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Recent Applications of HYDRUS Model: A Review

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ABSTRACT : *HYDRUS computer software packages are widely used for predicting and analyzing water flow and solute transport in vadose zone, variably saturated media, and groundwater. Applications involve a broad range of steady-state or transient water flow, solute transport, irrigation scheme and fate of contamination in subsurface flow constructed wetland. The HYDRUS models can be used for both direct problems such as solute transport and irrigation problems, as well as co-operated with CW2D and CWM1to simulate contaminate transfer in subsurface flow constructed wetland. In this article, a brief overview of the current developments on modelling of subsurface flow using HYDRUS model is provided. Physical and chemical nonequilibrium water flow (water storage in immobile domains and/or water flow in structured soils with macropores) is also discussed, and review various application approaches that have been used in the literature in combination with the HYDRUS codes.*

.***KEYWORDS***- *Constructed wetland, HYDRUS model, irrigation schemes, solute transfer, water flow*

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I. INTRODUCTION

Simultaneous water and/or solute transfer processes between the soil surface and the groundwater table is increasing evidence that flow and transport processes in soils often cannot be described using classical models that assume uniform flow and transport[1–5].

Accurate process-based modeling and solute transport remains a major challenge in vadose zone hydrology [6, 7].

The HYDRUS-1D and HYDRUS (2D/3D) computer software packages are widely used finite-element models for simulating water, heat, and solute movement in one, two- and three- dimensional variably saturated media [8,9].

HYDRUS program is a finite-element code that solves the Richards equation for saturated and unsaturated water flow and advection-dispersion equations for both heat and solute transport. The flow equations additionally include sink term to account for water uptake by plant roots. The governing convective-dispersive transport equations are written to include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, and linear equilibrium reaction between the liquid and gaseous phases. These equations also incorporate the effects of zero-order production, and two first-order degradation reactions: one which is independent of other solutes and one which provides the coupling between solutes involved in sequential first-order decay reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation which partitions the liquid phase into mobile and immobile regions. Attachment/detachment theory, including the filtration theory, is included to simulate transport of viruses, colloids, and/or bacteria. Moreover, the biochemical degradation and transformation processes for biochemical components are described [5, 8, and 10].

The different versions of HYDRUS models have been used over the years for a large number of applications including agricultural problems evaluating different irrigation schemes, water flow dynamics in soils containing macropores which governing water flow equations to define variables later used in the solute transport equations. In addition, many early applications focused mostly on biochemical transformation and degradation processes in subsurface-flow constructed wetlands.

The purpose of this article is to present in brief review some recent applications of the HYDRUS models that used for water flow and solute transport in the variably saturated zone, irrigation schemes and simulate processes in subsurface flow constructed wetlands.

II. WATER FLOW AND SOLUTE TRANSPORT

2.1 EQUILIBRIUM FLOW

The unsaturated zone play an important role in the hydrological cycle where the vadose zone is of great interest in evaluating infiltration, soil moisture storage, evaporation, plant water uptake, groundwater recharge, runoff, and erosion. Unsaturated water flow through a porous medium is generally described using the Richards equation.

Richards equation can described the uniform variably-saturated water flow in HYDRUS model as shown below [11]:

$$\frac{\partial\theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] - S \qquad (1)$$

Where: θ = volumetric water content [L^3L^{-3}]; h = pressure head [L]; z= the vertical coordinate positive upward [L]; K(h)= the unsaturated hydraulic conductivity function, often given as the product of the relative hydraulic conductivity; S = general sink/source term [T^{-1}] accounting for root water uptake; t = time [T].

Examples of applications of equilibrium flow processes in combination with relatively standard functions for the unsaturated soil hydraulic properties to a range of laboratory and field data are provided by [12-14]. They studied one-step and multi-step outflow experiments. Horizontal infiltration was studied by [15, 16]. While upward infiltration and centrifuge experiments were mentioned in a study by [17-20], finally, the steady-state water flow and single porosity in stony soils was estimated by [21-23].

2.2 NONEQUILIBRIUM FLOW

There is increasing evidence that water and contaminants moving through the vadose zone often cannot be described using classical models that assume uniform flow and transport [1, 4, and 24].

The Richards equation predicts unsaturated water flow through a porous medium on a macroscopic scale, while solute transport described using the classical advection–dispersion equation [11, 25]. Therefore, modifying macroscopically allow to use of spatially variable soil hydraulic properties (e.g., geometry of porous pathways).

A variety of dual-porosity or dual-permeability models was used to describe preferential flow in macro porous soils and fractured rocks [25, 26]. Dual-porosity models assume that both water and solute can move into and out of the immobile domain, while dual permeability models allow the transfer of both water and solutes within the soil or rock matrix.

Equations 2 and 3 describe dual-porosity whereas 4 and 5 define dual-permeability formulas for water flow based on a mixed formulation of the Richards equation (1) augmented with a mass balance equation. These equations describe water flow in each of two pore regions (one the inter-aggregate pores and fractures, macropore, and the intra-aggregate pores or the rock matrix comprising the micropores) as follows [27]:

$$\frac{\partial\theta_{mo}(h_{mo})}{\partial t} = \frac{\partial}{\partial x_i}\left[K(h_{mo})\left(K_{ij}^{A}\frac{\partial h_{mo}}{\partial x_j} + K_{iz}^{A}\right)\right] - S_{mo}(h_{mo}) - \Gamma_w \qquad (2)$$

$$\frac{\partial\theta_{im}(h_{im})}{\partial t} = - S_{im}(h_{im}) + \Gamma_w \qquad (3)$$

$$\frac{\partial\theta_{f}(h_{f})}{\partial t} = \frac{\partial}{\partial x_i}\left[K_f(h_{f})\left(K_{ij}^{A}\frac{\partial h_{f}}{\partial x_j} + K_{iz}^{A}\right)\right] - S_{f}(h_{f}) - \frac{\Gamma_w}{w} \qquad (4)$$

$$\frac{\partial\theta_{m}(h_{m})}{\partial t} = \frac{\partial}{\partial x_i}\left[K_m(h_{m})\left(K_{ij}^{A}\frac{\partial h_{m}}{\partial x_j} + K_{iz}^{A}\right)\right] - S_{m}(h_{m}) + \frac{\Gamma_w}{1-w} \qquad (5)$$

Where h_{im} and h_{mo} = pressure heads for both regions [L]; S_{im} and S_{mo} = sink terms for both regions [T^{-1}]; and Γ_w= transfer rate for water from the inter- to the intra-aggregate pores [T^{-1}]; the mobile liquid phase (flowing, inter-aggregate), θ_{mo}, and immobile (stagnant, intra-aggregate), θ_{im} [L^3L^{-3}]; w = ratio of the volumes of the macropore or fracture domain and the total soil system ($0 < w < 1$); θ_f , θ_m,represented volumetric water content of the fraction and matrix pore system respectively [L^3L^{-3}] such that $\theta = w\theta_f + (1-w)\theta_m$ [25].

Many laboratory and field experiments have demonstrated the presence of dual-porosity models and dual-permeability models. Both equilibrium and nonequilibrium models in HYDRUS to simulate water flow and tracer movement are provided by [25], and [28-38].

2.3 SOLUTE TRANSPORT

HYDRUS models assume that solutes can exist in all three phases (liquid, solid, and gaseous) and that the decay and production processes can be different in each phase. The solute not only could be transported by advection and dispersion in the liquid phase, but also by diffusion in the gas phase, that accounts sequential first-order decay chain reactions. The equations for solutes in a variably saturated rigid porous are given by [27]:

$$M_k = \theta C_k + \rho C_k + a_v g_k \qquad k = 1, N_s \qquad (6)$$

$$J_{si,k} = -\theta D^{w}_{ij,k} \frac{\partial C_k}{\partial X_j} - a_v D^{g}_{ij,k} \frac{\partial g_k}{\partial X_j} + q_i C_k \qquad (7)$$

$$\emptyset_k = -(\mu_{w,k} + \mu'_{w,k})\theta C_k - (\mu_{s,k} + \mu'_{s,k})\rho S_k - (\mu_{g,k} + \mu'_{g,k}) a_v g_k - SC_{r,k} + \vartheta(\mu'_{w,k-1}\theta C_{k-1} + \mu'_{s,k-1}\rho S_{k-1} + \mu'_{g,k-1} a_v g_{k-1}) + \gamma_{w,k}\theta + \gamma_{s,k}\rho + \gamma_{g,k} a_v \qquad (8)$$

Where ; M =mass of solute [ML^{-3}]; J_{si} = solute flux density [ML^{-2}T^{-1}]; C = solute concentrations in the liquid [ML^{-3}]; g = solute concentration in the gaseous phase [ML^{-3}]; μ_w, μ_s and μ_g= first-order rate constant for solutes in the liquid, solid and gas phases [T^{-1}], respectively; μ'_w,μ'_s and μ'_g = similar first-order rate constants providing connections between individual species in the decay chain; γ_w , γ_s and γ_g= zero-order rate constant for the liquid [ML^{-3}T^{-1}], solid [T^{-1}] and gas phases [ML^{-3}T^{-1}], respectively. a_v= air content [L^{3}L^{-3}]; D^w_{ij} and D^g_{ij}= diffusion coefficient tensor [L^{2}T^{-1}] for liquid and gas phases, respectively; and N_s= number of solutes involved in the chain reaction. The subscripts w, s, and g correspond with the liquid, solid and gas phases, respectively; while the subscript k represents the kth chain number. The parameter ϑ is zero for k=1. ρ = soil bulk density [ML^{-3}]; S = sink term in the water flow equation (1); Cr = concentration of the sink term [ML^{-3}]; $\emptyset$ Typical examples of HYDRUS applications involving First-order degradation rate constants following a series of chain reactions are the transport of trichloroethylene, c2s-dichloroethylene, vinylchloride and ethene [39].

The fate and transport of hormones [40]; saturated column transport experiments were conducted with 2, 4, 6-trinitrotoluene, hexahydro-1, 3, 5-trinitro-1, 3, 5-triazine, and the explosive formulation. Composition B in solid and dissolved forms [41] and finally the fate of nitrogen that contaminate ground waters was studied by [42].

Physical nonequilibrium transport as implemented in HYDRUS may be formulated to reflected both dual-Porosity and dual-permeability models. In addition, it divides the matrix domain into mobile and immobile subregions.

[32, 33, 43, and 44] are examples of dual-porosity, dual-permeability and physical nonequilibrium mobile–immobile models for solute transport.

Reference [44] studied physical nonequilibrium mobile–immobile for solute transport. There result showed that mobile–immobile transport parameters were very similar for Levenberg–Marquardt optimization that combines with the HYDRUS-2D model. The study by [34] showed that both hydrograph and solute breakthrough data might help to identify of hydraulic and transport dual permeability model parameters to characterize preferential flow and solute transport. A mobile immobile solute transport model, a dual-porosity approach, and a dual-permeability formulation were used by [43] to compare different preferential flow and/or transport. There result showed that the dual-permeability approach most accurately simulated preferential drainage flow, mobile–immobile approach largely failed to capture the preferential flow process while the dual porosity approach was able to predict much more distinct and higher drainage flow as compared to the dual-permeability approach.

The triple-porosity with dual-permeability and physical nonequilibrium mobile–immobile models was employed by [4] to study herbicide transport under variably saturated flow conditions.

Chemical nonequilibrium transport in HYDRUS assumes that the sorption sites can be divided into two fractions: one fraction of the sites, S^e [MM^{-1}] (type 1), is assumed to be instantaneous, while sorption, S^k [MM^{-1}] (type 2) on the remaining sites is considered to be time-dependent. The concept of type 2, nonequilibrium sites, is assumed a first-order kinetic rate process as shown in equation 9 [27]:

$$\rho \frac{\partial S^k}{\partial t} = \alpha_k\, \rho [S^k_e - S^k] - \phi_k \qquad (9)$$

Where α_k= first-order rate constant describing the kinetics of the sorption process [T^{-1}]; S^k_e= sorbed concentration that would be reached at equilibrium with the liquid phase concentration [MM^{-1}]; ϕ_k= sink/source term that accounts for various zero- and first-order or other reactions at the kinetic sorption sites [ML^{-3}T^{-1}].

Two chemical nonequilibrium, miscible-displacement models were used by [40] to describe the 17β-estradiol sorption to the soil; one without transformations and the other with transformations.

However, physical and chemical nonequilibrium transport models could be occurring simultaneously at the two sites, on one hand chemical process of attachment/detachment could be responsible of one fraction of sorption sites, on the other; physical process of straining could be associated with the second fraction of sorption sites. Then the kinetic processes are described as follows [27]:

$$\rho \frac{\partial S_1^k}{\partial t} = K_{a1}\theta C - K_{d1}\rho S_1^k - \emptyset_{k1} \qquad (10)$$

$$\rho \frac{\partial S_2^k}{\partial t} = K_{a2}\theta C - K_{d2}\rho S_2^k - \emptyset_{k2} \qquad (11)$$

S_1^k,S_2^k = concentrations of the first and second fraction of kinetic sorption sites [MM^{-1}] respectively, K_{a1},K_{a2}= attachment coefficients for the first and second fraction of kinetic sorption sites [T^{-1}], respectively, K_{d1}, K_{d2}= detachment coefficients for the first and second fraction of kinetic sorption sites [T^{-1}], respectively, $\emptyset_{k1}$, $\emptyset_{k2}$= sink/source terms for the first and second fraction of kinetic sorption sites [T^{-1}], respectively.

[45-47] mentioned that the two kinetic sites might be used to describe different processes. While the first kinetic process could be used for attachment models, which successfully optimized the colloid transport data, the second kinetic process could simultaneously considers both chemical attachment and physical straining of colloids or pathogenic microorganisms. In addition of attachment and detachment and straining models, exclusion that modelled by adjusting transport parameters for colloid-accessible pore space where studied by [48].

III. IRRIGATION SCHEMES

Trees play a significant role in controlling the water and energy balance at the land-air surface. Both hydrological and tree responses are affected by the changing of soil water content, by regulate the stream flow transpiration rates, and ecosystem functions.

HYDRUS model allows simulating the relevant soil hydrodynamic processes in different irrigation schemes, such as pesticide transport processes, soil water redistribution and deep percolation, as well as water uptake by roots and the effects of soil water stress on tree transpiration.

As a result of application of pesticides to cultivated fields, pesticides have been detected in many aquifers and surface waters. Biodegradation and sorption kinetics seems to be the main process that controls pesticide fate through the unsaturated zone of soils [49]. However, rapid nonequilibrium flow through soil macropores can cause pesticide leaching to ground water before it can degrade or be adsorbed by the soil [50].

Pesticide leaching process is described as a complex process and it can be controlled by a range of soil and environmental conditions. Accordingly, many studies have demonstrated the fate and transport of a variety of pesticides in different soils.

HYDRUS model package has the ability to simulate solute movement in the vadose zone. In this model, first-order degradation and convection-dispersion equation is included and extended to calculate preferential transport of a parent pesticide and its metabolites formed [25].

Examples of HYDRUS applications that consider the simultaneous of fate and transportation of pesticide is given by [4]; [43]; [6] ;[51]; [8]; [52] and as discussed in solute transport above.

To prevent downward leaching and deep percolation, an application of water below the surface (drip irrigation system) can keep water and nutrients in the root zone [53]. However, this technology can lead to upward flow of water and solutes, which accumulate at the surface. On the other hand, when saline irrigation water was used as irrigation resource, salt also accumulated at the surface.

In order to deepen understanding of water and solute distribution patterns in root zone, field tests provide a more realistic assessment, but due to the high cost and time-consumption of the field experiments, the use of simulation models of water movement in the soil is highly recommended.

HYDRUS was used to model salt accumulation and salinity distribution from subsurface drip irrigation in the root zone [53, 54]. These studies showed that a better understanding of the processes that occur at the field scale, such as volumetric soil water content in root zone, root growth and distribution, and plant water uptake, is essential for model's ability to predict water and solute transport with drip irrigation. While [55] used HYDRUS to simulate the salinity distribution in and around the overlap zone (a region of confluence between each pair of emitters in which plants are grown).

Not only was the salinity distribution from drip irrigation in and around root zone was simulated using HYDRUS model, but also optimizing the operational parameters that are available to irrigators were simulated [56, 57]. However, there are limitations in these studies where the length of simulation was short and the absence of plant roots.

Another optimizing factor such as spatial distribution of water and solutes in the root zone, soil moisture under field, the effect of different installation geometries and main dimensions of the wetted soil volume surrounding the emitter during drip irrigation were also simulated by HYDRUS model [58–62].

Water uptake by plant and their spatial and temporal distribution, another irrigation schemes, found to be essential for both agricultural and hydrological viewpoint. Root water uptake patterns may employ a large degree of control on the water fluxes to the atmosphere and the ground water.

The result from [63] showed that water stress factor, actual root uptake with actual evapotranspiration play as key factors for accurate simulations. They coupled HYDRUS-1D and the crop growth model WOFOST to improve crop production prediction. Multidimensional root water uptake was studied by [64] using HYDRUS-2D. While three-dimensional HYDRUS models need spatial characterization of root water uptake data, where there is a lack of these data to support multidimensional root water uptake parameters [65]. However, a study by [66] evaluated spatial and temporal compensated and uncompensated root water uptake patterns of a flood-irrigated mature using HYDRUS (2D/3D).

IV. CONSTRUCTED WETLAND

Numerical modelling of subsurface flow constructed wetlands (CWs) gained increasing interest during the last years. CWs are engineered wastewater treatment and purification system with conditions found in natural environments; consequently, CWs is a complex system that is difficult to understand where the interaction between soil, vegetation, water and microorganisms are active in parallel and were they mutually influence each other.

Numerical simulators, on the one hand, represent valuable tools for analysing and improving our understanding the insight in dynamics and functioning of the complex CW system by governing the biological and chemical transformation and degradation process in detail. As these models are complex and therefore rather difficult to use there is, on the other hand, a need for simplified models for CW design.

CWs are generally categorized into surface flow and subsurface flow wetlands. Subsurface flow wetlands are the most common CWs type; such systems have been consistently effective in the removal of biochemical oxygen demand, suspended solids, and pathogenic organisms [67]. Past on the direction of water flow through the porous medium, subsurface flow CWs are further subdivided into horizontal flow (HF) and vertical flow (VF) systems.

HYDRUS-2D wetland module includes two biokinetic model formulations simulating reactive transport in CWs: CW2D and CWM1. While aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorous are taken into account in CW2D, aerobic, anoxic and anaerobic processes for organic matter, nitrogen, and sulphate are considered in CWM1. In order to obtain realistic predictions for the treatment efficiency of CWs, the HYDRUS implementation was able to simulate fixed biomass [68].

A comparison results for HF CWs using both CW2D and CWM1 modules showed that CWM1 produces more reasonable results than CW2D. That is may be because that CWM1 considers anaerobic degradation processes [68].

A study by [69] applied HYDRUS-2D software with CW2D to simulate the behaviours of both HF and VF pilot scale treating municipal wastewater. HYDRUS-2D software was applied for flow and single-solute transport, while tracer and chemical wastewater analyses were carried out to calibrate and validate the transport model. The multi-component reactive transport module CW2D was used to model the transformation and elimination processes of organic matter, nitrogen and phosphorus. Their results demonstrated that the modelling results adequately fit the experimental data for water flow, tracer and pollutant removal processes.

The variable chemical oxygen demand and ammonia inflow to the HFCWs was simulated using HYDRUS-CWM1 by [70]. While ammonia reduction in pilot scale storm water HF CWs was simulated in a study by [71] using HYDRUS-CW2D. Their results showed almost perfect agreement in pollutant removal efficiencies for both simulating and measuring data.

A difficult hydraulic characterization, due to the use of matrix of porous mineral material and organic matter as filter material in VF CW, is simulated successfully used HYDRUS-1D by [72].

The fate of nitrogen in VF CW using gravel treating directly domestic raw wastewater is simulated by [73] using CW2D. In their work, they measured values for the hydraulic parameters and the maximum autotrophic growth rate. Moreover, oxygen re-aeration rate and adsorption coefficients of ammonium were calibrated to reduce the difference between predictions and measurements.

The result from these studies showed that HYDRUS-CWM1 and HYDRUS-CW2D could be a powerful tool to simulate the response of HF and VF CWs under different conditions.

V. CONCLUSION

HYDRUS model is found to be a very attractive tool for analyzing different applications, which can conclude in below:

1. The HYDRUS model may be used to simulate not only one- and multi-dimensional water flow, solute transport in variably saturated media, the mean soil water content in the root zone, but also to increase our

understanding of the fundamental processes of transformation and elimination of pollutants in subsurface flow in constructed wetland.

2. While the classical model using Richards equation have proved to be useful for analyzing uniform water flow and solute transport, the traditional physical and chemical nonequilibrium models, to more complex dual-permeability models that consider both physical and chemical causes of nonequilibrium.
3. The most common applications of HYDRUS model can be described in three categories. The first one deals with transport of hormones, nitrogen explosive formulation pathogenic microorganisms and pesticide under variably saturated flow conditions. In this application, the chemical nonequilibrium transports have the ability to simulate processes such as attachment/detachment to the solid phase or gas-water interface, or straining.
4. The second group addresses water and solute distribution patterns in root zone, salt accumulation and salinity distribution from subsurface drip irrigation, optimizing the operational parameters that are available to irrigators and water uptake by plant to simulate by HYDRUS model.
5. Several more complex models and modules are being developed at present. For instance, the use of CW2D and CWM1code that couples the HYDRUS-2D water flow and solute transport model. Different studies used HYDRUS-CW2D or HYDRUS-CWM1to show the fate and transportation of nitrogen, ammonia, organic matter and phosphorus in subsurface flow constructed wetland.

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