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REGULAR ARTICLE

Modeling and simulation of trifluralin herbicide movement due to its application on soils by chemigation

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Abstract

The Trifluralin (TFN) is a pre-emergent herbicide which is widely used in agriculture. Usually, this pesticide is directly applied to the soil, where it can remain for long periods or can be transported. In this sense, knowing the dynamics of an herbicide soil transport is essential to avoid environmental contamination problems and risks to human health. Thus, this study aims to model and simulate TFN movement on soils with two different textures, a sandy loam and clay loam soil. It was considered that the herbicide was applied via chemigation trough a subsurface drip irrigation system, under a non-steady regime. Therefore, the transport parameters of TFN in these soils and physical-hydric characteristics of these were used, while the physical environment modeling were conducted using the Hydrus 2D software. The results showed that both in sandy and clayey soils, the TFN tends to be retained by the soil, close to where it was applied, not exceeding a layer greater than 2.5 mm outside the dripper radius, even in more favorable conditions such as the presence of irrigation. Finally, it could be concluded that this herbicide movement in the soil is of low potential, due to this product high solid-liquid partition coefficient (Kd), even in sandy soil, which has low cation exchange capacity (CEC).

Keywords

Contaminant transport; Hydrus 2D; Subsurface drip irrigation.

Introduction

Subsurface drip irrigation (SDI) is an irrigation technique that consists of supplying water, which may contain diluted agrochemicals, directly to the root zone of crops. This technology is used worldwide, and its popularization is due to its advantages, such as high water use efficiency, reduced deep percolation, soil evaporation and weeds growth around the crop (Wang et al., 2022). In addition, this system use can be an efficient solution for irrigation in corners where the center pivot cannot reach, what can increase 15 to 20% of the available area in a square parcel (Sorensen et al., 2021; Tilley et al., 2016). However, in SDI the emitters are buried in the ground and can become clogged by root intrusion, reducing the system efficiency and its useful life (Cai, et al. 2019; Lima et al., 2014).

The Trifluralin (α,α,α-trifluoro-2−6-dinitro−NN-dipropyl-p-toluidine), TFN, is an herbicide of the chemical group Dinitroaniline, widely used in agriculture since 1960 (Coleman et al., 2020; Epp et al., 2018). This pre-emergent herbicide is efficiently used to control grasses and some small-seeded dicotyledonous species (Coleman et al., 2020; Li et al., 2021) and is also capable of minimizing root intrusion in subsurface drippers (Lima, 2011; Mendonça et al., 2020). At a global scale, it is estimated that around 4,400 tons of TFN are currently used per year, mainly for the cultivation of cotton, alfalfa, and soybeans (Maggi et al., 2019).

Usually, this pesticide is applied directly to the soil where, due to its physicochemical characteristics, it tends to remain for long periods of time (Li et al., 2021). Zhichkina et al. (2020) point out that the residual time of TFN at the soil can reach up to three years. In addition to being bioaccumulative and persistent, TFN is a potentially toxic compound, especially to aquatic environments, and possibly carcinogenic to humans (Friedrich et al., 2021).

Once at the soil, solutes tend to interact with its liquid and solid phases and can be transported, which creates risks of environmental contamination and for people's health (Lelis Neto et al., 2020). According to Oliveira et al. (2000), this is

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the main contamination process of groundwater and surface water.

The mobility of a pesticide in the soil, especially when applied directly to it, by spraying or chemigation, depends on several factors such as the characteristics of the product itself and the physical and hydraulic properties and characteristics of the soil (Cruciani et al., 1996; Hatzisymeon et al., 2021; Oliveira et al., 2000). Therefore, knowing the transport dynamics of an agrochemical at a soil makes its use more efficient and conscious. Thus, the objective of this work is to model and simulate the movement of TFN, applied via chemigation through SDI, in two soils with different physical and hydraulic properties and characteristics.

Materials and methods

From the physical and hydraulic properties and characteristics of a sandy loam soil (77%, 5% and 18% of sand, silt and clay, respectively), a clay loam soil (25, 35 and 40% of sand, silt and clay, respectively) and the TFN transport parameters for these soils (Table 1) presented in Faria (2011), modeling of the soil profile and of a dripline in subsurface condition for water and herbicide application were carried out, using the Hydrus 2D software version 2.05.027 (Simunek et al., 1999).

Table 1. Physical and hydraulic properties and characteristics of soils used to model and simulate the movement of Trifluralin.

Properties and characteristics	Sandy Soil	Clayey Soil
Bulk density (mg cm^{-3})	1480	1210
Residual moisture (cm^3 cm^{-3})	0.093	0.208
Saturated moisture (cm^3 cm^{-3})	0.626	0.734
α (1 cm^{-1})	0.02203505	0.02203637
n	2.096998	2.182286
Saturated hydraulic conductivity (cm dia^{-1})	110.880	299.280
Tortuosity	0.500	0.500
Soil-water partition coefficient, Kd (cm^3 mg^{-1})	5.210	6.250
Soil water velocity, v (cm h^{-1})	97.440	39.420
Dispersion-diffusion coefficient, D (cm^2 h^{-1})	386.840	87.120

Source: Faria (2011).

For the computational modeling, it was considered that chemigation with TFN was performed twice a week, by an irrigation system with subsurface drip emitters. The model geometry information was determined for two dimensions, X and Y, forming a rectangular profile 100 cm deep and 75 cm wide. An emitter was added at the left corner of the profile, buried at a depth of 20 cm.

Subsequently, it was programmed that the simulation would occur for water flow together with standard transport of solutes. The time information was defined considering a 7-days total period. A non-steady water application regime was simulated, i.e., a variable flow boundary condition modeled on the dripper surface. Thus, applications were determined on the first day with a duration of 0.1 day, and after 3.5 days, another application of 0.1 day, with a flow of -60 cm day^{-1} m^{-1}, which represents the intensity of water application that occurs per meter of dripline through its lateral area, calculated using its external diameter (approximately 12.7 mm), when considering a flow rate of 1 $L.h^{-1}.m^{-2}$. The application of the solute (TFN) was defined for a concentration of 44.5 mg cm^{-3}.

To represent the hydraulic characteristics of the soil, the van Genuchten – Mualem model (van Genuchten, 1980) was selected, without considering the soil hysteresis. The parameters used, related to the hydraulic modeling for each soil, are presented in Table 1. The initial soil condition was defined by the water matric potential, considering a value of -100 cm wc (approximately 10 kPa) for the entire profile.

A finite element mesh refinement was made close to the dripper, and 17 observation nodes were placed on the horizontal axis from the dripper surface, spaced apart at 2.5 mm intervals (Table 2).

Table 2. Distance of the observation nodes in the geometry modeled at Hydrus 2D software.

Observation node	Distance from the dripper surface on the horizontal axis (cm)
1	0.00
2	0.25
3	0.50
4	0.75
5	1.00
6	1.25
7	1.50
8	1.75
9	2.00
10	2.25
11	2.50
12	2.75
13	3.00
14	3.25
15	3.50
16	3.75
17	4.00

The TFN soil adsorption modeling was obtained by a linear solute adsorption mathematical model, by the soil-water partition coefficient, Kd (Table 1). In addition, the value of TFN diffusivity in pure water of 0.5327513 cm^2 dia^{-1}; longitudinal dispersivity (Equation 1, Table 1) of 2.21 cm for clayey soil and 3.97 cm for sandy soil were considered, for a concentration of the herbicide active ingredient of 44.5 mg cm^{-3} (Faria, 2011).

$$\lambda = \frac{D}{v} \tag{1}$$

where,

D - Dispersion-diffusion coefficient (cm^2 h^{-1})

v - Soil water velocity (cm h^{-1})

The diffusivity of the solute in pure water was calculated using the empirical equation of Wilk-Chang (1955), Equation 2.

$$D_{cl} = \frac{7.4 \times 10^{-8} (\varphi_w^o \times m_w)^{0.5} T}{\mu_V \, V_c^{0,6}} \tag{2}$$

where,

D_{cl} - Molar diffusivity coefficient of pesticide in water (cm^2 s^{-1})

T - Absolute temperature (K)

φ_w^o - Association factor for the solvent (2.6 for water)

m_w - Molecular weight of water (18.0 g mol^{-1})

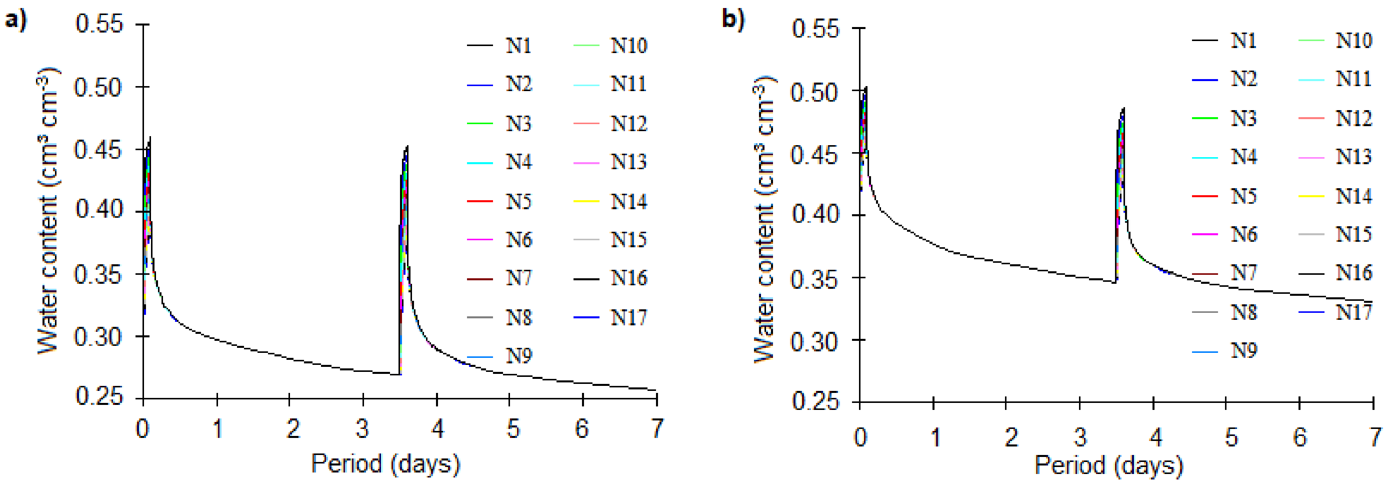
μ_v – water viscosity (8.9 x 10^{-1} cP)

Vc - Molar volume of the pesticide (250.6 cm^3 mol^{-1} for TFN).

Results and discussion

From the Figure 1 analysis, it is possible to observe the moments of the water solution and TFN applications to the soils. It is noted that soon after the solution application, there is a gradual reduction of moisture, which occurs due to the redistribution of water in the soil. In addition, water flow was verified at all observation nodes when the emitter was operated, with greater differences of moisture between nodes for the sandy soil.

Figure 1. Soil moisture variation with time at observation nodes fixed for the sandy soil (A) and clayey soil (B).

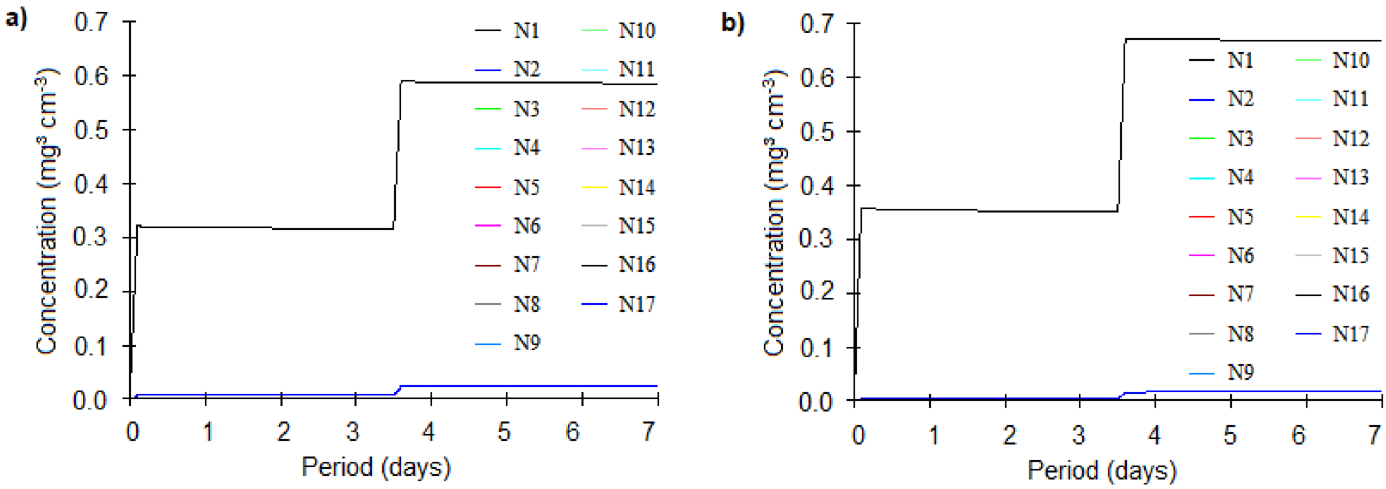


Chen et al. (2019) and Fagundes et al. (2012) explain that the matric potential is relatively large in relation to the gravitational potential when the soil is dry, which leads to water redistribution; however, with the gradual wetting, the matric potential gradient is reduced, leading to the gravitational potential gradient to have greater importance in the movement of water.

It is also observed, by Figure 1 analysis, that the moisture in the clayey soil, due to its greater volume of pores and greater water retention capacity (Edeh et al., 2020), was higher at all observation nodes. In contrast, there is clearly a greater drainage, as expected, for the sandy soil (Yost et al., 2019), which could reflect in a greater movement of the TFN to deeper layers of this soil.

As can be seen in Figure 2, the TFN concentration for both soils increased at the moment of the herbicide application, with the concentration value for the clayey soil, at the node closest to the emitter, approximately 0.1 mg cm^{-3} higher than the value found for the sandy soil. Thus, as reported by Lima (2011), it was found that the soil with a greater presence of clay has a greater capacity to retain TFN. In addition, the moisture redistribution to nodes farther away from the emitter was greater for clayey soil, due to its physical and hydraulic characteristics, which contributes to a higher TFN dilution.

Figure 2. TFN concentration variation with time at the observation nodes fixed for sandy (A) and clayey (B) soils.



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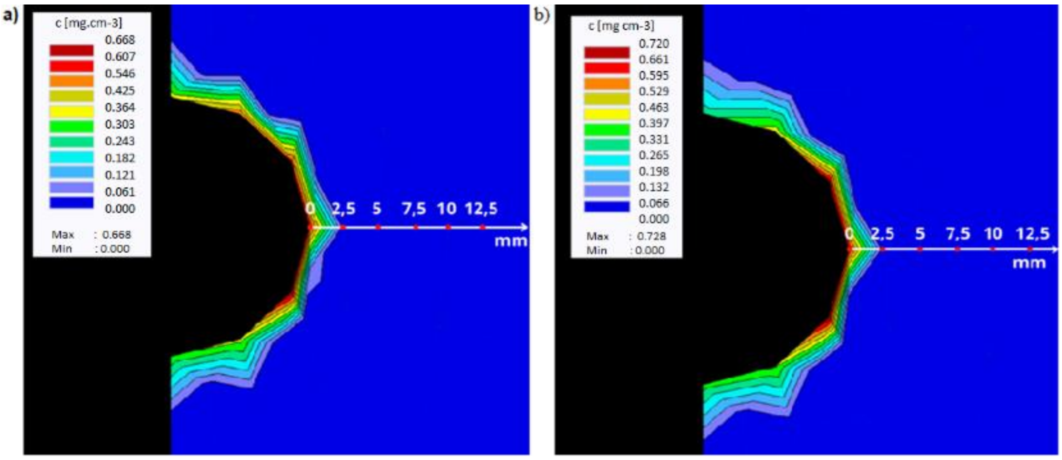
When analyzing Figure 2, it is also noted that the behavior trend of the TFN concentration in the soil over time at the second observation node, was similar to that of the first node, however, on a smaller scale. With the verification of TFN concentrations at nodes 1 and 2, the greater movement of TFN to the sandy soil is evident, compared to the clayey one.

The TFN distribution in the profile of both soils at the final time of application is shown in Figure 3. As can be seen, in both soils, concentrations of this pesticide were not observed beyond the distance of 2.5 mm outside the dripper radius, not even at the regions below and farther horizontally from the emitter, what could lead to environmental contamination.

Figure 3. Graphic representation of the TFN concentration distribution at the sandy (A) and clayey (B) soil profile at the final time.



According to Cruciani et al. (1996) and Li et al. (2021), even in the presence of water flow, TFN does not have a considerable displacement in the soil profile, which is due to its physicochemical properties, what give to it low mobility, such as: low solubility in aqueous media, high volatilization and retention to colloidal soil particles, consequently, high values of Kd, which could be verified even in sandy soil (Faria, 2011), which has a lower cation exchange capacity (CEC), one of the phenomena responsible by the binding increase of molecules to colloids.

One of the main disadvantages of the SDI is the possibility of emitters clogging due to root intrusion, due to the moisture near the drippers. Chemigation with TFN is able to avoid this problem, since at each application, an amount of the herbicide is accumulated near the emitter's outlet, forming an acidic environment which can inhibits root growth and, consequently, its intrusion into the emitters orifice (Cai et al., 2019; Lima et al., 2014). This technique has been widely recommended as a preventive in field measure, especially in crops extremely sensitive to water stress, such as sugarcane cultivars (Dalri et al., 2021; Lima et al., 2014; Simões et al., 2018).

Conclusions

In both sandy and clayey soils, TFN tends to be retained in the soil, close to where it has been applied, not exceeding a layer greater than 2.5 mm, even in more favorable conditions, such as in the presence of irrigation, which generates extra energy for the solution movement through the soil. This fact is due to this pesticide physicochemical properties that give it low mobility.

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