Modelling and Simulation of Pollutant Transport in Porous Media—A Simulation and Validation Study

M. R. Dhanraj and A. Ganesha

Abstract In this paper, the transport of pollutants is simulated with COMSOL multi-physics in a transition-based cross-sectional model to trace the path and flow of pollutants after infiltration from the point of discharge of treated domestic sewage. The study is investigated using soil columns with known porosity and permeability and with various other boundary conditions. The solutions are tested using a finite-element numerical model built with COMSOL Multi-physics. It is found that the simulation model holds good in pollutant removal in comparison with the physical pilot scale model. It is also found that there is a strong correlation between the inlet and outlet parameters in removing the pollutants with naturally available media (soil). Also, the removal efficiency in BOD and COD in soil media is 54.54 mg/l and 50.13 mg/l respectively. The results of the reliability check also showed good agreement between the measured and the simulated value for both BOD and COD with ($R^2 = 0.83$), ($R^2 = 0.99$), respectively. Hence the results obtained from horizontal transport of pollutant is more significant.

Keywords Transport of diluted species (TDS) · Infiltration · Biochemical oxygen demand (BOD) · Chemical oxygen demand (COD)

1 Introduction

Water is the main source for any creatures to survive on the planet earth. In a country like India due to the diversified culture people are adopted to a different lifestyle. Due to the consistent increase in population growth, mostly in urban areas, the managing of wastewater has become a tedious process. The water demand is increasing day by day and generation of the wastewater is increasing, with the lack of proper management of wastewater disposal is a burning issue in almost all the cities in the present scenario. Adopting a systematic way to attain sustainability in the present scenario is very important due to the pollution, climate change, and deforestation the natural

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existing water sources are deteriorating day by day. In India presently, as per the estimation 61,754 million liters of water per day (MLD) of sewage is generated per day, 22,963 MLD of sewage is treated and 62% of sewage is discharged directly into the water bodies without the treatment. By 2025 demand for industry and domestic usage may increase to 29.2 BCM population is expected to cross the 1.5 billion mark by 2050 [1]. So therefore the aim is to utilize the treated sewage as an alternative source of the main source to replenish and conserve it for future purposes using artificial recharge technique. This may increase the efficiency in water use by the approach of conjunctive use of groundwater thereby reducing the demand for freshwater sources. Though we have adopted the practice of stormwater recharge, the significant effects are still unknown after recharge for seasonal emerging pollutants. Water reuse plays a prominent role in future development, there are many forms of disposal of treated sewage the disposal is done either on surface or subsurface. Since because of the mandatory rules from the state pollution control board the disposal of the treated sewage has become a very big hectic planning. Zero effluent discharge for commercial, gated communities, institutions might be more troublesome to overcome such circumstances. Future this would not only be domestic, but even industry also treated waste would face problem is disposal of such a large quantity of water generated after treatment. A study was conducted to anticipate the reliability of the model using comsol to predict the outcome using the 2D model and its effectiveness for effective examination [2]. So, this research would give a solution to such problem of disposal which mega industries and domestic treatment plants are facing today. The amount of energy spent on treatment must reward back by some means, or in another way the treated sewage has to be utilized completely. There are many situations where the treated wastewater may be used completely, in developed countries after the tertiary treatment. But the stigma toward the developing countries for recycling and reuse is being present, due to a lack of concern. Therefore, adopting the groundwater recharge will overcome the disposal problem and also helps in replenishing as well as the withdrawal of water at any point in time for irrigation purposes [3]. For the present study, the water is being considered from the secondary clarifier, the considerations are being shown in the flowchart along with the treatment process (Fig. 1).

Analyzing the risk associated with the contamination of soils and identification of the sources of its propagation and fate processes is needed [4]. According to Jiang and Chen [5], their study suggested that both the physical (advection, diffusion,

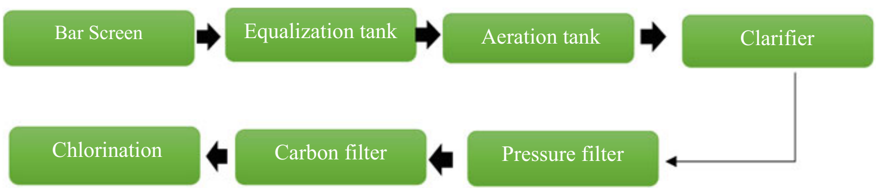


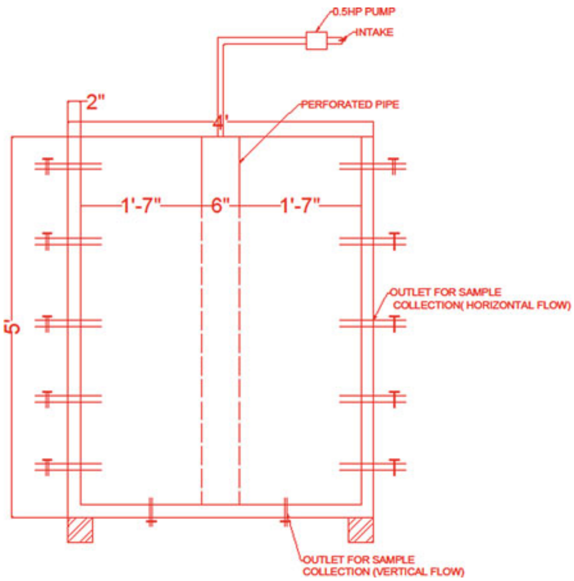
Fig. 1 Flowchart of STP

dispersion) and reaction (adsorption and degradation) process controlling contaminant transport should be analyzed in the numerical model. Lie et al. [6] in their study solved the one-dimensional advection-dispersion equation in a heterogeneous porous media coupled linear and nonlinear sorption or decay using the generalized integral transforms technique. Gao et al. [7] studied one-dimensional model convective diffusion in the soil contaminant transport subjected to time-dependent boundary conditions. Comsol multi-physics software based on a partial differential equation. It is to solve the linear or nonlinear problem, and the steady-state or transient problem which was related to geometry mode of 1D, 2D, 3D problems. Comsol was mainly used to study at present in earth science research of groundwater flow and the soil water infiltration applied the software to simulate the migration of pollutant in soil and unverified the applicability of comsol to simulate soil solute transport. In this study based on comsol 5.5, 3d transient cross-sectional models were used to investigate water and solute transport in the soil column denoting variable sand column forms. These research gap findings with horizontal transport of pollutants would help generate the baseline data on removal of pollutant concentration after infiltration and serve the purpose of disposal after the treatment. Also, this will help to find the distance of pollutant transport from the point of discharge in the same directions.

2 Methodology

The working model is made up of concrete with a diameter of 1.2 m and a height of 1.5 m consists of a perforated pipe at the center with a diameter of 0.15 m. This center pipe acts as a well for recharge, and it also includes outlets for sampling. The water is pumped from the clarifier using a 0.5HP pump with a controlled flow to the recharge well. The water is being allowed to percolate and tried with two types of media. The water which comes out of the model is tested for various parameters such as BOD, COD and then checked for efficiency under inlet flow conditions, with the same existing media of sand, followed by the same parameters. The water sample is collected using polyethylene cans. Further, it is being transported and stored in a deep freezer at 4 °C for further analysis. A total of 50 samples were collected to check the consistency in the media used for the study. BOD and COD are the two important water quality parameters required to assess the waste assimilative capacity in the soil media [8]. BOD is employed as a gross measure of the oxygen demanding potential of the effluent. Assimilative capacity varies following variations in hydrodynamic conditions and other ecological processes. COD is employed as an indicative measure of the amount of oxygen that can be consumed by reactions in a measured solution (Fig. 2).

Fig. 2 Pilot-scale model



2.1 BOD and COD Analysis

The analysis of water samples is done in the laboratory by collecting the water samples from both inlet and outlet. The collected water samples are stored in polyethylene bottles and stored at 5 °C while transportation. BOD_5 @20 °C is measured by the dilution method. Samples have undergone three trials and the best two values have been considered. The COD of the water is measured by the closed reflux method using potassium dichromate by colorimetric method (IS 10500:2012) (Fig. 3).

2.2 Model Characteristics

COMSOL Multi-physics modules were used to simulate and trace the pollutant transport in subsurface porous soil media. To verify the efficiency of the simulated model, experimental data is required. The COSMOL program, which simulates the velocity, pressure head, and the concentration distribution based on the boundary condition using an implicit iteration solution, has been used in developing and understanding the efficient working conditions of the model. A detailed description of the model is presented on the COMSOL website. In the following sections, a brief description of the main features of the model is presented (Tables 1 and 2).

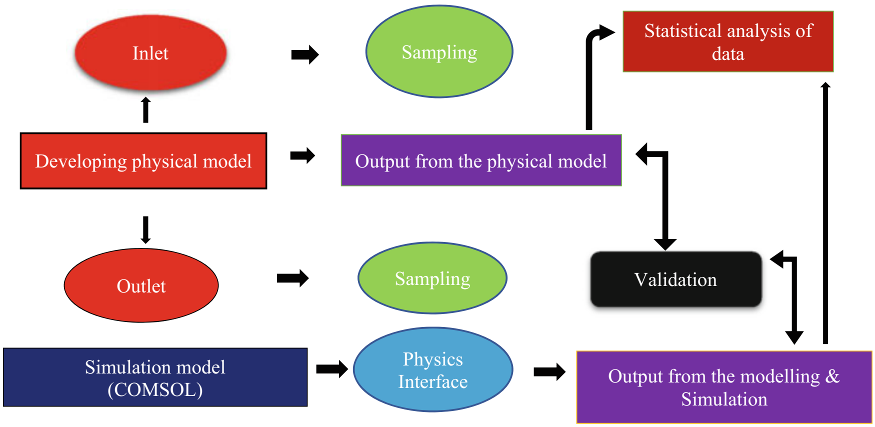


Fig. 3 Methodological flowchart of the study

Table 1 Boundary and initial conditions

Parameters	Soil
Permeability (cm/sec)	1.79×10^{-5}
Density (gm/cm$^{3)}$	1.46
Specific gravity	2.54
Grain size (uniformity coefficient)	1.44
Porosity	0.3

Table 2 Flow measurements

Parameters	Value
Velocity (m/s)	0.28
Discharge (m^3/s)	0.044
Hydraulic head (m)	1.5
Pressure head (m)	1.38

2.3 Model Calibration and Governing Equations

Model calibration is a trial-and-error adjustment of parameters until the model solution matches the field physical model. In general, the calibration aims to design a steady state model for head distributions to be used as an initial condition for a transient state simulation after applying and trying different states of scenarios on it. Model calibration also includes a successive refinement for model input parameters from the initial condition to improve the fit between observed input and model predicted results. The calibration procedure typically begins with the definition of parameters also based on the availability of data with an initial conceptual model of the hydrogeology systems. The parameters chosen for the calibration process include soil permeability, porosity and materials used for the study purpose. Several adjustments to the calibration parameters were made until the final calibration was achieved. Once calibrated then the physics used for the study purpose is applied to the model.

Phase transport in porous media for study controlled under time-dependent conditions is given by

$$\frac{\partial \varepsilon_p \rho_{s_i} s_i}{\partial t} + \nabla \cdot \mathbf{N}_i = 0 \tag{1}$$

By assuming the time-dependent equation this will be

$$\mathbf{N}_i = \rho_{s_i} \mathbf{u}_i, \ \mathbf{u}_i = -\frac{\kappa_{rs_i}}{\mu_{s_i}} \kappa \nabla \rho_{s_i}$$

When the outflow is set for the model $-\mathbf{n} \cdot \mathbf{N}_i = -\mathbf{n} \cdot \left(\rho_{s_i} \mathbf{u}_i\right)$.

3 Results and Discussion

See Tables 3 and 4.

3.1 COMSOL Multi-physics for Simulation and Modelling

This study traced the contaminant transport in a horizontal direction and analyzed it using a 2D-model transport of pollutant in porous media with controlled discharge using COMSOL multi-physics created with soil matrix for water recharge of treated domestic sewage. The study's objective is to understand the concentration distribution in the saturated porous media of the system. Based on the different time the variations in the concentration is observed at the Outlet. A study using COMSOL multi-physics software for the Artificial recharge in Jordon compares the measured and the software modeling (Azad et al. 2010). The validation work has applied the same approach. A study was conducted in the vadose zone to model the solute transport and their travel times toward groundwater bodies. The study to understand the impact of the unique state of soil in terms of spatial infiltration of solute-rich water [9] is needed in COMSOL to trace the pollutant transport in soil concerning time (Fig. 4).

Table 3 Summary of the BOD results from the physical model

Parameter (mg/l)	Influent (mg/l)	Measuring range	Saturation time (min)	Effluent (mg/l)	Mean	Samples numbers	SD	SEM	Median
BOD_5 @20 °C	30.06	30	30	15.96	10.26	10	7.34	2.32	6.20
COD	94.66	30	30	56.37	66.93	10	43.61	10.90	46.3

Table 4 Summary of the BOD results from the simulation model

Parameter (mg/l)	Influent (mg/l)	Measuring range	Saturation time (min)	Effluent (mg/l)	Mean	Samples number	SD	SEM	Median
BOD_5 @20 °C	30.06	30	30	23	9.8	10	6.66	2.10	6.20
COD	94.66	30	30	39.06	39.05	10	22.62	5.19	26.2

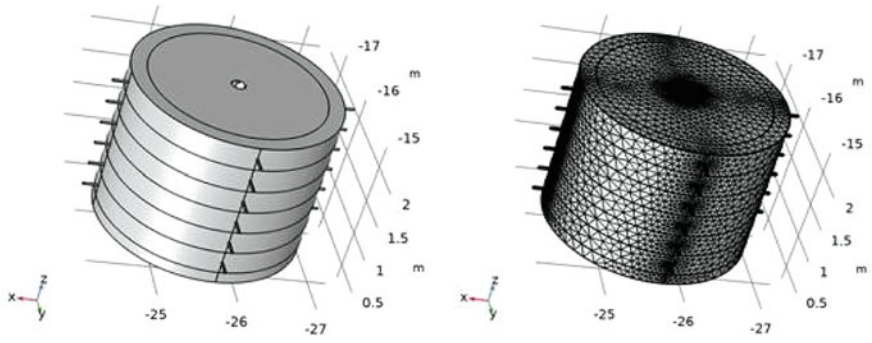


Fig. 4 Physical model developed using COMSOL

3.2 *Performance Measures Between Measured Values and Simulated Values for BOD and COD*

There is a significant reduction in the output of the model after the horizontal movement. The presented graph shows the variations at the inlet and outlet from the physical and simulation model of the study.

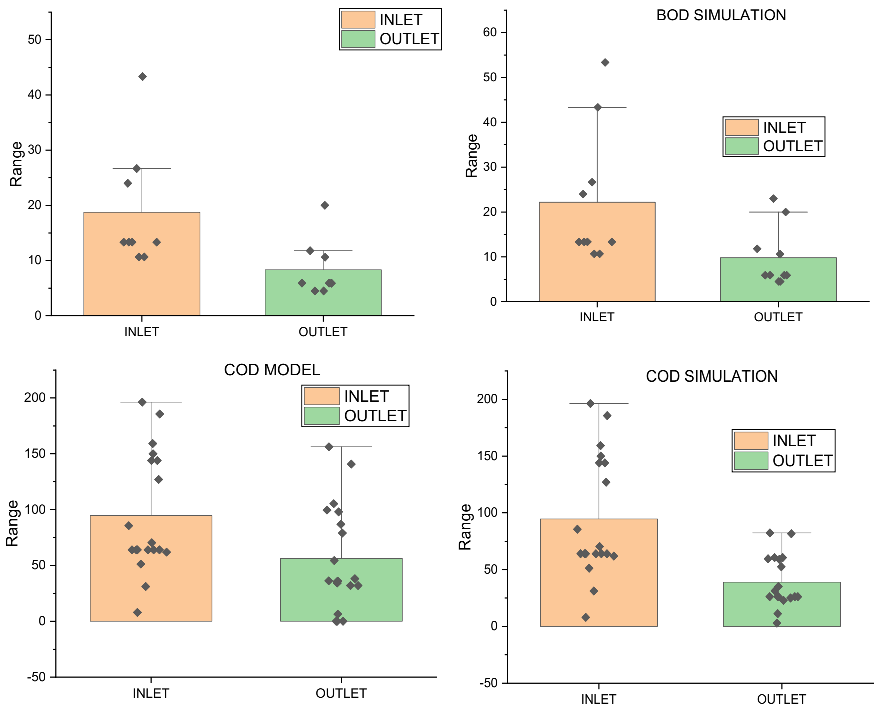


Fig. 5 Validation of pollutant transport in horizontal direction based on transient condition

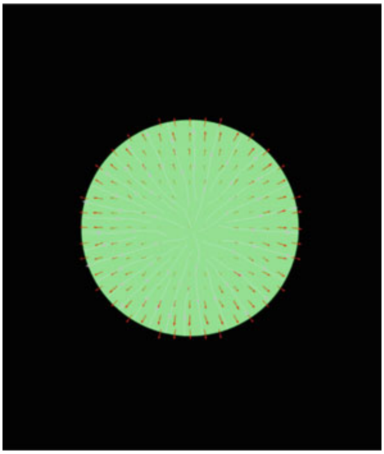
3.3 Particle Trace Trajectories for Validation Using Simulation

This Figure clearly shows the transport of pollutant in the horizontal direction. The distribution of concentration is observed at a time interval of $t = 30$ min (Fig. 5).

3.4 Dispersion of Pollutants

Horizontal displacement of the pollutant is not introspected well because the focus toward the recharge was always toward the vertical transport of species. Here Fig. 6 shows the horizontal transport from the point of discharge in different directions, this will be helpful in tracing the pollutant from the point of discharge.

Fig. 6 Particle dispersion in different directions

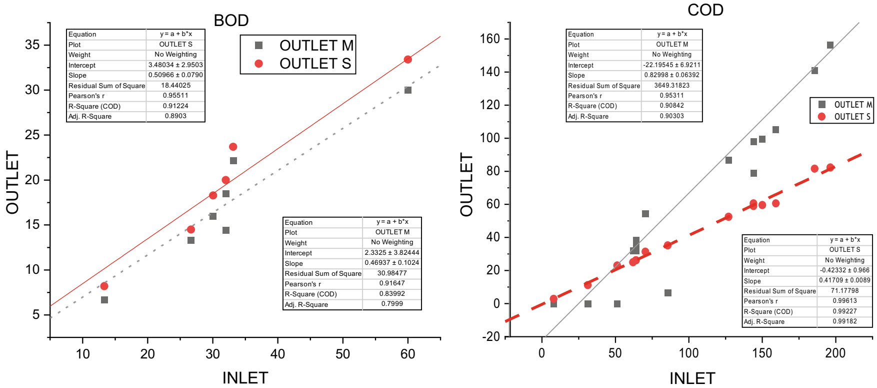


3.5 *Numerical Analysis of BOD and COD Profiles*

For data consisting of x and y subjected to each x corresponds to y and vice-versa which causes at least two distinct straight lines, correlation analysis, and various significance tests. The curve fitting is standardized with 95% confidence level. Therefore, from this analysis, the results obtained from the physical model and simulation model have a strong correlation with an R^2 value of 0.8 or more with good significance. Also, for all the measured value between the inlet and outlet samples has an R^2 value of 0.8 or more for the simulation value with good significance. The below-mentioned chart represents the graph drawn between the Inlet (influent) and Outlet (effluent) of measured value/Simulated value for soil media (Graph 1).

4 Statistical Analysis of Models

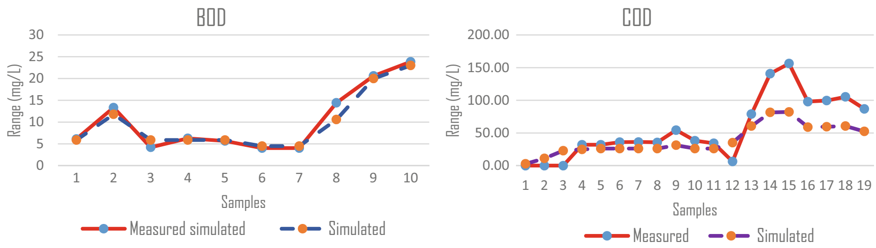
See Table 5.



Graph 1 Regression analysis of BOD and COD

Table 5 Regression

Models	Parameter	R^2
Measured value	BOD_5	0.91
Simulated value	BOD_5	0.83
Measured value	COD	0.90
Simulated value	COD	0.99



Graph 2 Validation between measured and simulated

4.1 Validation of the Results

In this paper, to tackle the common issues in the prediction process of simulation models the COMSOL multi-physics is used and validated with the measured values which are done on a pilot scale in the college campus. The main objective of the study was to prove the lateral movement in soil porous media. The forecasted data of pollutants for BOD and COD was measured for a year from January to December 2020. From the obtained results it is found that the measured and simulated are in good agreement with less than 10% error. The results from the simulation and measure are represented further using statistical analysis. Also, from the statistical analysis, it is found that there is a strong acceptance of data between measured data from the simulation model (Graph 2).

5 Discussion

The Effluent variations were closely observed and it is found that the influent has an impact and primly effected the target value at the Effluent. The comparison pertaining to pollutant removal efficiency between the measured and the Simulation holds good is contributing a good amount of pollutant removal after infiltration. The BOD removal concept remains the same as the water gets recharged. The retention time attained during transport reduces the pollutant concentration in the outlet and also in the simulation model. The chemical oxidations also go well during the horizontal infiltration after the recharge, which is also closely observed in BOD due to the relationship between BOD and COD. Therefore, the organic matter removal also takes place in the horizontal direction resulting in the impact of artificial recharge.

6 Conclusion

Artificial recharge and its removal of pollutants is the simplest form of disposal of treated domestic sewage. Where a high-quality consistent value is required. It is found that the permeability of the soil medium has a direct influence on the removal efficiency. The BOD removal is found to be 54.54 mg/l and COD removal is 50.13 mg/l. Also, the results obtained from the physical model and simulation model have a very strong correlation, i.e., R-square = $(0.7 < |r| \leqq 1)$. The model can also be used to understand the pollutant travel distance for zero transport from the point of discharge. Therefore, artificial recharge of treated domestic sewage has an impact on unconfined aquifer with reduction of pollutant concentration from influent to effluent and hence artificial recharge can be used as a method of disposal for treated domestic sewage (used after secondary treatment). However, as a safety measure, regular monitoring of the recharge water quality and ground water quality in the surrounding area of recharge site is essential.

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