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SHORT COMMUNICATION

Validation of Gas Diffusivity Models with Chilean Soil Samples

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Abstract

This study compares the goodness of fit of 10 empirical models used to predict gas diffusivity ($D_p\,D_0^{-1}$) with experimental data obtained from Chilean soil samples from different soil management practices. Nine sites under different soil management practices were sampled at different depths. In total, 275 soil cores were obtained. The gas diffusion coefficient (D_p) was determined at different matric potentials using a gas diffusion chamber saturated with free-oxygen (O_2) nitrogen (N_2) as the gas that diffuses and oxygen as the measured gas inside the diffusion chamber with a gaseous oxygen sensor. Complementary soil properties were measured in order to modelate the diffusivity with several models. The use of statistical indexes, i.e., determination coefficient (r^2), root mean square error (RMSE), mean bias error (BIAS), the agreement index (d), and the mean absolute error (MAE), to rank the models according to the fit of goodness was proposed. The models of Millington and Quirk (M-Q), Penman Water Linear Reduction Model (P-WLR), Millington Water Linear Reduction Model (MI-WLR), and Marshal Water Linear Reduction Model (MA-WLR) showed a high simplicity and had a better prediction of gas diffusivity than more complex models. The Three-Porosity Model (TPM) showed the worst performance among the models. Thus, the use of more complex models does not guarantee a better prediction of gas diffusivity. However, it is necessary to test other complex models that incorporate soil management practices and have presented better results than those used in this work. Also, incorporating new soil management could be the base to develop a more accurate comparison. Finally, the P-WLR and TPM models had the best and worst performances above all models. It is suggested to test new models and to increase soil management in future research.

Keywords Gas diffusivity models · Goodness of fit · Air-filled porosity · Tortuosity

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1 Introduction

The air exchange between the soil and the atmosphere is one of the most critical soil functions and directly impacts the environment and crop productivity, where soil physical properties define the soil-gas movement mainly by pore-size distribution, pore continuity, and water saturation (Blackwell et al. 1990; Hillel 1998; Piccoli et al. 2017). One example of how the soil conditions affect the soil-gas transport is the case of the nitrification process, where flooded soils are the most feasible conditions for denitrification. On the contrary, upland soils without the lacking of oxygen (O_2) exhibit nitrification (Bollmann 2010). In this sense, air transport is strongly affected by tillage management (Martínez et al. 2016; Mentges et al. 2016; Schjønning and Rasmussen 2000) and soil moisture is an important driver for soil-gas transport (Ball 2013; Chamindu Deepagoda et al. 2020).

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The air permeability (ka) primarily controls the near-surface transport of gases (Stepniewski et al. 1994; Schjønning et al. 2002) and diffusion is the process of dominating gas exchange in subsoil (Taylor 1950; Troeh et al. 1982; Glinski and Stepniewski 1985), while the convective processes have minor importance (Moldrup et al. 2004). The gas transport processes in the soil, by diffusion or advection, under natural conditions depend on variations in soil-water content, soil texture, soil structure, and soil organic matter content (SOM) (McCarthy and Brown 1992; Horn et al. 2000; Czyz 2004; Fujikawa and Miyazaki 2005; Dörner and Dec 2007; Chamindu Deepagoda et al. 2019, 2020), where the effect of SOM on the soil-gas movement has been poorly studied; however, SOM is essential to improve, maintain, or remediate soil structure as a binding agent (Six et al. 2000; Tejada and Gonzalez 2007; Clark et al. 2009; Arthur et al. 2011; Eden et al. 2011).

Under steady-state condition, the gas diffusion follows Fick's first law (Eq. 1):

$$q = -D_p \left(\frac{\partial C}{\partial x} \right) \tag{1}$$

where q is the gas flux (cm^3 air cm^{-2} soil s^{-1}), D_p (cm^3 air cm^{-2} soil s^{-1}) is the effective diffusion coefficient of the gas in soil, and $\partial C/\partial x$ is the gas concentration gradient (cm^{-3} air cm^{-1} soil). The gas diffusivity (D_p $D_0{}^{-1}$) corresponds to the ratio between D_p and the gas diffusion coefficient in free-air at atmospheric pressure (D_0, cm^2 air s^{-1}). D_p is a function of air-filled porosity related to the transport effectiveness, continuity-tortuosity, and the restrictions in the soil pore matrix. In this regard, the water content and the presence of solids in the pores act as barriers that restrict transport (Weerts et al. 2000; Caron and Nkolongo 2004).

The gas diffusivity was determined in several experiments using soil samples under different conditions, like undisturbed or sieved-repacked soil cores, showing different behaviors on the soil-gas diffusivity according to its soil physical properties. Under natural conditions, gas diffusion depends on the type and structure of soil (Schjønning et al. 1999); also, the presence of allophane, clay with unique chemical and physical properties, increases the soil-water retention in volcanic soil (Resurreccion et al. 2007), affecting the gas diffusion negatively. Because organic soils have high water retention capacity, they also present a porosity restriction that reduces the gas diffusivity (Hamamoto et al. 2012).

Arthur et al. (2013) quantified the newly formed structure of 22 field-incubated physically disturbed (2-mm sieved) samples of varying clay mineralogy (illite, kaolinite, and smectite) amended with organic material (7.5 Mg ha^{-1}). The results showed that soil pore organization was similar for both natural and incubated soils. Nevertheless, pore network complexity increased as follows: sieved and repacked < incubated < natural soils, where the increase of pore network complexity reduces gas diffusivity. Schwen et al. (2015) tried to deduce and apply a scaling rule for gas diffusivity and analyze spatio-temporal variations of soil respiration and gas diffusivity under conventional tillage and no tillage, concluding that scaling factors for soil-water retention, hydraulic conductivity, and gas diffusivity for flow pathways were not the same for water and gases. Piccoli et al. (2017) evaluated the effect of conservation agriculture practices on gas transport in 144 undisturbed soil cores from Northeastern Italy, in two depths: 3–6.5 cm and 20–23.5 cm. The results showed that treatments only affected the transmission properties in the coarsest studied soil, causing a reduction of air permeability in the deeper layer and relative gas diffusivity in both layers. Furthermore, recent studies recognize the environmental importance of the gas diffusivity, evidencing its importance as a predictor of nitrous oxide (N_2O) fluxes (Balaine et al. 2016; Owens et al. 2016; Owens et al. 2017; Chamindu Deepagoda et al. 2019).

D_p is the most critical parameter in the gas diffusion equation (Neira et al. 2015). However, its measurement is hugely laborious; thus, several empirical and semi-empirical models have been developed based on soil physical properties as total porosity (Φ), air-filled porosity (ε), soil-water content or water-filled porosity (ϕ), or pore connectivity-tortuosity (τ). Buckingham (1904) developed the first gas diffusivity model, and it was the base for different models considering different conditions. The D_p models are classified into six groups, where the first three groups are empirical models based on the soil physical properties and are the most commonly used; the other three groups are more complex and rarely used (Moldrup et al. 2000b, 2004). Moldrup et al. (2013) proposed the general form of soil-gas diffusivity prediction models (Eq. 2) as a function of air-filled porosity and total porosity:

$$\frac{D_p}{D_0} = P * \varepsilon^X * \left(\frac{\varepsilon}{\Phi} \right)^{T_a} \tag{2}$$

where D_p is the soil-gas diffusion coefficient (cm^3 air cm^{-1} soil s^{-1}), D_0 is the air-gas diffusion coefficient (cm^2 air s^{-1}), ε is the air-filled porosity (cm^3 soil-air cm^{-3} soil), Φ is the total soil porosity (cm^3 porous space cm^{-3} soil), and P, X, and T_a are the adjustment parameters of the models (unitless).

Some studies have tested the predictive capacity of different gas diffusivity models in different types of soils and substrates under different conditions. For example, Mostafid et al. (2012) determined the gas diffusivity for wood chip compost and green residues collected from landfill bio cover and biofilters under variable saturation conditions. In their study, a D_p $D_0{}^{-1}$ prediction model that assumed inactive pore space was used, obtaining good prediction results. Pokhrel et al. (2011) measured D_p values in compost with variable saturation conditions and soil-compost mixtures based on methane (CH_4) diffusion experiments. They used $D_p D_0^{-1}$ prediction models without good results; thus, they proposed an empirical model with four adjustment parameters. Dilrukshi et al. (2015) used soil, compost, and compost-soil mixtures at different matric potentials. In all cases, experimental D_p increased linearly with the increase in air content. Jayarathne et al. (2019) used 11 porous literature media corresponding to seven agricultural soils and four manufactured porous media to determine $D_p D_0^{-1}$ and determine the predictive capacity of six models. The results showed that recent models, which incorporated the bimodal behavior of soil porosity, had a better performance than the classic models. Jayarathne et al. (2020) proposed a new soil-gas diffusivity model that considered inter and intra-aggregate porosity that was tested on agricultural land in Sri Lanka and compared to eight literature models. The results of this work showed that the proposed model obtained better results than the literature models.

Considering the agronomic and environmental importance of the soil-gas diffusivity, few studies have measured this physical soil property in Chilean soils, like the works by Neira (2015) and Haas et al. (2018); however, none tested the predictive capacity of different soil-gas diffusivity models considering different physical properties, agronomic management, and soil types present in Chile. This work aims to compare the predictive capacity of ten empirical soil-gas diffusivity models from different Chilean soil samples.

2 Materials and Methods

2.1 Soil Sampling

Nine sites under different agronomic management practices were sampled at different depths (Fig. 1). Table 1 and

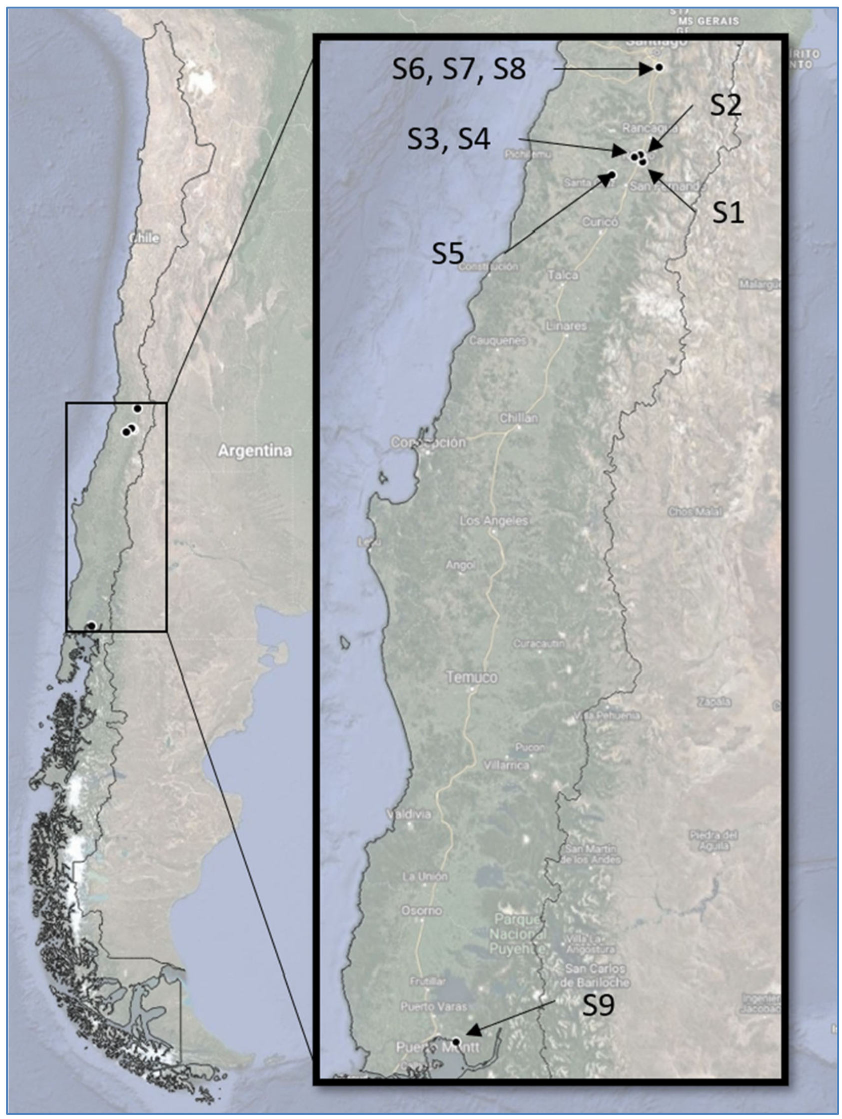

Fig. 1 Geographic location of the sample sites

Table 1 Time and agronomic management developed in each sampled sites at the moment of sampling

Site	Agronomic management
S1	Apple orchard in which the pruning residue is chipped and mixed in-depth with the soil once a year
S2	Cherry orchard in which pruning residue is removed
S3	Plum orchard where the pruning residue is chipped and spread superficially, this had been performed for 15 years
S4	Apple orchard where the pruning residue is chipped and spread superficially, this had been done for 8 years
S5	Plum orchard located in soil of lacustrine origin, where the pruning residue is chipping and spreading superficially
S6	Non-tillage has done for more than 15 years
S7	Traditional tilling
S8	Non-tillage has done for 8 years
S9	Native forest renewal located in a volcanic ash soil near the coast

Table 2 describe the agronomic management and the physical soil properties of the samples, respectively. According to the soil classification system of the United States Department of Agriculture (USDA) (Soil Survey Staff 2006), site 1 is a Mollisol (thermic Aquic Haploxerolls), S2 is an Inceptisol (thermic Typic Xerochrepts), and S3 and S4 are Mollisols (thermic Aquic Haploxerolls). S5 is a Mollisol (thermic Aquic Argixerolls) in a flat position and imperfectly drained under 100 cm. S6, S7, and S8 are Mollisols (thermic Entic Haploxerolls) with a soft slope (0.5–2%). S9 is an Andisol located in the Katalapi Park (median family, amorphic, isomeric Acrudoxic Durudands) developed from Holocene volcanic ash with moderate to strong ripples.

Soil sampling considered disturbed and undisturbed soil samples at different depths. The disturbed samples were collected in 34 plastic bags and undisturbed soil samples in 270 cores. Sites S1, S2, S3, and S4 had four sampling depth: 0–5 cm, 5–10 cm, 10–20 cm, and 20–50 cm; S5 had two sampling depths: 0–5 cm

Table 2 Summary of the soil physical properties of the Chilean soil samples at different sampled sites

Site	Depth (cm)	Φ (%)	SOM (g g^{-1})	ρb (g cm^{-3})	ρs (g cm^{-3})	Water retention curve (kPa)					
						− 0.2	− 6	− 10	− 30	− 100	− 1500
S1	0–5	58.7 ± 4.7	0.0314	1.1 ± 0.14	2.6 ± 0.03	0.43 ± 0.1	0.23 ± 0.1	0.21 ± 0.1	0.20 ± 0.1	0.17 ± 0.1	0.16 ± 0.1
S1	5–10	54.2 ± 6.6	0.0312	1.2 ± 0.16	2.6 ± 0.08	0.43 ± 0.1	0.25 ± 0.1	0.24 ± 0.1	0.23 ± 0.1	0.22 ± 0.1	0.20 ± 0.1
S1	10–20	49.4 ± 3.6	0.0278	1.3 ± 0.11	2.6 ± 0.03	0.33 ± 0.1	0.22 ± 0.1	0.20 ± 0.1	0.20 ± 0.1	0.18 ± 0.1	0.17 ± 0.1
S1	20–50	50.4 ± 3.3	0.0173	1.3 ± 0.09	2.7 ± 0.02	0.36 ± 0.1	0.21 ± 0.1	0.19 ± 0.1	0.19 ± 0.1	0.17 ± 0.1	0.15 ± 0.1
S2	0–5	47.9 ± 10.4	0.0304	1.3 ± 0.26	2.5 ± 0.06	0.37 ± 0.0	0.21 ± 0.0	0.19 ± 0.0	0.16 ± 0.0	0.14 ± 0.0	0.13 ± 0.0
S2	5–10	48.9 ± 7.2	0.0210	1.3 ± 0.18	2.6 ± 0.04	0.34 ± 0.0	0.21 ± 0.0	0.19 ± 0.0	0.15 ± 0.0	0.13 ± 0.0	0.12 ± 0.0
S2	10–20	51.0 ± 3.4	0.0185	1.3 ± 0.08	2.6 ± 0.03	0.35 ± 0.0	0.21 ± 0.0	0.18 ± 0.0	0.14 ± 0.0	0.12 ± 0.0	0.11 ± 0.0
S2	20–50	47.2 ± 9.4	0.0175	1.4 ± 0.24	2.6 ± 0.03	0.33 ± 0.0	0.21 ± 0.0	0.19 ± 0.0	0.15 ± 0.0	0.13 ± 0.0	0.12 ± 0.0
S3	0–5	47.2 ± 7.8	0.0325	1.3 ± 0.17	2.4 ± 0.04	0.35 ± 0.1	0.22 ± 0.0	0.22 ± 0.0	0.18 ± 0.0	0.16 ± 0.0	0.13 ± 0.1
S3	5–10	46.7 ± 4.3	0.0290	1.3 ± 0.07	2.5 ± 0.10	0.33 ± 0.0	0.19 ± 0.1	0.18 ± 0.1	0.13 ± 0.1	0.11 ± 0.1	0.09 ± 0.1
S3	10–20	47.5 ± 1.9	0.0289	1.3 ± 0.05	2.6 ± 0.03	0.32 ± 0.1	0.19 ± 0.1	0.19 ± 0.1	0.14 ± 0.1	0.13 ± 0.1	0.10 ± 0.1
S3	20–50	45.0 ± 4.4	0.0250	1.4 ± 0.05	2.5 ± 0.14	0.31 ± 0.0	0.17 ± 0.0	0.17 ± 0.0	0.13 ± 0.0	0.11 ± 0.0	0.09 ± 0.0
S4	0–5	53.0 ± 1.8	0.0290	1.2 ± 0.05	2.5 ± 0.01	0.41 ± 0.0	0.23 ± 0.0	0.20 ± 0.0	0.14 ± 0.0	0.10 ± 0.0	0.09 ± 0.0
S4	5–10	50.9 ± 1.9	0.0272	1.2 ± 0.05	2.5 ± 0.02	0.35 ± 0.0	0.21 ± 0.0	0.19 ± 0.0	0.14 ± 0.0	0.11 ± 0.0	0.10 ± 0.0
S4	10–20	50.4 ± 3.3	0.0226	1.2 ± 0.05	2.5 ± 0.07	0.35 ± 0.0	0.21 ± 0.0	0.19 ± 0.0	0.14 ± 0.0	0.12 ± 0.0	0.10 ± 0.0
S4	20–50	47.8 ± 2.7	0.0181	1.3 ± 0.07	2.4 ± 0.07	0.33 ± 0.0	0.22 ± 0.0	0.20 ± 0.0	0.15 ± 0.0	0.13 ± 0.0	0.12 ± 0.0
S5	0–5	67.9 ± 3.2	0.0130	0.6 ± 0.04	1.9 ± 0.08	0.56 ± 0.0	0.47 ± 0.0	0.45 ± 0.0	0.40 ± 0.0	0.36 ± 0.0	0.33 ± 0.0
S5	5–10	64.8 ± 4.3	0.0130	0.6 ± 0.04	1.8 ± 0.14	0.57 ± 0.0	0.50 ± 0.0	0.49 ± 0.0	0.41 ± 0.0	0.38 ± 0.0	0.38 ± 0.0
S6	0–2	48.2 ± 4.7	0.0526	1.2 ± 0.09	2.4 ± 0.09	0.54 ± 0.0	0.33 ± 0.0	0.33 ± 0.0	0.25 ± 0.0	0.21 ± 0.0	0.15 ± 0.0
S6	2–5	45.5 ± 2.9	0.0344	1.4 ± 0.08	2.5 ± 0.10	0.48 ± 0.1	0.34 ± 0.1	0.34 ± 0.1	0.26 ± 0.1	0.23 ± 0.1	0.20 ± 0.0
S6	5–15	43.4 ± 3.8	0.0200	1.4 ± 0.05	2.5 ± 0.09	0.41 ± 0.2	0.33 ± 0.2	0.32 ± 0.2	0.26 ± 0.2	0.23 ± 0.1	0.19 ± 0.1
S6	15–35	46.1 ± 2.2	0.0162	1.4 ± 0.07	2.5 ± 0.10	0.44 ± 0.2	0.34 ± 0.2	0.33 ± 0.2	0.28 ± 0.1	0.25 ± 0.1	0.21 ± 0.1
S6	35–55	44.8 ± 3.6	0.0155	1.4 ± 0.07	2.5 ± 0.08	0.42 ± 0.2	0.33 ± 0.2	0.32 ± 0.2	0.27 ± 0.1	0.24 ± 0.1	0.19 ± 0.1
S7	0–2	47.1 ± 1.6	0.0171	1.3 ± 0.05	2.5 ± 0.08	0.60 ± 0.1	0.35 ± 0.1	0.35 ± 0.1	0.29 ± 0.1	0.25 ± 0.1	0.24 ± 0.1
S7	2–5	47.9 ± 3.4	0.0188	1.3 ± 0.09	2.5 ± 0.02	0.64 ± 0.1	0.42 ± 0.1	0.39 ± 0.1	0.36 ± 0.1	0.30 ± 0.1	0.29 ± 0.1
S7	5–15	46.0 ± 4.6	0.0204	1.3 ± 0.12	2.4 ± 0.09	0.70 ± 0.2	0.53 ± 0.1	0.51 ± 0.1	0.44 ± 0.1	0.41 ± 0.1	0.39 ± 0.1
S7	15–35	41.0 ± 3.2	0.0180	1.4 ± 0.10	2.4 ± 0.22	0.67 ± 0.1	0.54 ± 0.1	0.52 ± 0.1	0.45 ± 0.1	0.42 ± 0.1	0.40 ± 0.1
S7	35–55	45.0 ± 5.8	0.0164	1.3 ± 0.09	2.4 ± 0.19	0.64 ± 0.2	0.47 ± 0.2	0.44 ± 0.1	0.36 ± 0.1	0.33 ± 0.1	0.31 ± 0.1
S8	0–2	44.8 ± 9.9	0.0173	1.3 ± 0.24	2.4 ± 0.04	0.81 ± 0.1	0.61 ± 0.2	0.62 ± 0.2	0.53 ± 0.2	0.49 ± 0.2	0.48 ± 0.2
S8	2–5	51.1 ± 10.9	0.0155	1.3 ± 0.28	2.6 ± 0.06	0.70 ± 0.1	0.55 ± 0.1	0.52 ± 0.1	0.49 ± 0.1	0.43 ± 0.1	0.42 ± 0.1
S8	5–15	37.6 ± 6.1	0.0129	1.4 ± 0.08	2.2 ± 0.16	0.80 ± 0.1	0.70 ± 0.1	0.70 ± 0.1	0.64 ± 0.1	0.61 ± 0.1	0.58 ± 0.1
S8	15–35	48.4 ± 1.8	0.0128	1.4 ± 0.05	2.6 ± 0.02	0.76 ± 0.1	0.65 ± 0.1	0.65 ± 0.1	0.58 ± 0.1	0.54 ± 0.1	0.52 ± 0.1
S8	35–55	41.5 ± 3.0	0.0160	1.4 ± 0.07	2.4 ± 0.11	0.75 ± 0.1	0.65 ± 0.1	0.65 ± 0.1	0.59 ± 0.1	0.56 ± 0.1	0.55 ± 0.1
S9	0–10	68.4 ± 4.5	0.0700	0.5 ± 0.06	1.4 ± 0.00	0.67 ± 0.1	0.52 ± 0.1	0.50 ± 0.1	0.42 ± 0.1	0.42 ± 0.1	0.41 ± 0.1

Φ , soil total porosity; *SOM*, soil organic matter content; *ρb*, bulk density; *ρs*, particle density and 5–10 cm; sites S6, S7, and S8 had five sampling depths: 0–2 cm, 2–5 cm, 5–15 cm, 15–35 cm, and 35–55 cm; finally, site S9 had only one sampling depth: 0–10 cm. Also, the following physical soil properties were determined: particle density (ρ_s), bulk density (ρ_b), water retention curve, and gas diffusion coefficient. The determination of ρ_s was done using the pycnometer method (Blake and Hartge 1986b), while for ρ_b, the core method (Blake and Hartge 1986a) was used. Moreover, the water retention curve was determined according to Klute (1986), and the gas diffusion coefficient was computed according to Rolston and Moldrup (2002), both with soil cores. The samples initially were saturated with water and then drained in a sand box at − 0.2 kPa, − 3.0 kPa, − 6.0 kPa, and − 10.0 kPa and then in pressure plates at − 30 kPa, − 100 kPa, and − 1500 kPa. The gas diffusion coefficient was determined at each matric potential using a gas diffusion chamber. The measurement chambers were flushed and saturated with oxygen-free N_2 (nitrogen), and oxygen (O_2) was used as the diffusing gas, and its concentration was measured every minute inside the chamber with a gaseous oxygen sensor (SO-110 Apogee Instrument). Equation 3 was used to standardize D_p at 20 °C (Currie 1960) and correct the effect of the room temperature fluctuation on D_p determination:

$$D_{p\ T2} = D_{p\ T1} * \left(\frac{T2}{T1}\right)^{1.72} \tag{3}$$

where $D_{p\ T1}$ and $D_{p\ T2}$ are the gas diffusion coefficients measured at temperatures T_1 and T_2 (°K), respectively. It was set at 20 °C as the standard temperature (T_2), while T_1 was the average temperature during the measurement period of each sample in each potential matric. Finally, gas diffusivity is the ratio between $D_{p\ T2}$ and D_0 at 20 °C.

2.2 Gas Diffusivity Prediction Models

Ten models described in the literature were used, where the Millington and Quirk (1961) model was used as the standard result. The physical soil properties in Table 2 are used to complete each model requirement. The predicted models are described below:

Penman Water Linear Reduction Model (P-WLR) (Moldrup et al. 2000a):

$$\frac{D_p}{D_0} = 0.66*\varepsilon*\left(\frac{\varepsilon}{\Phi}\right) \tag{4}$$

Marshal Water Linear Reduction Model (MA-WLR) (Moldrup et al. 2000a):

$$\frac{D_p}{D_0} = \varepsilon^{\frac{3}{2}}*\left(\frac{\varepsilon}{\Phi}\right) \tag{5}$$

Millington Water Linear Reduction Model (MI-WLR) (Moldrup et al. 2000a):

$$\frac{D_p}{D_0} = \varepsilon^{\frac{4}{3}}*\left(\frac{\varepsilon}{\Phi}\right) \tag{6}$$

Buckingham Water Linear Reduction Model (BU-WLR) (Moldrup et al. 2000a):

$$\frac{D_p}{D_0} = \varepsilon^{2}*\left(\frac{\varepsilon}{\Phi}\right) \tag{7}$$

where D_p is the soil-gas diffusion coefficient (cm^3 air cm^{-1} soil s^{-1}), D_0 is the air-gas diffusion coefficient (cm^2 air s^{-1}), ε is the air-filled porosity (cm^3 soil-air cm^{-3} soil), and Φ is the total soil porosity (cm^3 soil porous space cm^{-3} soil). Equations 4 to 7 are modifications of the classical models used to predict gas diffusion in dry soils; to include the effect of water in these equations, Moldrup et al. (2000a) included a concept called linear reduction induced by water, expressed as ε/Φ.

Buckingham-Burdine-Campbell model (BBC) (Moldrup et al. 1999):

$$\frac{D_p}{D_0} = \Phi^2*\left(\frac{\varepsilon}{\Phi}\right)^{\left(2+\frac{3}{b}\right)} \tag{8}$$

b is a parameter derived from the soil moisture curve, determined as the slope of the soil moisture curve in a system log (cm^3 soil-water cm^{-3} soil) vs. log (pressure, kPa). Moldrup et al. (1996, 1999, 2000a) describe b as a parameter related to the pore-size distribution and describe the effect of soil types (soil texture and soil structure) on D_p in undisturbed samples.

Three-Porosity Model (TPM) (Moldrup et al. 2004):

$$\frac{D_p}{D_0} = \Phi^2*\left(\frac{\varepsilon}{\Phi}\right)^{\left(\frac{\log\left(\frac{2\varepsilon_{100}{}^3+0.04\varepsilon_{100}}{\Phi^2}\right)}{\log\left(\frac{\varepsilon_{100}}{\Phi}\right)}\right)} \tag{9}$$

where ε_{100} is the air-filled porosity (cm^3 soil-air cm^{-3} soil) at − 100 cm of water matric potential (≈ − 10 kPa), and according to Resurreccion et al. (2008), this parameter is related to the soil macroporosity. Moldrup et al. (2004) considered the equation log $[(2\varepsilon_{100}{}^3 + 0.04\varepsilon_{100})/\Phi^2]$/log (ε_{100}/Φ) as a description of the connectivity-tortuosity of porous matrix.

Three-Porosity-Encased (3POE) (Moldrup et al. 2005b):

$$\frac{D_p}{D_0} = \Phi^2*\left(\frac{\varepsilon}{\Phi}\right)^{\left(2+\frac{\log\left(\varepsilon_{100}{}^{\frac{1}{4}}\right)}{\log\left(\frac{\varepsilon_{100}}{\Phi}\right)}\right)} \tag{10}$$

Organic Matter Fraction Dependent Model (OMF-WLR) (Hamamoto et al. 2012):

$$\frac{D_p}{D_0} = (\varepsilon - \varepsilon_{th})^{X'} \tag{11}$$

where ε_{th} is the air-filled porosity (cm^3 soil-air cm^{-3} soil), and the gas diffusivity is equal to zero, depending on soil type and management (Eq. 12), X' is a parameter related to the connectivity-tortuosity of the porous matrix (Eq. 13). Both parameters are determined according to the volumetric fraction of the soil organic matter (OMF, $m^3\ m^{-3}$), being calculated based on the SOM content (g SOM g^{-1} soil), according to Eq. 14.

$$\varepsilon_{th} = 0.01e^{(2.5*OMF)} \quad (12)$$

$$X\ddot{E} = 1.8 + 1.4*OMF \quad (13)$$

$$OMF = \frac{SOM}{1 + \frac{(1-SOM)}{2.7}} \quad (14)$$

Structure-Dependent Water-Induced Linear Reduction Model (S-WLR) (Moldrup et al. 2013):

$$\frac{D_p}{D_0} = \varepsilon^{(1+cm\Phi)}\left(\frac{\varepsilon}{\Phi}\right) \quad (15)$$

with *cm*, a parameter that reflects the complexity of the porous soil matrix. The *cm* values depend on the type and management of soil; when the soil is sieved and repacked *cm* is equal to 1; in mineral soils, independent of their SOM content, *cm* is equal to 2; finally, in organic and volcanic ash soils *cm* is equal to 3.

Millington and Quirk (1961):

$$\frac{D_p}{D_0} = \varepsilon^{\frac{4}{3}}*\left(\frac{\varepsilon}{\Phi}\right)^2 \quad (16)$$

The parameters for the gas diffusivity models (Table 3) were determined using the information on the Table 2 and the equations described above.

Table 3 Parameters required for each model for the soil-gas diffusivity models according to each sample site. The parameters were determined using the soil physical properties and the equations in the methodological section

Site	Depth (cm)	*cm*	OMF	ε_{100} (%)	ε_{th} (%)	*b*	X'
S1	0–5	2	0.080	37.7	1.2	7.91	1.91
S1	5–10	2	0.080	28.4	1.2	12.70	1.91
S1	10–20	2	0.072	28.1	1.2	12.07	1.90
S1	20–50	2	0.045	31.2	1.1	9.33	1.86
S2	0–5	2	0.078	30.5	1.2	7.26	1.90
S2	5–10	2	0.055	30.9	1.1	7.79	1.87
S2	10–20	2	0.049	32.9	1.1	6.81	1.86
S2	20–50	2	0.046	29.4	1.1	7.35	1.86
S3	0–5	2	0.083	25.2	1.2	8.84	1.91
S3	5–10	2	0.075	28.2	1.2	6.79	1.90
S3	10–20	2	0.074	29.0	1.2	7.00	1.90
S3	20–50	2	0.065	28.2	1.2	6.73	1.89
S4	0–5	2	0.075	32.6	1.2	4.96	1.90
S4	5–10	2	0.070	31.9	1.2	6.10	1.89
S4	10–20	2	0.059	31.0	1.2	6.31	1.88
S4	20–50	2	0.047	27.8	1.1	7.54	1.86
S5	0–5	3	0.287	23.0	2.1	15.55	2.20
S5	5–10	3	0.287	16.1	2.1	16.25	2.20
S6	0–2	2	0.130	15.5	1.4	6.69	1.98
S6	2–5	2	0.088	12.5	1.2	9.09	1.92
S6	5–15	2	0.052	15.9	1.1	10.46	1.87
S6	15–35	2	0.043	15.7	1.1	10.37	1.86
S6	35–55	2	0.041	16.8	1.1	10.86	1.86
S7	0–2	2	0.045	12.9	1.1	8.38	1.86
S7	2–5	2	0.049	10.0	1.1	10.12	1.87
S7	5–15	2	0.053	5.6	1.1	11.32	1.88
S7	15–35	2	0.047	5.0	1.1	15.92	1.87
S7	35–55	2	0.043	0.0	1.1	19.24	1.86
S8	0–2	2	0.045	0.1	1.1	14.72	1.86
S8	2–5	2	0.041	8.3	1.1	15.76	1.86
S8	5–15	2	0.034	0.0	1.1	24.17	1.85
S8	15–35	2	0.034	0.1	1.1	24.69	1.85
S8	35–55	2	0.042	1.1	1.1	20.93	1.86
S9	0–10	3	0.190	18.8	1.6	15.49	2.07

cm, parameter that reflects the complexity of the porous soil matrix and it is used in the S-WLR model; ε_{100}, air-filled porosity (cm^3 soil-air cm^{-3} soil) at − 100 cm of water matric potential (≈ − 10 kPa), used in the TPM and 3POE models; *b*, parameter derived from the soil moisture curve, determined as the slope of the soil moisture curve in a system log (cm^3 soil-water cm^{-3} soil) vs. log (pressure, kPa); X', parameter related to the connectivity-tortuosity of the porous matrix, used in the OMF-WLR model; ε_{th}, air-filled porosity (cm^3 soil-air cm^{-3} soil) where the gas diffusivity is equal to zero, used in the OMF-WLR model; *OMF*, soil organic matter calculated based on the SOM (g SOM g^{-1} soil), used in the OMF-WLR to estimate X' and ε_{th}

2.3 Statistical Analysis

For this study, the model evaluation was done using the determination coefficient (r^2), the root mean square error (RMSE), the mean bias error (BIAS), the agreement index (*d*), and the mean absolute error (MAE). They were computed using R software (R Core Team 2018) with the library hydroGOF (Zambrano-Bigiarini 2020), and their equations are the following:

$$RMSE = \sqrt{\frac{\sum_i^n\left(\widehat{y}_i - y_i\right)^2}{n}} \quad (17)$$

$$BIAS = \frac{\sum_i^n \widehat{y}_i - y_i}{n} \quad (18)$$

$$d = 1 - \frac{\sum_i^n\left(\widehat{y}_i - y_i\right)^2}{\sum_i^n\left(\left|\widehat{y}_i - \overline{y}_i\right| + \left|y_i - \overline{y}_i\right|\right)^2} \quad (19)$$

$$MAE = \frac{\sum_i^n\left|\widehat{y}_i - y_i\right|}{n} \quad (20)$$

To determine the best model, they were ranked according to the statistical performance from 1 to *n*, where 1 is the best model and *n* the worst. In the case of a tie between two or more models, they were assigned with the same ranking. Also, it was defined as a *standard score* of the index obtained by dividing the ranking value by *n* (equivalent to the worst performing model). Finally, the models were compared by the average of the standard scores.

3 Results and Discussion

Figure 2 shows the relation between the observed and predicted data, wherein almost all cases are under the 1:1 line. The main concern of applying the method proposed by Rolston and Moldrup (2002) on undisturbed samples is the effect of the microorganism's respiration on the diffusion coefficient. However, Moldrup et al. (2000a, 2004) consider this value negligible after measured the oxygen consumption rates in soil samples at − 100 cm of water (≈ − 10 kPa) for 48 h. The results showed that the error in the measurement of the D_p value did not exceed 1.5%. The time used in measuring the samples varied between 20 and 60 min, depending on the water content.

Table 4 shows the results of the statistical indices and the goodness of fit between the soil-gas diffusivity predicted by the models and the soil-gas-diffusivity measured with Chilean soil samples. Table 5 shows the ranking of the prediction model according to the goodness of fit between the predicted and the measured data, showing that P-WLR was the best model with the best statistical values for MAE, BIAS, and RMSE. In contrast, BU-S-WLR and S-WLR showed the worst values in the RMSE, BIAS, MAE, and *d*. Thus, BU-S-WLR and S-WLR could be considered as inadequate models to predict the soil-gas diffusivity in similar conditions.?]

On the contrary, the model P-WLR was the most adequate model to predict the soil-gas diffusivity in our samples. M-Q model was considered as a classical model from literature and has three considerations (Moldrup et al. 2003): (i) used initially in restructured soils, such as coarse sandy soils with a random particle distribution of uniform size; (ii) derivative for cases of permeability rather than diffusivity; and (iii) does not take into account the effect of pore-size distribution on gas diffusivity. Despite these apparent limitations in its development, this model has been tested in various situations with good results (Moldrup et al. 2000a, b, 2013). In this study, even with limitations, the M-Q performance was better than more complexity models (fifth place). Moldrup et al. (2013) found that P-WLR performed better than M-Q. However, we did not include repacked soils as Moldrup et al. (2013) considered as unimodal soils.

The models BBC, TPM, 3POE, OMF, and S-WLR could be considered more complex models since their parameters required physical soil properties with laborious laboratory determination. This complexity could be

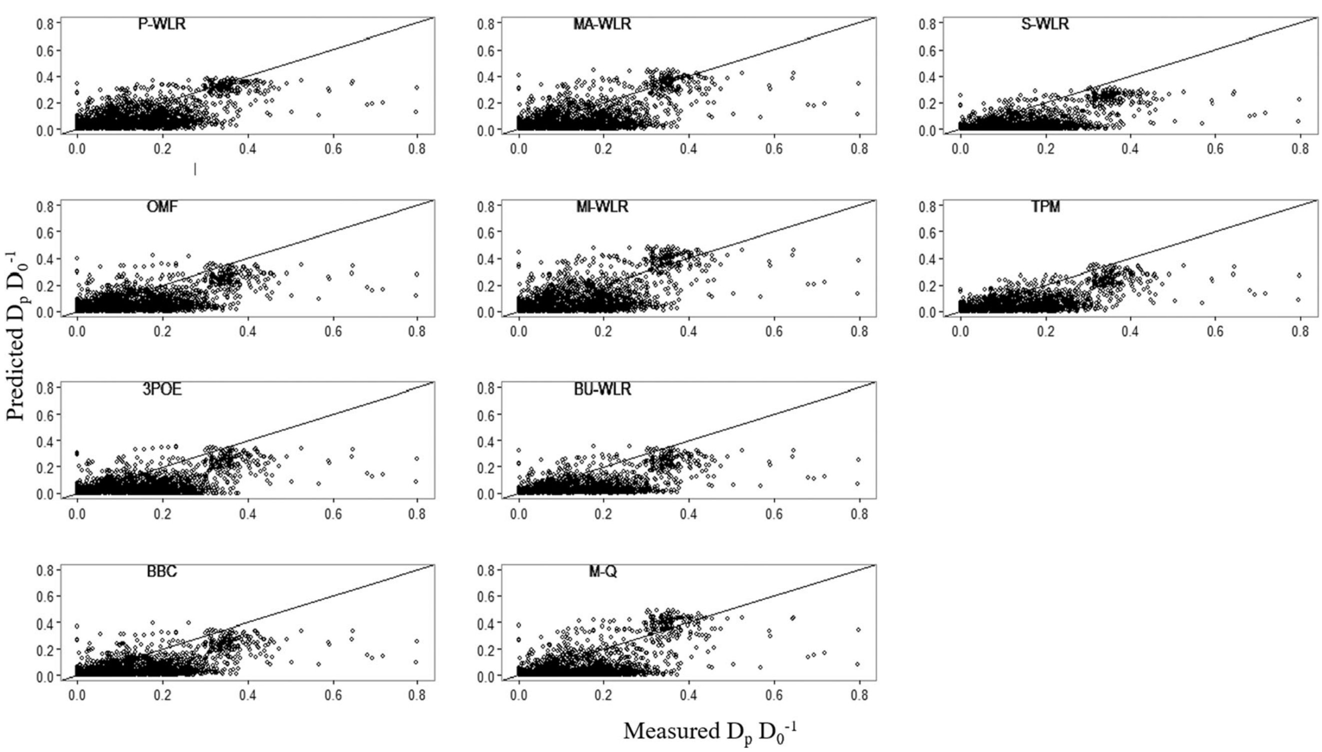

Fig. 2 Comparison of the predictive capacity of gas diffusivity ($D_p\,D_0^{-1}$, cm air cm^{-1} soil) models. The *x*-axis is the data determined at the laboratory (measure data), and the *y*-axis represents the predicted values from each model (predicted data). The black line indicates the 1:1 relation between predicted and measured data

Table 4 Performance of soil-gas diffusivity models against the laboratory data of soil-gas diffusivity, from Chilean soil samples, in terms of MAE, RMSE, *d*, r^2, and BIAS

Model	Abbreviation	Statistical indices				
		MAE	RMSE	*d*	r^2	BIAS
Penman Water Linear Reduction	P-WLR	0.08	0.11	0.74	0.37	−0.05
Marshal Water Linear Reduction	MA-WLR	0.09	0.12	0.73	0.35	−0.06
Millington Water Linear Reduction	MI-WLR	0.09	0.12	0.76	0.36	−0.05
Buckingham Water Linear Reduction	BU-WLR	0.10	0.13	0.64	0.34	−0.09
Millington and Quirk	M-Q	0.09	0.13	0.73	0.36	−0.07
Structure-Dependent Water-Induced Linear Reduction	S-WLR	0.10	0.13	0.64	0.36	−0.09
Organic Matter Fraction Dependent	OMF	0.09	0.12	0.68	0.32	−0.07
Three-Porosity	TPM	0.10	0.13	0.65	0.33	−0.09
Three-Porosity-Encased	3POE	0.09	0.13	0.67	0.35	−0.08
Buckingham-Burdine-Campbell	BBC	0.09	0.12	0.69	0.42	−0.06

MAE, the mean absolute error; *RMSE*, root mean square error; *d*, agreement index; *r*, determination coefficient; *BIAS*, mean bias error. BIAS, MAE, and RMSE are in the same units of the soil-gas diffusivity, *d* varies between 0 (no agreement at all) to 1 (perfect match), and r^2 varies between 0 (0 means that the dependent variable cannot be predicted from the independent variable) to 1 (means the dependent variable can be predicted without error from the independent variable)

associated with the ability to differentiate soil management, soil structure, or pore-size distribution, even when they had similar values of ε and Φ; i.e., the soil density affects tortuosity and gas diffusivity, even when the samples have similar values of air-filled porosity and moisture content (Moldrup et al. 2005a, b).

Among these models, only BBC had an excellent performance (third place), while OMF, 3POE, S-WLR, and TPM obtained the sixth, seventh, eighth, and tenth place, respectively. Finally, according to our results, more complexity does not guarantee better performance than simpler models, contrary to what was proposed by Jayarathne et al. (2019) where models such as S-WLR and M-Q underestimated $D_p\,D_0^{-1}$ at low values of air-filled porosities and overestimated it to high values of air-filled porosities. Also, this is due to the low capacity to describe the characteristics of the porous soil matrix adequately.

According to Jayarathne et al. (2020), the use of models based on physical soil properties such as total porosity and air porosity results in weak predictions when not considering the presence of two different pore regions (inter and intra-aggregate porosity). On average, the RMSE of the proposed model was higher (average RMSE for all the analyzed situations was 0.019) than for the WLR-MA, M-Q, and S-WLR models (0.042,

Table 5 Ranking and score of the soil-gas diffusivity models according to their goodness of fit. The proposed ranking orders and compares the models according to the result of the statistical index, where 1 is the best model, and 10 is the worst model

Model	Abbreviation	MAE		RMSE		*d*		r^2		BIAS		Average score	
		R	S.S.	R	S.S.	R	S.S.	R	S.S.	R	S.S.		
Penman Water Linear Reduction	P-WLR	1	0.33	1	0.33	2	0.25	2	0.29	1	0.2	0.28	1
Marshal Water Linear Reduction	MA-WLR	2	0.67	2	0.67	3	0.38	4	0.57	2	0.4	0.54	4
Millington Water Linear Reduction	MI-WLR	2	0.67	2	0.67	1	0.13	3	0.43	1	0.2	0.42	2
Buckingham Water Linear Reduction	BU-WLR	3	1.00	3	1.00	8	1.00	5	0.71	5	1.0	0.94	9
Millington and Quirk	M-Q	2	0.67	3	1.00	3	0.38	3	0.43	3	0.6	0.61	5
Structure-Dependent Water-Induced Linear Reduction	S-WLR	3	1.00	3	1.00	8	1.00	3	0.43	5	1.0	0.89	8
Organic Matter Fraction Dependent	OMF	2	0.67	2	0.67	5	0.63	7	1.00	3	0.6	0.71	6
Three-Porosity	TPM	3	1.00	3	1.00	7	0.88	6	0.86	5	1.0	0.95	10
Three-Porosity-Encased	3POE	2	0.67	3	1.00	6	0.75	4	0.57	4	0.8	0.76	7
Buckingham-Burdine-Campbell	BBC	2	0.67	2	0.67	4	0.50	1	0.14	2	0.4	0.48	3

R, ranking, ranges between the best model (1) to the worst model (10); *S.S.*, standard score ranges between the best model (0) to the worst model (1); *MAE*, the mean absolute error; *RMSE*, root mean square error; *d*, agreement index; r^2, determination coefficient

0.059, and 0.074 respectively). The low value of RMSE obtained by this work, compared with our results in the same models, and the environmental importance of gas diffusivity, makes us think that there is a need to test new models and agronomical managements not included in this study.

4 Conclusions

The objective of this work is to test the predictive capacity of 10 soil-gas diffusivity models obtained from different agronomic managements for Chilean soils. According to our findings, models with lower complexity showed a better performance than more complex models. The Penman Water Linear Reduction Model (P-WLR) had the best performance among all models, while the Three-Porosity Model (TPM) showed the worst performance. The classical Millington and Quirk model (M-Q) presented a better performance than more complex models, even considering its design limitations. Therefore, in the sampled soils of this work, the use of simpler models is more appropriate than more complex models. However, in order to evaluate the real predictive capacity of the models used, as well as those models not considered in this study, it is necessary to include other soil management with agricultural, forestry, and environmental interest.

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Compliance with Ethical Standards

Conflict of Interest The authors declare that they have no conflict of interest.

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