marshall model was developed specially for repacked soils, according to Figure 3(g), this model has markedly underpredicted the results in wet region. The MQ (1961) model was not developed for gas diffusivity measurements, but it has been used widely used for predicting gas diffusivity in many numerical models. According to the Figure 3(f), the MQ (1961) model has underpredicted the results markedly in wet region as usual. Developed two-region model has accurately predicted the results for six soils. The best-fit model parameters of the descriptive model are given in Table 4.

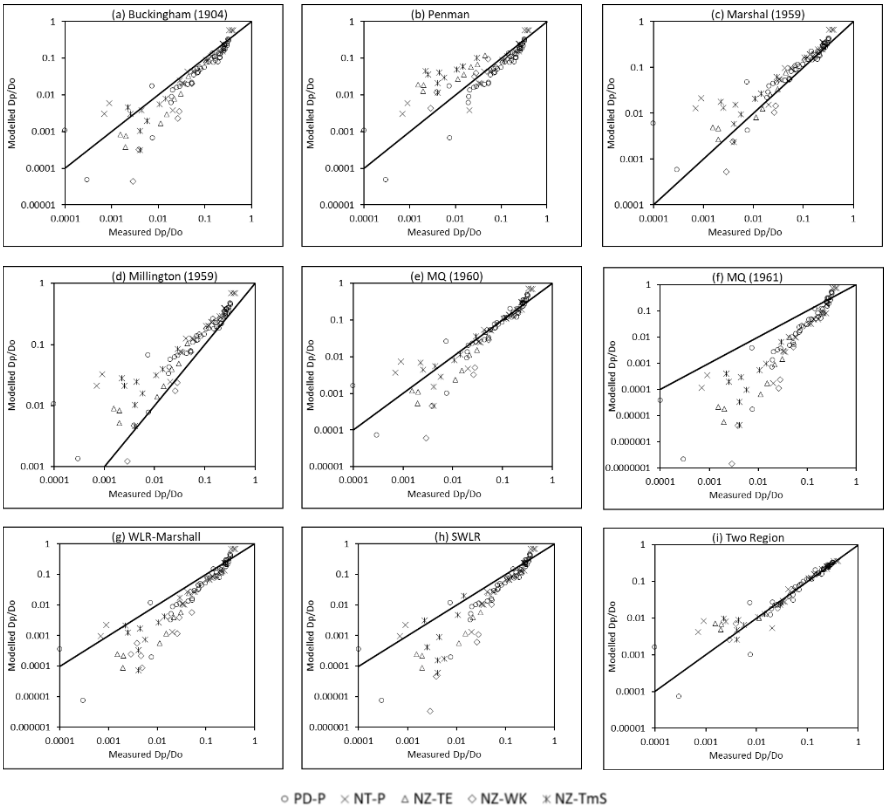

Figure 3: Measured and Modelled D_p/D_o in log scale for repacked soils

Table 4: Numerical characterization of soil-gas diffusivity in selected pasture soils

Soil	Soil-gas diffusivity Eq. (1)				
	A	B	ε_o	$\emptyset_{int}$	C
Wakanui, NZ	0.390	1	0	0	0
Temuka, NZ	0.250	1	0	0	0
Templeton, NZ	0.145	1	0	0	0
Peradeniya-1, SL	1.500	2	0	0.424	0.4
Peradeniya-2, SL	2.000	2	0	0.325	0.4
Nishi-Tokyo, JP	1.400	2	0	0.392	0.4

Tortuosity of Gaseous Phase

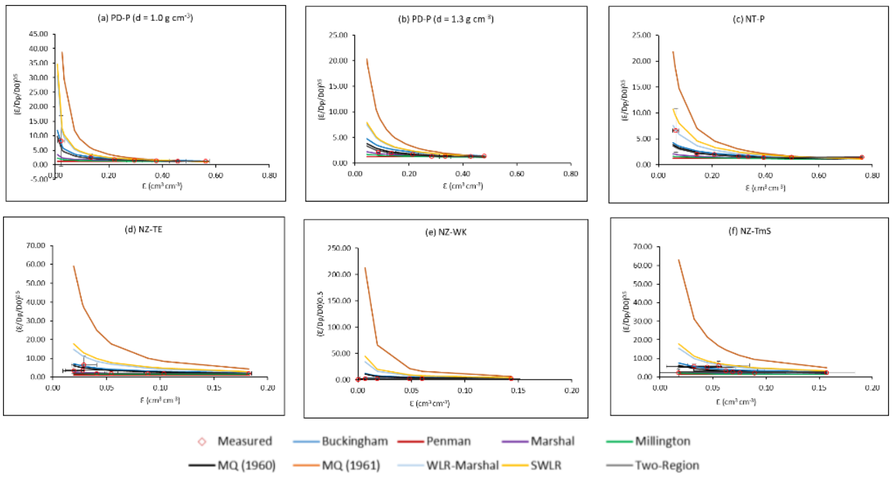

Figure 4: Pore tortuosity factor vs Air filled porosity for selected repacked soils

Figure 4 shows the pore tortuosity factor derived from measured gas diffusivity data, together with the model predictions. The Penman (1940) model showed a constant value of tortuosity across the total air-filled porosity variation, typically yielding a lower-limit tortuosity for all six soils, while the MQ (1961) model provides an upper limit for tortuosity for all the repacked six soils. Buckingham, MQ (1960), MQ (1961), WLR-Marshal and SWLR models showed nonlinear variation with decreasing tortuosity as the air-filled porosity increases. On the other hand, Marshal and Millington models showed constant value for high ε values and showed slight non-linear variation at high moisture contents as shown in Figure 4(a), 4(b), 4(c). The developed two-region descriptive model also exhibited a constant value at all the ε values for NZ soils. But for two Peradeniya soils and Nishi-Tokyo soil, the developed two-region model showed a slight non-linear variation with decreasing tortuosity as the air-filled porosity increases.

4. Conclusions

This study investigated the effect of soil structural status such as aggregation induced by compaction on soil-gas diffusivity in repacked soils sampled from pasture topsoil (0-5 cm). The selected six repacked soils from the literature were compared with eight recognized models for estimating soil-gas diffusivity and none of them considered the distinct two-region characteristics of aggregated soils. A descriptive model was developed to better characterize the two-region behaviour of each soil. The developed two-region model accurately predicted the measured gas diffusivity data and statistically outperformed the classic diffusivity models. The calculated gas phase tortuosity showed a nonlinear relationship with air-filled porosity and provided a good agreement with measured tortuosity values for all repacked soils.

It should be noted that the all measurements involved have been carried out in laboratory-controlled environments where natural environmental complexities (e.g., temperature, evaporation, wind speed and humidity) were eliminated. Such additional environmental factors were out of the scope of this study but must be accounted when making more realistic conclusions. Results, therefore, must be compared against field-measured data with caution.

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References

Buckingham, E. (1904). Contributions to our knowledge of the aeration of soils. Bur. Soil Bull (Vol. 25). Washington, DC: U.S. Gov. Print. Office.

Chamindu, D., Møldrup, P., Schjønning, P., de Jonge, L. W., Kawamoto, K., & Komatsu, T. (2011). Density-Corrected Models for Gas Diffusivity and Air Permeability in Unsaturated Soil. Vadose Zone Journal, 10(1), 226-238. https://doi.org/10.2136/vzj2009.0137

Chantigny, M. H., Rochette, P., Angers, D. A., Bittman, S., Buckley, K., & Masse, D. (2010). Soil nitrous oxide emissions following band-incorporation of fertilizer nitrogen and swine manure. Journal of Environment Quality, 39, 1545–1553. https://doi.org/10.2134/jeq2009.0482

Clough, T. J., Sherlock, R. R., & Rolston, D. E. (2005). A review of the movement and fate of N2O in the subsoil. Nutrient Cycling in Agroecosystems, 72, 3–11. https://doi.org/10.1007/s10705-004-7349-z

Currie, J.A. (1960). Gaseous diffusion in porous media. Part 2. Dry granular materials. British Journal of Applied Physics, 11, 318–324

Currie, J. A. (1984). Gas diffusion through soil crumbs: The effects of compaction and wetting. Journal of Soil Science, 35, 1–10.

Ding, F., Sun, W., & Huang, Y. (2019). Net N2O production from soil particle size fractions and its response to changing temperature. Science of The Total Environment, 650(1), 97–104.

Fujikawa, T.,&Miyazaki, T. (2005). Effects of bulk density and soil type on the gas diffusion coefficient in repacked and undisturbed soils. Soil Science, 170, 892–901.

Hamamoto, S., P. Moldrup, K. Kawamoto, and T. Komatsu. 2009. Effect of particle size and soil compaction on gas transport parameters in variably saturated, sandy soils. Vadose Zone J. 8:986–995.

Jayarathne, J.R.R.N., Chamindu Deepagoda, T.K.K., Clough, T.J., Nasvi, M.C.M., Thomas S., Smits, E.B., K., 2019. Gas-Diffusivity Based Characterization of Aggregated Agricultural Soils. Soil Sci. Soc. Am. J. https://doi.org/10.1002/saj2.20033.

Moldrup, P., T. Olesen, T. Komatsu, P. Schjønning, and D.E. Rolston. 2001. Tortuosity, diffusivity, and permeability in the soil liquid and gaseous phases. Soil Sci. Soc. Am. J. 65:613–623.

Myhre, G., D. Shindell, F.-M. Breon, W. Collins, J. Fuglestvedt, J. Huang, D. Koch, J.-F. Lamarque, D. Lee, B. Mendoza, T. Nakajima, A. Robock, G. Stephens, T. Takemura, and H. Zhang. 2013. Anthropogenic and natural radiative forcing In: T.F. Stocker, D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex, and P.M. Midgley, editors, Climate change 2013: The physical science basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge Univ. Press, Cambridge, U.K.

Pelster, D. E., Chantigny, M. H., Rochette, P., Angers, D. A., Rieux, C., & Vanasse, A. (2012). Nitrous oxide emissions respond differently to mineral and organic nitrogen sources in contrasting soil types. Journal of Environment Quality, 41, 427–435. https://doi.org/10.2134/jeq2011.0261

Rolston, D.E., and P. Moldrup. 2002. Gas diffusivity. p. 1113–1139. In J.H. Dane and G.C. Topp (ed.) Methods of soil analysis. Part 4. SSSA Book Ser. 5. SSSA, Madison, WI.

Schjønning, P. (1985). A laboratory method for determination of gas diffusion in soil. (In Danish with English summary.) Rep. S1773. Danish Inst. of Plant and Soil Sci., Tjele.

Schjønning, P., Thomsen, I. K., Møberg, J. P., de Jonge, H., Kristensen, K., & Christensen, B. T. (1999). Turnover of organic matter in differently textured soils: I. Physical characteristics of structurally disturbed and intact soils. Geoderma, 89, 177–198.

Taylor, S. A. (1949). Oxygen diffusion in porous media as a measure of soil aeration. Soil Science Society of America Journal, 14, 55–61.