STUDIES ON GAS DIFFUSION IN COMPACTED SOILS

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Abstract

For modeling gas transport in soils and other porous media is necessary to know the diffusion coefficient. Gas diffusion in soil is a dominant process when convective transport is minimal. Gas molecules from soil are constantly moving as the kinetic theory of gases. Soil compaction has a major impact on gas transport characteristics. Over the years many models have been developed for determining the gas diffusion coefficient in soil, defined as the ratio of gas diffusion in soil (D) and the gas in the air (D_0). Millington and Quirk (1960) and Moldrup (1999) determined the variation of diffusion coefficient for different soil types, based on Penmann's numerical and empirical models(1940). Diffusion models tend to perform better in some soils than in others. Knowledge of the diffusion coefficient is essential for developing accurate predictive models for gas transport in porous media and to improve our understanding of the basic processes involved in transport. Gas diffusion measurements on different samples of different sizes is an important goal in research diffusion. In this context, based on experimental research and extensive bibliographical studies, the authors determined the relationship between the soil suction curve and moisture. Suction curve was used to estimate the permeability of which is subsequently used in modeling the behavior of soil. Nowadays, significant contributions were made by researchers in determining and measuring suction curve. However, almost all measurement models of suction have deficiency, including such aspects as reliability, cost, method of application and practicality. Therfore, there is still a need for improved techniques for measuring suction.

Key words: gas diffusion, numerical modeling, Millington-Quirk-Moldrup models, suction curve, diffusion coefficient

Current knowledge about gas diffusion are due to famous scientists Thomas Graham and Adolf Eugen Fick. Graham's gas diffusion research was guided by a hollow glass diffusion apparatus, which ends with a semi-permeable plug at one end. The tube was filled with hydrogen, while the other end was introduced into the water. The results of his experiment were simple and decisive, indicating that the diffusion flow is proportional to the difference between the tube and the hydrogen concentration in the air. The next important step in the diffusion theory result from the work of Adolf Fick. Knowing that dynamic molecular diffusion is a process, Fick developed the laws of diffusion, in analogy with Fourier's heat law (Crank, 1975, Jaynes and Rogowski, 1983; Rolston, 1986; Cussler, 1997, Ball and Smith, 2001).Therefore, one-dimensional gas diffusion in soil can be described by:

$$\frac{V_{gaz}}{At} = V_{gaz} = -D_g \frac{\partial c}{\partial x} \qquad (1.1)$$

where V_{gaz} is the amount of gas released, A is cross-sectional area of soil, t is time, C is the concentration of soil gas phase, x is the distance of soi land D_g is gas diffusion coefficient in soil.

However, although useful in soil science, Fick's law must be applied cautiously in diffuse process because is suitable only for certain cases, such as diffusion of a gas in a mixture of several echimolar gases.

A great effort was made to measure in laboratory soil gas diffusion coefficient (Penmann, 1940; Currie, 1960; Ball, 1981; Rolston, 1986). However, determining the gas diffusion is time consuming and difficult. Therefore, researchers have introduced mathematical formulas to determine the gas diffusion (diffusion coefficient ratioa of gas in the soil, D_g, and free air, D_0, for example, D_g/D_0), which include easily measured soil properties as porosity and the total volumetric content of air, $(a = PT - \theta)$.

Penmann (1940) proposed a universal formula for saturated porous media,

$$\frac{D_g}{D_0} = \frac{1}{\tau} a \qquad (0 < a < 0,7) \quad (1.2)$$

where τ indicates a constant convolution (approximately equal to 2), for example, τ does not depend on air cobntent,a. Then, adapted Penmann equation (1.2) to experimental data and obtained a known linear expression:

$$\frac{D_g}{D_0} = 0,66 a \qquad (1.3)$$

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where 0,66 is the universal coefficient of sinuosity for all porous media. Since the the variation of volume decreases when the air content increases (Hillel, 1980; Xu, 1992), the constant 0,66 is valid only for certain volumetric air content values and cause an overestimation of the diffusion coefficient for low air content.

Marshall (1959) showed that the formula of Penmann (1940), equation (1.3) did not take into account air phase discontinuities. Therefore , he examined the effects of air on its conductivity. Following research, Marshall concluded that the constant 0,66 from equation (1.3) should be replaced by $a^{1/2}$, assuming that the porous medium whose pores capillary is equal diameter, or:

$$\frac{D_g}{D_0} = a^{2/3} \tag{1.4}$$

In addition, to overcome the limits of equation (1.4), Millington (1959) modified the equation of Penmann, introducing a coefficient of sinuosity as a function of air-filled porosity ($\tau = 1/a^{1/3}$), so:

$$\frac{D_g}{D_0} = a^{4/3} \tag{1.5}$$

But, this formula overestimated the diffusion coefficient for high levels of air content. Similarly, Currie (1960) established a link between the empirical diffusion capacity and air content in the soil, and this formula fits more porous material consisting of particles of the same size:

$$\frac{D_g}{D_0} = \varphi a^{\xi} \tag{1.6}$$

where φ (≤ 1) and ξ (≥ 1) are constant for a granular material, representing the shapes of pores. In equation (1.6), φ is a constant, but is a function of total porosity, This formula can not be applied to wet materials, the geometry of the pores filled with air change depending on water content. Although, equation (1.6) is recommended for low porosity, and not where the largest pores are filled with water, was used the following empirical formula (Currie,1961):

$$\frac{D_g}{D_v} = \left(\frac{a_f}{a_v}\right) \tag{1.7}$$

where a_f is fractional air volume, a_v is the volume occupied by the largest pore space and D_v is diffusion coefficient when only a is filled with air. This equation is difficult to enforce because of the determination of a_v. By analogy with the unsaturated conductivity, the relationship between

the diffusion capacity of gas and air content was introduced as an exponential function of air content and porosity (Millington and Quirk, 1960):

$$\frac{D_g}{D_0} = \frac{a^{10/3}}{pT^{2/3}} \tag{1.8}$$

In this equation it is assumed that all pores filled with water contribute equally to diffusion. Recently, Sallam (1984), Xu (1992), Petersen (1994), Washington (1994), Jin and Jury (1996) and Moldrup (1996) compared the equation (1.9) with other forms of diffusion capacity. Although usually the equation (1.8) gave lower results of diffusion capacity, for certain soils it gave good results. Another type of relationship, the Millington – Quirk relationship:

$$\frac{D_g}{D_0} = \frac{a^2}{pT^{2/3}} \tag{1.9}$$

was designed to give much better results of diffusion capacity for different soils with different textures (Jin and Jury, 1996, Washington, 1994). On the other hand, Peterson (1994) demonstrated that equation (1.9) underestimates the diffusion coefficient of several gases, especially when the air content is high. However, when the air content is low, this formula is appropriate.

Gas diffusion capacity in the soil type (texture, structure, horizon, mining) control gases in homogeneus soils, where the diffuse gas transport is predominant compared to gas transport by convection.

SUCTION CURVE. DETERMINING THE RELATIONSHIP BETWEEN HUMIDITY AND SUCTION METHOD (SANDBOX)

This sandbox is used to analyze a range of pressures for pF 0 (saturation) up to pF 2.0(-100hPa). The sand from the box it is used to transfer the suction from the installation of desorbtion to soil samples. Sand surface is flexible, which facilitates contact between it and reinstall the soil samples after they were removed for weighing. This leads to better transmission of suction by sandy material, to the porous flat for this instrument.

The results of measurements made with this sand box correspond to points on the curves of drying of samples; is associated with decreasing pressure. These pressure values are usually standard values of water potential.

Wetting curve, on the other hand is determined graphically representing the water content according to increasing values of pressure. This curve is identical to that of drying because the

water content does not respond instantly to changes in pressure (Hysteresis Curve).

"The principle of raising the water" is used to apply suction to soil samples. Height difference between the regulator and central suction of soil samples is the difference in pressure. Pressure values between 0 and 100 cm can be applied. Suction regulator is adjusted for application of specific pressure of soil samples. Finally, samples are dried and weighed so that the water content can be inferred for each specific pressure.

The laboratory must have a constant temperature between measurements. If there will be changes in temperature when water changes its viscosity and therefore values of the retention capacity. If the volume is less than the volume of soil sample ring, or if the sample has changed during transport should not be subject to analysis. Also, will be removed stones from the sample if it contains something.

Figure 1 **Sandbox for measuring suction curve**

The samples were taken from the area Pacurari, Iasi.

RESULTS AND DISCUSSIONS

The SOILPARA program has developed a soil texture diagram, which only requires information about the content of clay, silt and sand (percentage) and soil bulk density.
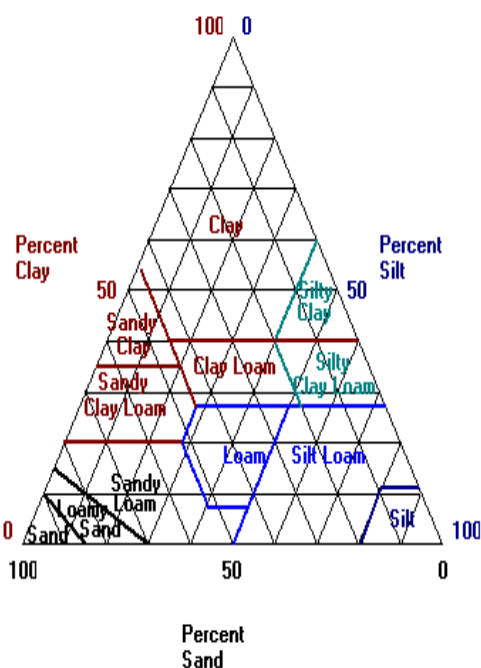

Figure 2 **Soil texture diagram**

In the texture diagram, on the left is clay, which increases from bottom to top. On the right side is sludge, which increases from the top to bottom. At the bottom of the graph, the amount of sand increases from left to right. Soil texture classes include: sand, loamy sand, clay and sandy soi land clay.

Bulk density must be less than 2,65 g/cm^3 (2, 65 is the density of solids). Water retention curve establishes a link between soil – water matrix potential and soil structure, water retention curve can be considered a psyhical characteristic of soil. Determination of the retention curve is achieved by execution of six steps:

1. File name;
2. Selection formula;
3. Conductivity/diffusion capacity;
4. Program control;
5. Parameter estimation;
6. Execution of the program.

This steps are used to plot the curve of the characteristics of ground water, and the air entry value of the absorbtion can be determined. Air entry value of soi lis absorbed when the air starts to enter into the largest pores of the soil. Θw (in percent) is the peak of the curve an dis the intersection of two tangents.
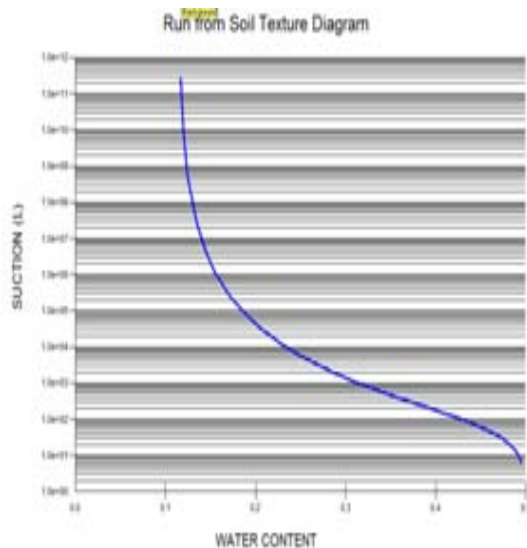
Table 1

Measurements results

No. sample	No. of ring	pF	Water column (cm) (hPa)	Wet weight (sample,ring,clo th,elastic) A	dry weig(sample ,ring,cloth, elastic) B	Weight of ring, cloth, elastic C	Weight of soil with water D=A-B	Weight of dry soil E=B-C	W W=D/E	Bulk density DA	Volumetric content of water
1	57			241	192,19	112	48,81	80,19	60,86794	2,32	141,21362
2	67	0,0	1,0	259	203,47	115	55,53	88,47	62,76704	2,32	145,61953
3	58			267	206,48	113	60,52	93,48	64,74112	2,32	150,1994
4	59			276	217,75	113	58,25	104,75	55,60859	2,32	129,01193
1	57			241	192,19	112	48,81	80,19	60,86794	2,32	141,21362
2	67	0,4	2,5	253	203,47	115	49,53	88,47	55,98508	2,32	129,88538
3	58			262	206,48	113	55,52	93,48	59,39238	2,32	137,79033
4	59			276	217,75	113	58,25	104,75	55,60859	2,32	129,01193
1	57			241	192,19	112	48,81	80,19	60,86794	2,32	141,21362
2	67	1,0	10	250	203,47	115	46,53	88,47	52,5941	2,32	122,01831
3	58			262	206,48	113	55,52	93,48	59,39238	2,32	137,79033
4	59			274	217,75	113	56,25	104,75	53,69928	2,32	124,58234
1	57			223	192,19	112	30,81	80,19	38,42125	2,32	89,137299
2	67	1,5	31,6	238	203,47	115	34,53	88,47	39,03018	2,32	90,550017
3	58			242	206,48	113	35,52	93,48	37,99743	2,32	88,154004
4	59			258	217,75	113	40,25	104,75	38,42482	2,32	89,145585
1	57			217	192,19	112	24,81	80,19	30,93902	2,32	71,778526
2	67	1,8	63,1	232	203,47	115	28,53	88,47	32,24822	2,32	74,81587
3	58			236	206,48	113	29,52	93,48	31,57895	2,32	73,263158
4	59			251	217,75	113	33,25	104,75	31,74224	2,32	73,642005

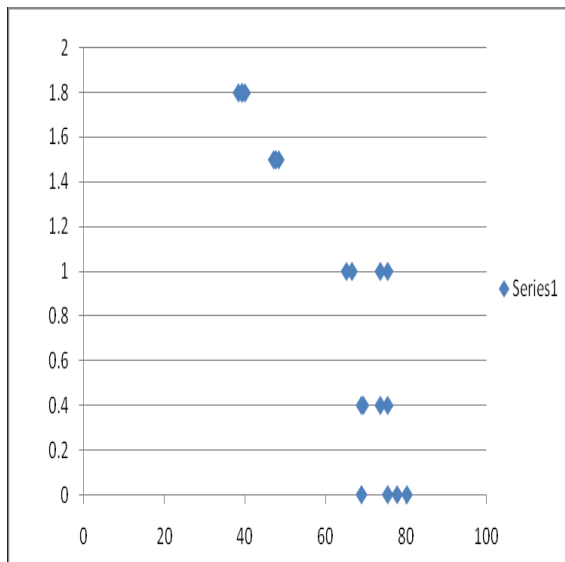Figure 3 **Suction curve of soil from Pacurari (Soilpara)**

Figure 4 **Suction curve of soil from Pacurari (Laboratory determinations)**

Gas diffusion and its dependence on soil porosity filled with air controls most of the gas diffusion processes in the soil.

Table 2
Determination of the diffusion coefficient of soil gases

	D_p/D_0			
	0,66 a	$a^2/PT^{2/3}$	$a^{10/3}/PT^2$	$PT^2(a/PT)^{2+3/b}$
Păcurari	0.181	0.124	2.677	0.052

CONCLUSIONS

Knowledge of soil characteristics and features is a fundamental scientific material for sustainable exploitation of a territory, which includes, besides edaphic information and the information of environmental conditions.

Soil quality is given on the one hand by its natural qualities, which sometimes can cause restrictions on use, and on the other hand, the characteristics acquired as a result of human intervention, which may change positively or negatively natural qualities. Currently, in national and international literature are found more and more studies and research on mathematical models to determine the diffusion coefficient in soil gas. Physical analysis, chemical and biological performed in laboratories, are often used only to calibrate mathematical models. This is aimed at actually reducing the cost of investigation.

Mathematical models in the field have become increasingly complex, providing a modeling soil properties and processes more closely to real conditions. They have as input parameters many of essentail characteristic of the soi land contain specific sub-shaping processes are involved in the soil mineral and organic compounds. They also provide a range of results and better accuracy of data. Some of the programs developed to determine the diffusion coefficient in soil gas are easy to use, expeditious and are used in studies prepared for practical sustainable use and protection of soil quality. Others are very complex, requiring advanced knowledge in Soil Science and Mathematical modelling, are used in scientific research.

Gas diffusion in soi land its dependence on the characteristics of diffuse oxygen transport controls, gas emissions of pollutants and volatile organic agriculture, forest and urban soils. Appropiate formulas are required to determine gas diffusion as a function of air- filled soil porosity in natural soil homogeneous.

Key parameters in the soil gas transport, gas diffusion capacity and air permeability and their variation depending on soil type plays an important role in problems of gas leakage from the soil, including chemical volatisation from the poluted areas, production and gas release emissions. Knowing the diffusion coefficient is very important to develop formulas for gas in the porous media and to improve basic understanding of transport processes involved.

Thus, for determining the gas diffusion coefficient in soil, we made a series of laboratory tests like: soil moisture, size distribution by sieve, texture, pH, stability of aggregates, bulk density, total density, porosity, suction curve. Gas molecules perform a random motion duet o thermal energy. By diffusion, the molecules move as a result of pressure and concentration. Diffuse transport is the main mechanism responsible for the movement of gas in the soi land provide exchanges between soil and atmosphere (Troeh,

1982; Rolston, 1986, Arah and Ball, 1994; Kruse, 1996). The most important soil processes are affected by gas diffusion, including: soil aeration (Glinsk and Stepniewski, 1985), the movement of water vapor in soil (Kirkham and Powers, 1997) and volatization of organic compounds(Petersen, 1994, Amalia, 1996; Arands, 1997).

Recent formulas of soil gas diffusion take into account the effects of soil structure and explained the development of anaerobic zones of the components. In clay soils anaerobic conditions persist for a long time in larger components, but quantitative assessment of anaerobic volume is complicated by the uncertainty about the value of the diffusion coefficient of oxygen in wet soils.

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