

## EXPERIMENTAL AND CFD- SIMULATION OF POLLUTANT TRANSPORT IN POROUS MEDIA

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**Abstract:** Efforts were made in this search to design a physical and computer model using the CFD techniques to simulate the problem of transporting pollutants through a porous media in unsteady state case. A physical model was built to measure the transmission of a copper nitrate pollutant at an initial concentration of 25 mg/l in a medium consists of (sand + gravel) and study the movement of the pollutant through. Then the results of the pollutant transport through used in the physical model were entered as entry data to the CFD simulated model using COMSOL 5.4. Software. The results of the CFD simulated model showed that the change in the inlet velocity to more than 20% of the initial velocity increases the pollutant concentration and reduces the time wanted to reach the highest value of the pollutant, while reducing the inlet velocity to less than 20% of the initial velocity, cause to decrease the concentration and increase the time to reach the highest pollutant value. When changing the porosity by (30%, -15%) of the initial porosity, it was noticed that increasing the porosity value reduces the pollutant concentration and increases the time required to reach the highest value of the pollutant. while when the porosity decreases to 15% of the initial porosity, the concentration increases the time decreases to reach the highest value of the pollutant at all control points. The adsorption factor has a noticeable effect on the emergence of the pollutant, while the temperature change was almost imperceptible for all degrees. However, the results of laboratory work were compared with the results of the CFD simulated model, which showed a good match between them.

**Keywords:** Soil contaminant, porous media, contaminant numerical modeling, FCD model.

### 1. Introduction

One of the main causes of pollution of water, soil and air is the rapid development of industrial activities over the past few decades, according to the reports of the World Health Organization 1984 the most important minerals are lead, cadmium, copper, cobalt, aluminum, chromium, manganese, iron and mercury. One of the most important areas of research and development is the development of low-cost adsorbents to reduce toxic ions. Various treatment techniques including adsorption, sedimentation, and ion exchange have been used to remove or reduce toxic ions concentrations in the wastewater. The removal of heavy metals from wastewater and runoff from landfills has become a very important environmental issue in all aspects. Water and soil adsorption is one of the most important methods for removing pollutants from water. A number of low-cost

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adsorbents have been reported to remove heavy metals (ions) from aqueous solutions. Activated charcoal is highly effective in removing metal ions, but it is readily soluble in very low and high pH conditions [1]. There are many adsorbents that are low in cost, such as waste agricultural products, soils of various types and natural clays and low-quality raw materials [2,3,4]. And industrial wastes that are formed after and during the production process [3,5] as potential adsorbents to dilute poisonous cations from water levels. The presence of heavy elements in soil additions for agricultural purposes or landfill waste in addition to heavy elements added to fertilizers and pesticides and what falls directly from the air or rain as a result of air pollution from the gases emitted from power plants and factories and car exhaust are all sources of soil pollution with heavy elements such as copper [6]. Soil susceptibility to heavy element adsorption is affected by several factors including different soil tissue components and a Installation of ion balance solution [7,8]. The transfer of pollutants through different soils or various porous media is one of the many problems that the environment is exposed to at this time. To understand the process of transporting different pollutants, especially heavy metals, through different types of porous media, many researchers have made experimental investigations through laboratory and real-life studies at the work site. Many researchers are working on analytical and numerical studies to simulate the movement and transport of pollutants in soil and groundwater. With the introduction of high-energy computers, digital modeling has taken a broad base and is in fact very important in this matter. Mathematical models are very good techniques for indicating the estimated amount of dissolved pollutant and its quantity after it is transported in soil, porous media, or underground water originating from factories and lands Agro-composting [9].The

researchers used the green process method to generate 1D, 2D and 3D limited resources with in aquifers of finite depth [10]. The researchers worked out an analytical solution to calculate the solute transport of a contaminant in a 3D form using decomposition in a vertical plane source of a constant concentration [11]. Other researchers presented a solution to two models considered to be elementary to the diffusion flow for a quantity of the distributions of primary solute and solute concentrations with fixed boundaries [12]. Other researchers developed the Dominica 3D solution (1987) and have demonstrated that if there is a zero value for linear dispersion, the solution provides suitable analytical results [13,14]. Currently, it turns out that numerical models are away to typical resolve the tricky and complex outlines states of the problems of groundwater and subterranean soil. Researchers have used the particle force interchange way to propose a numeral model that is of a two-dimensional type to passively simulate the problem of transporting pollutants [15,17]. The way of fabrication for modeling in unsaturated and saturated porous medium has also used to simulate a three-dimensional transition of dissolved contaminants below the surface [18]. The general structure of the finite difference method of two-dimensional flow and dispersion equations was examined to find a solution to the problem of pollutant transport through the soil [19]. The transport of pollutants by 3D surface was also simulated using the Lagrangian - Eulerian bounded item method [20]. A new class group of algorithms was provided to solve the problem of pollutants by solving two-dimensional transient scattering models [21]. A numerical and numerical model was made to solve problems of adsorption, dispersion and convection the model problem is well simulated [22]. Contaminant transport in compressible porous media was also studied through

experimental and numerical research by other authors [23]. Has been defined a numerical model and laboratory works using a conservative tracers, the results indicated that a better experimental set-up and a numerical assessment method were established [24]. Laboratory experiments with a multi-tracer bench have been used to simulate and design a pore scale for various homogeneous porous media and relating to both unsaturated and saturated porous media [25]. A large amount of research work has been submitted for experimental investigation or by using the analytical solution and numerical method to solve the problem of pollutants and simulations [26]. The rationality of the adsorption coefficient approach of Triassic sandstones - a common type of aquifer around the world - is better studied to better measure bonding with metal ions [27]. Computational fluid dynamics frames are proposed with soil, and it is evident that the interaction between tubes and sand can be successfully analyzed by modeling the fluid with a single phase system in soil [28]. Introduced [29] a new non-interlaced approach to artificial intelligence to model pollutant transport in porous media, where the model proposed a solution to pollutant transport using computational fluid dynamics. In this research was evaluated the absorption properties of atrazine using a linear one and nonlinear isothermal formulas with results of adsorption data from the laboratory formula, the results indicated that the behavior of both organic matter and the adsorption coefficient is linear in the soil [30]. Researchers have studied pollutant transport simulation under hydraulic structures using a physical model and CFD simulation was also studied using physical and CFD models the results of that study indicated that the adsorption process plays a large role in these problems for all the cases studied, the two models turned out to be a very good results [16].

The main objective of this paper is to study the state of unstable pollutant transport across porous media, taking into consideration the effect of hydraulic properties and properties of soil used as a porous medium on altering pollutant concentration and pollutant distribution across media. Also noted that all results and solutions obtained in this research were conducted on the basis of a saturation of water pores.

## **2. Description of Copper Transmission and Adsorption Motion**

Copper is one of the toxic heavy metals that affect humans by its effect on soil and water. In this research, we drew a picture of the ability to adsorb copper by the sandy medium with gravel and also take a look at its interaction with agricultural soils that contain organic compost. A study of what happens to a concentration when it is moving and moving within a certain distance copper is a toxic heavy metal that affects humans through its influence on soil and water. In this paper, the efforts was conducted to study the ability of the simulation the problem of the absorb the copper in the sandy gravel medium using the CFD techniques with the help of COMSOL 5.4 software.

## **2. Material and Method**

### **2.1 Laboratory Model**

The physical model is designed to study the transport and absorption of copper through the porous media of its component materials, which thus simulates the adsorption of copper and takes an idea of its effect on agricultural lands and lands whose components are mainly gravel and sand, such as Iraqi lands, and a statement of the ability of these soils to adsorption. It consists of a main polyethylene tube with a length of 3 meters and a diameter of 4 cm installed on an iron stand with a height of 150

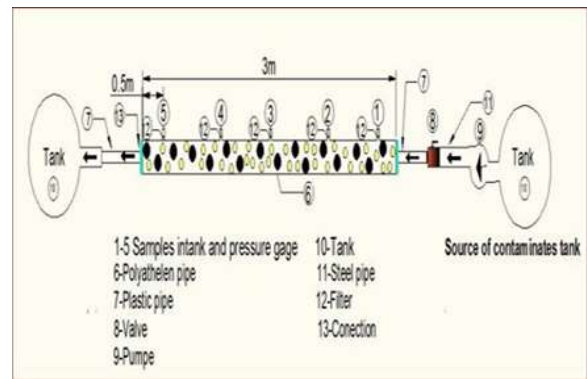
cm. At each 50 cm on the pipe there is a small hole connected to a small polyethylene tube of 3 cm length and 12 mm diameter for sampling collection and water pressure measurements using a mercury-sensitive type pressure gauge to know the pressure distribution of the water passing through the porous medium inside the main tube of the system. The polluted water was supplied to the system from an elevated tank of a 250 liter tank using a 30 l/min pump connected to the inlet of the main tube by a plastic hose. For the outside, the tube was provided with a filter to prevent penetration of the porous medium. Also, the disposal flow from the outlet was collected in another 250 liter tank capacity, see Fig.1, Fig.2 for more explanation and details.



Figure 1. Physical model



(a)



(b)

Figure 2. Representation of the physical model (a) General system layout (b) Main polyethylene tube

2.2 Porous Media

Soil sample was collected to fill in a main pipe by a crushed sand and gravel. Sandy soil was obtained from sand used in construction work. The gravel is obtained from the job site of the type crushed stone. The sample was washed with distilled water and placed in a drying oven for two hours at a temperature of 300 ° C. Then 60% of the gravel was mixed with 40% of the passing sandy soil from a 2 mm sieve to less than 0.75 mm to obtain a working soil model , see fig.3. Then large quantities of these percentages were prepared for the purpose of preparing them for sieve analysis in the Central Soil Laboratory. Fig. 4 represents the results of the sieving analysis for the gradient of grains. Also, some essential laboratory tests were performed for porosity, mass density, and measuring the surface area for minutes, as shown in Table 1.

Table 1. Properties of soil sample.

Porosity	0.32
Bulk Density (kg/m <sup>3</sup> )	1587
Surface area m <sup>2</sup> /g	2.673
Particle Size Distribution	0.61
Mean grain size d <sub>50</sub> (mm)	2
Uniformity coefficient	3.93
Adsorption isotherm m <sup>3</sup> /kg	0.003
Coefficient of hydraulic	0.0074
Conductivity (m/s)	
Tissue class	Sand gravel



Figure 3. The soil model

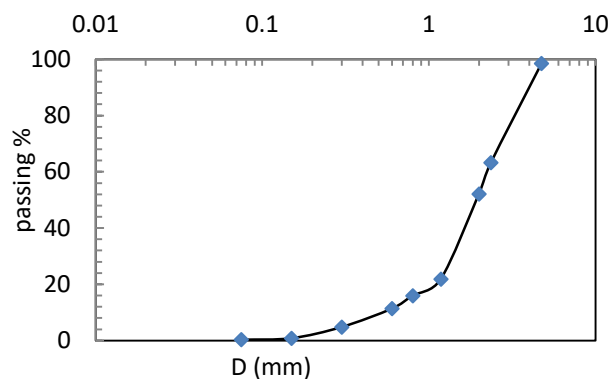


Figure 4. Sieve analysis test

### 2.3 Contaminated Water Preparing

Aqueous blue copper nitrate  $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$  was used as a heavy metal contaminating soil. Where the contaminated water was prepared with a weight of 26.6 g of aqueous copper blue nitrate by a sensitive balance, then it was added to a tank filled with tap water of 250L capacity with a pH 6 and a temperature of 13 degrees Celsius and the water was mixed with copper nitrate for 10 minutes to be completely dissolved in order to get A pollutant at a concentration of 25 mg/L aqueous copper blue nitrate.

### 2.4 Adsorption Coefficient Estimation

The adsorption coefficient is the ratio between the concentrations of the primary pollutant when

it is passed into the soil and its percentage in the soil after moving for a certain distance or interacting with the soil for a affective phase of time, as time is an influencing factor, that is, the extent to which the pollutants are distributed in the soil, [31]. The copper ion is absorbed from its aqueous solutions using a batch method using (0.5 grams) of soil consisting of gravel and sand by adding 40 ml of the prepared solution consisting of different concentrations of copper ranging. From (10, 20, 30, 40, 50) mg/l with a pH of 6. The samples were incubated in a centrifuge and run at 300 rpm for 3 hours, then the samples were filtered with filter paper (Watt Man No. 42). After that, the concentration of the remaining copper in the sample was measured using atomic spectroscopy in the laboratories of the Iraqi Ministry of Science to calculate the amount of copper remaining in the water sample after its incubation with the soil. These experiments were used to calculate the coefficient of adsorption ( $K_d$ ) and also to take an idea of the absorption capacity of copper from its aqueous solutions by the soil used in this research. The adsorption percentage and the values of the distribution coefficient were found after knowing the copper ion concentration of a residue in an aqueous solution after treatment. Samples were taken from the solutions and examined in the atomic flame device to find the residual copper concentration ( $C_e$ ), and then the equilibrium concentration ( $q$ ) is calculated through the following equations (1). The average  $K_d$  value represents the gradient of the best fit line of the equilibrium concentration  $q$  verse the final concentration of copper ion  $C_e$ .

$$q = ((C_i - C_e) / W) * V \quad (1)$$

$$k_d = \frac{\Delta q}{\Delta C_e} \quad (2)$$

$q$  Equilibrium concentration, mg/g

$C_i$  Primary concentration of copper ion, mg/l

$C_e$  Final concentration of copper ion, mg/l

$K_d$  Coefficient of adsorption, l/g



V The volume of copper ion solution, ml  
W Soil weight

### 3. CFD Simulation Model

Mathematical modeling can be used to sense, forecast & improve flow conditions in closed and open systems. Mathematical modeling is used in many environmental issues, as it has been used in gas in traffic road flow modeling, and the results showed a good match with the physical model [32]. The results of the comparison with the prepared statistics showed a good match in predicting the transmission of new diseases as Covid 19, using dynamic modeling [33]. The CFD technique was also used to model the airflow containing three pollutants; it was communicated in one direction with the CFD model. Physical verification was achieved on the model that was designed as an air filter. The validated model was used to predict the effect of 3D pore geometry on pollutant mass transfer in the gas phase using cfd [34]. In our research, simulations were used to represent the transport of pollutants through sandy porous media. A two-dimensional CFD model was constructed by COMSOL software to match the dimensions used in the experimental work of the physical model the flow is considered unsteady state condition through a saturated homogeneous soil. In fact, two types of flow are encountered in this problem as follows.

#### 3.1 Porous Subdomain

In this type of flow, Brinkmann's equations together with Forchimer's equation define the flow after correcting the flow using the following equations, [35].

$$\frac{\mu}{k} \mathbf{u} = \nabla \cdot \left[ -p \mathbf{I} + \frac{\mu}{\epsilon} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right] - \frac{\rho \epsilon C_f}{\sqrt{k}} \mathbf{u} |\mathbf{u}| \quad (3)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (4)$$

$$C_f = \frac{1.75}{\sqrt{150 n^3}} \quad (5)$$

$\mu$  The active Viscosity (Pa.s)

$u$  The Velocity in the porous media (m/s)  
 $\rho$  The fluid's density (kg /m<sup>3</sup>)  
 $p$  The pressure (Pa).  
 $k$  The permeability of the porous medium (m<sup>2</sup>)  
 $n$  The porosity  
 $C_f$  Friction coefficient

#### 3.2 Type Flux out of Porous Media (Advective and Spared Transfer)

Contaminated material gets into the groundwater by diffusion that results from the groundwater flow scattering due to the process of mechanical jumbled and diffusion that is partial and residual of the pollutants after the adsorption process. The mathematical relationship between these operations will be like this:

$$\frac{\partial}{\partial x} (uc) + R \frac{\partial c}{\partial t} + \frac{\partial}{\partial y} (vc) = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + r + s \quad (6)$$

$$R = n + \rho Kd \quad (7)$$

$c$ : Concentration of contaminants, Kg/m<sup>3</sup>

$u$ : Velocity field in the x- direction, m/s

$v$ : Velocity field in the y- direction, m/s

$D_x$ : Coefficient of dispersion in the x- direction, (m<sup>2</sup>/s)

$D_y$ : Coefficient of dispersion in the y- direction (m<sup>2</sup>/s)

$r$ : Average of engender, function of  $c$

$s$ : Rate of external source, aim of  $C$

$R$ : Residues resulting from its absorption

$n$ : Porosity

$Kd$ : Adsorption isotherm (kg/m<sup>3</sup>)

$\rho$ : The density kg/m<sup>3</sup>

These partial differential equations, have been solved. From (3) to (7) depending on CFD technologies. Among the many software and Available programming for these purposes, the work here has been done in COMSOL Multiphasic version 5.4. Already pre-defined with multi-physics interface types and porous

media streams, this complex dual-flow system is intended to make this complex dual-flow system easy to set up, apply and fix.

### 3.3 Initial Limitations and Conditions

The boundary and premier state were convinced by the point:

For entry,  $u = V_0$  and  $C = C_0$

For exit,  $P = 0$ ,  $(\nabla \cdot u + (\nabla \cdot u) \cdot T) = 0$ , pressure and no sticky stress.

To all tube wall, the pipe was set as no-slip wall boundary conditions

Initial value,  $u = 0$  and  $C(x, y) = 0$  at time  $t = 0$ .

The CFD model has a physical control mesh of extremely coarse type with a gross number items of 31<sup>9</sup> and edge items of 814, see Fig. 5 (a) and (b).

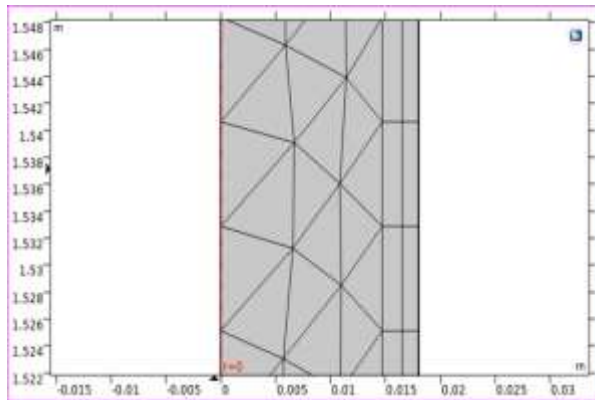


Figure 5. Simulated model design, control mesh

Also, It was considered that  $r = f(c)$  and  $s = g(c)$ . The rate of generation ( $r$ ) is considered to represent the effect of the chemical properties between the copper and the soil. While, the rate of external source ( $s$ ) is assumed to consider the effect of the sedimentation of the copper in soil where the soil will play a filter role against the contaminates transport. However, function  $g$  was assumed to be zero since there is no external source. While, the function  $f$  is estimated to be  $r = -0.006 c^2$ . This was done assuming several trials forms for  $r$  in the simulated model until gain the optimum results that provides the minimum differences between the actual results and the results of CFD model.

To verify the CFD emulation model, the results of the computational sample will be provided

using the same geometry and entry data used in the physical model. Then a comparison is made between the practical results and the results of the Computational fluid dynamics simulated sample in order to discussed and determine whether the CFD model is able to be considered to predict the required results of such problems suitable to be used for other cases or not.

## 4. Results and discussion

### 4.1 Result of Adsorption Factor (Kd)

Fig. 6 shows the value of the adsorption factor ( $K_d$ ) estimated experimentally as previously explained to be about (0.003 l/g). A rather small percentage is considered because the sample contains a quantity of sand that is considered an inert material and does not contain effective sites for adsorption or interaction with the pollutant to be removed from its aqueous solution. The effectiveness of the distributing factor is important in the process of transporting or retaining pollutants in the soil. The study of the adsorption factor ( $K_d$ ) plays an important role in taking a typical idea of the transmission process and in deducing the means that are the easiest transmission of pollutants than others. The absorption capacity of the soil increases with the increase of fine particles, especially the clay minerals, where clay minerals play an important role in a high capacity for adsorption. The internal as well as the exchange with the external surfaces of the sites with permanent negative charges. If the model contains organic matter, which is characterized by its containment of carboxyl groups, it contributes to the retention of contaminated [35]. As for sand, most of the silica components are characterized by few ions on their surface that may interact with the pollutant and lead to its removal. The surface area also in it has an important impact the adsorption process of the pollutant on the surface of the soil particles. So,

the surface area of the surface sand particles was equal to 2.673 m<sup>2</sup>/g. Therefore, the adsorption process was less when compared to the adsorption process for other soil particles.

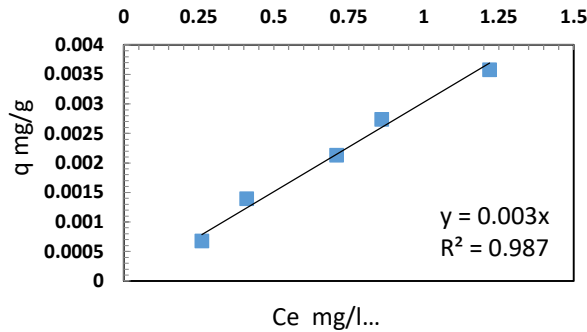


Figure 6. Coefficient of adsorption factor kd

#### 4.2 Simulation and Verification Model

A mathematical model was designed to simulate the transmission of pollutants through the models used in this study using COMSOL 5.4 software. Where all the required data provided to the CFD simulated model were obtained from laboratory experimental work and typical to the geometry and boundary condition of the physical model, see Fig.7 and Table 2.

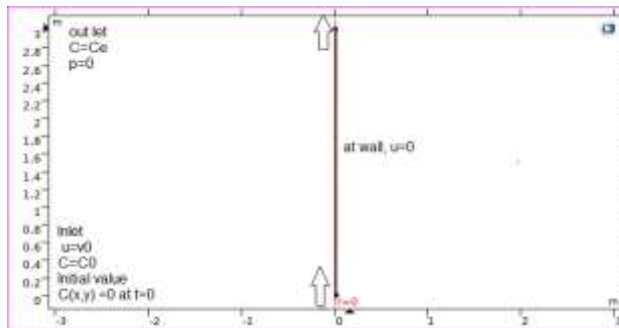


Figure 7. Geometry of the physical model used CFD simulation

Table 2. Data entered to the CFD simulated model's parameters

Name	Value	Description
T <sub>iso</sub>	300 K	Temperature
k <sub>f</sub>	0.006	constant
ro	0.018 m	Raduise
z <sub>1</sub>	0.01 m	inlet part
z <sub>2</sub>	3 m	Catalyst part
z <sub>3</sub>	0.01 m	outlet part
eps <sub>p2</sub>	0.32	porosity

v0	0.0065	inlet velocity (m/s)
Cf	0.789	Friction coefficient
fs	1	Switch for Forchheimer
kappa2	7.566E-10	Permeability m <sup>2</sup>
kd	0.003 m <sup>3</sup> /kg	Adsorption isotherm
rof	1000 kg/m <sup>3</sup>	fluid density
ros	1587 kg/m <sup>3</sup>	fluid soil
segx	0.5 m	segements for points
C <sub>t</sub>	0.395	Ce at tank

Fig.8 shown the results of the simulated sample for the values of the concentrations at the five control points, while Fig.9 shows a comparison between the same results with the contradictory results obtained in a laboratory using the physical model. As the figures indicate, the concentrations decrease as we move away from a source of contamination, due to the adsorption processes the soil particles that adsorb the pollutants, the longer the distance or the longer the detention period.

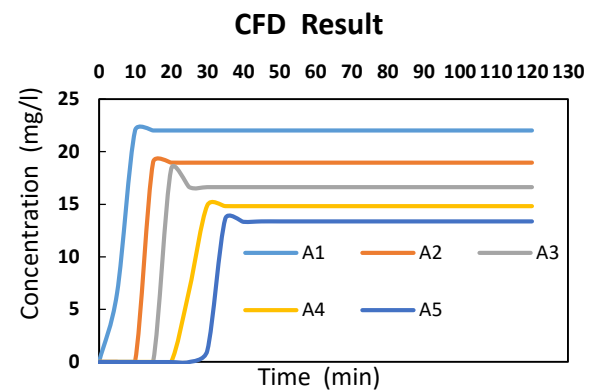
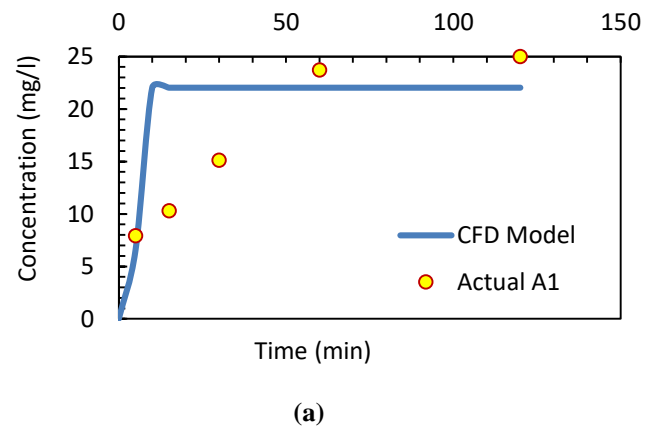


Figure 8. The results of the simulated sample for the values of the concentrations at the five control points





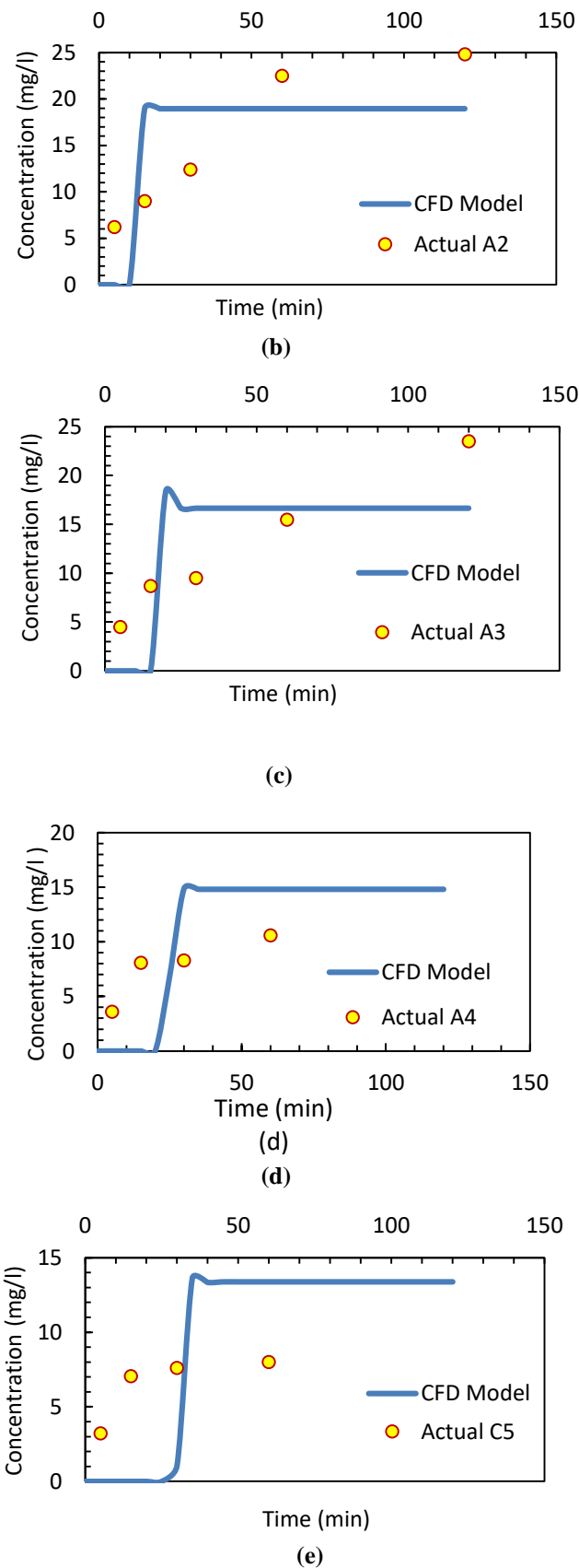


Figure 9. CFD simulated and physical models verification results at the five control points

### 4.3 Results of Statistical Verification

Verification was also tested according to several standard statistical indexes according to the equations (8 to 10). Based on the results of the statistical tests listed in Table 3, the CFD Simulation model provided a good reliability supported it to be a very good tool to simulate our problem without the physical model needed in order to reduce cost, time and effort. In addition, having a mathematical model that can simulate the problem and provide acceptable results close to the physical model helps us a lot in studying the effect of many factors and variables on the spread of pollutants in porous media, which is very difficult and cost to be studied in the laboratory. Therefore, the model is now ready to analyze and study the effect of a wide range values of many variables on this complex phenomenon. Thus, the effect of the flow velocity, temperature change, adsorption coefficient, porosity of the media will studied below depending on the simulated model only in order to decrease the efforts, cost , time.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^N (C_m - c_s)^2} \tag{8}$$

$$MSE = \frac{1}{n} \sum_{i=1}^N (C_m - c_s)^2 \tag{9}$$

$$MAE = \frac{1}{n} \sum_{i=1}^N |C_m - c_s| \tag{10}$$

$$RSE = \frac{\sum_{i=1}^N (C_m - c_s)^2}{\sum_{i=1}^N (C_m - C_m)^2} \tag{11}$$

Table 3. Statistical analysis verifications tests

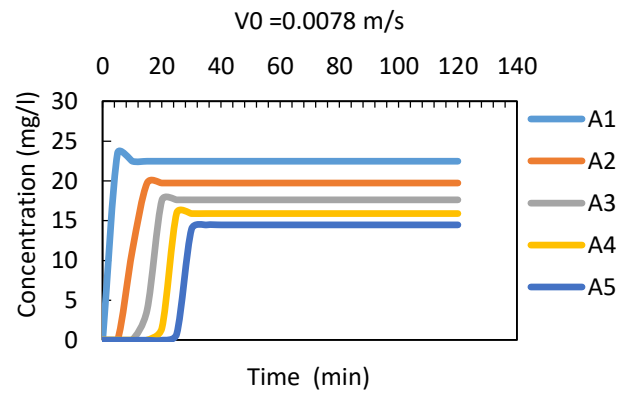
Point	RMSE	MSE	MAE	RSE
A1	6.32579	40.01564	4.95200	0.83841
A2	6.75230	45.59352	6.42800	0.83662
A3	6.24946	39.05576	5.66800	0.89861
A4	5.77264	33.32332	5.54000	1.12620
A5	5.38011	28.94558	5.15800	1.39863

#### 4.4 Prediction of CFD Simulated Model

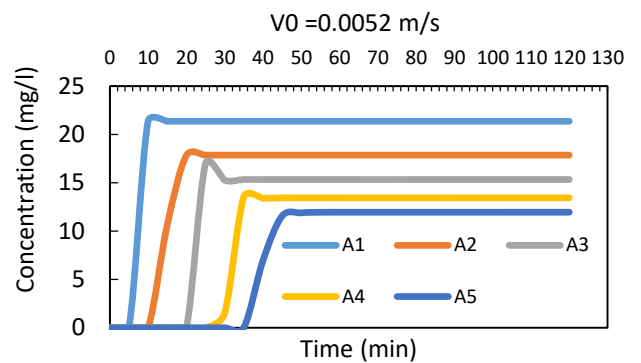
In the following paragraphs, the CFD simulated model will be run to study the effect of the important variables on the process of pollutant transport within the porous media to know the effect of each factor. These are the most important benefits of the simulated models to provide the required results with less time, effort and cost, and in a form that cannot be easily obtained in a laboratory depending on the physical models.

##### 4.4.1 Velocity Consideration

The velocity of flow in porous media has an important influence on the transport and diffusion of pollutants in the soil as it also affects the time required for the diffusion process and affects the external concentration and its quantity in the porous media. In this step, the effect of velocity change on the results obtained from the program was studied and the variable velocity values were imposed between (-20% to 20%) of the original laboratory value of (0.0065 m/s). The results showed that when increasing the speed, the concentration exiting from the abstraction points increased from (22 mg/l to 24 mg/l) due to the short period of time that the pollutant interacted with the soil minutes, which leads to a decrease in its adsorption process by the soil. This leads to an increase in the concentrations as well as to decrease in the time required to reach the highest value of the concentration in each points (i.e acceleration in the transmission of the pollutants), see Fig.10. Contrast, when the velocity value is reduced, the pollutant concentration decreases significantly because the pollutant takes a greater opportunity to interact with the soil and adsorb the pollutants and precipitate them before moving to the next distance (i.e delay in the transmission of the pollutants), see Fig.11.



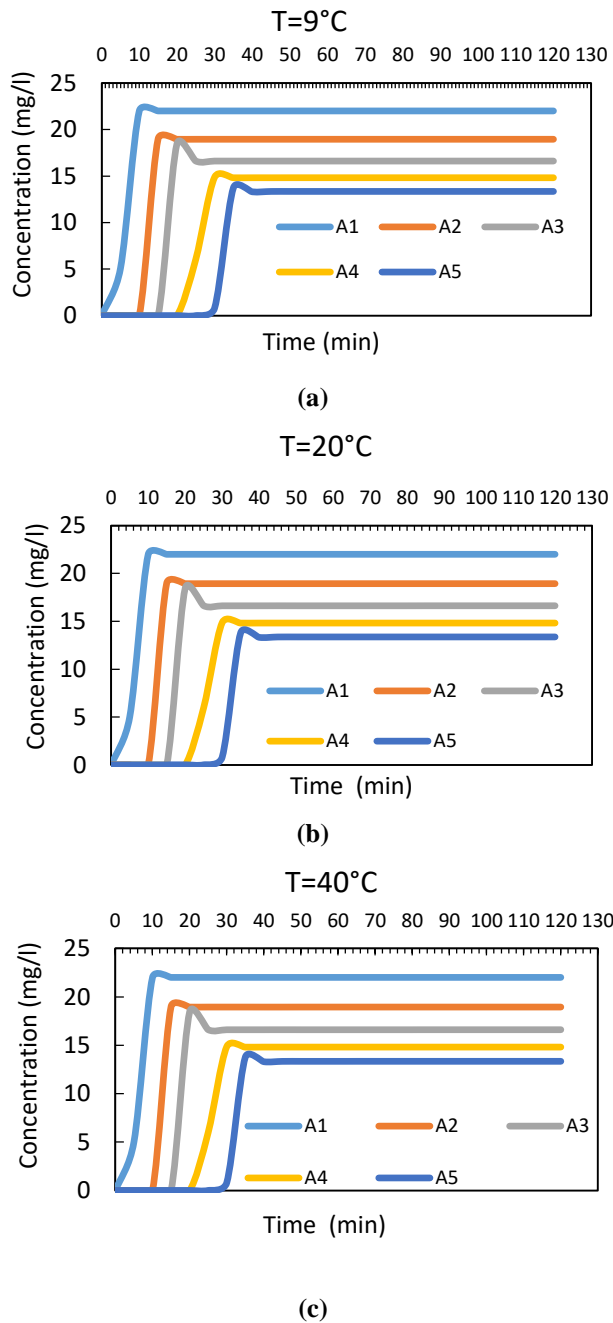
**Figure 10.** Concentration behavior under,  $V=+20\% VO$



**Figure 11.** Concentration behavior under inlet different velocity,  $V_0 = -20\%$  from initial value

##### 4.4.2 Temperature Effect

Temperature is a factor affecting related to the transport of pollutants through different porous media. To show the effect of the temperature on the nature of the transport through the porous media, a range of changed in the temperature of (9, 20, 40) degrees Celsius were assumed for this purpose. The results of the CFD simulated model indicated that the temperature it has little effect on the problem of pollutant transmission for the sample as explained in the Fig.12.

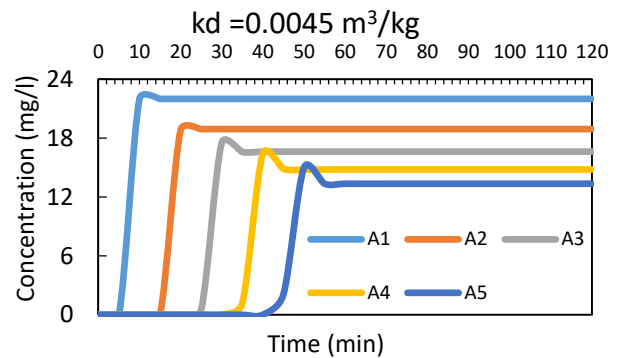


**Figure 12.** Concentration behavior under the effect of a range temperature values

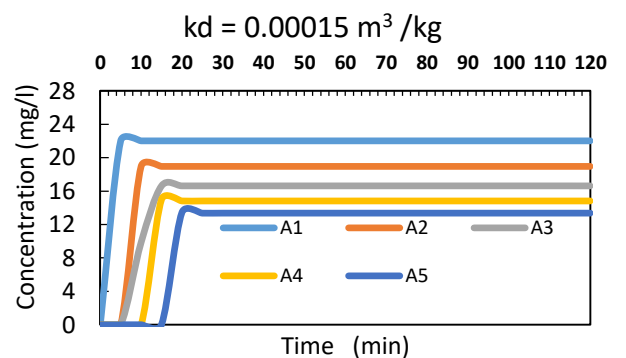
**4.4.3 Kd Consideration**

For the purpose of understanding the true role that the adsorption coefficient  $K_d$  plays in the pollutants transport process, the simulation was performed by imposing an increase and decrease in the adsorption coefficient equivalent to half of its initial laboratory value of ( $0.003 \text{ m}^3 / \text{kg}$ ). Increasing the adsorption coefficient means

increasing the ability of the soil to absorb heavy metals and thus an increase in the time required to reach the highest value of the concentration compared to the original sample (i.e delay in the transmission of the pollutants), as shown in Fig.13. This is because when the adsorption coefficient increases, this means that the pollutant will not come out early with high concentrations from the withdrawal points. But, when the  $k_d$  value is reduced to the half, it is noted an increase in the concentration coming out of the withdrawal points, as well as a decrease in the time to reach a high value of the concentration (acceleration in the transmission of the pollutants), as in Fig.14.



**Figure 13.** Adsorption coefficient effect for  $k_d = + 50 \%$  of the initial value



**Figure 14.** Adsorption coefficient effect for  $k_d = - 50 \%$  of the initial value

**4.4.4 Porosity Effect**

Porosity expresses the amount of spaces between particles in the soil and has an essential role in a factor velocity & transport Of

pollutants as it directly affects the surface area of the particles that make up the soil sample. In this step, the study was performed by changing the porosity of the porous medium to a ratio of (+ 30% and -15%) from the original value of the media of 0.32, while keeping the other data (velocity,  $K_d$ , temperature and other values) fixed under the same laboratory working conditions of the physical model. The results showed that when the porosity was increased to 30% of the initial porosity to be (0.416), the media is brought closer to the porosity of clay soil. Thus, it was noted an increase in the time required to reach the highest value recorded by the pollutant exiting from the control points due to the assumption that the surface area of the minutes it becomes more valuable with changing the porosity value to 30 percent which provides a high adsorption occurs, (i.e delay in the transmission of the pollutants), see Fig.15 the concentration of pollutants increased significantly at the sites of the five inspection points But when the porosity is reduced to 0.274 (15% of the initial value), this leads to less time to reach the highest value of the pollutant due to the small surface area of soil particles that work to absorb pollutants. Therefore, the lack of surface area means that there are no effective sites that absorb the pollutants and thus the pollutant will escape from the sample at a time that is relatively less than the time at the porosity before the increase, (i.e acceleration in the transmission of the pollutants), as shown in Fig.16. For the concentrations, the results indicated that there are insignificantly differences for both cases especially in the stable or maximum values.

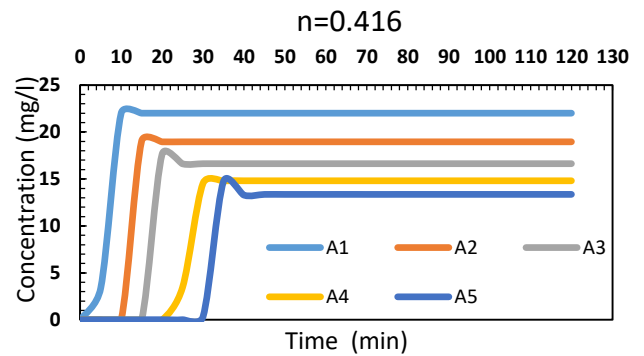


Figure 15. Porosity effect for  $n = +30\%$  from initial value

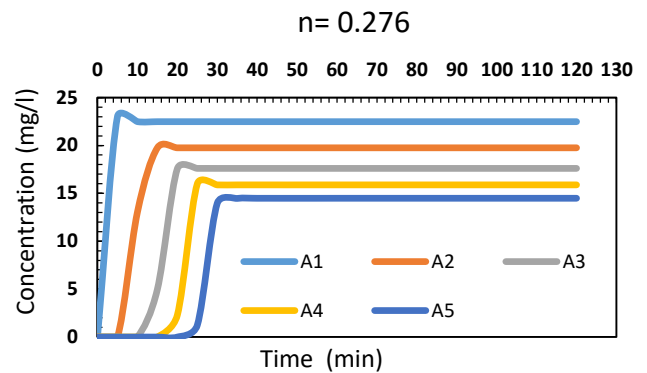


Figure 16. Porosity effect for  $n = -15\%$  from initial value

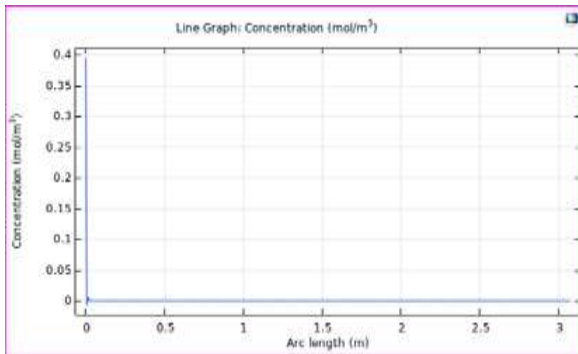
#### 4.5 Simulation of Contaminate Transportation

Fig.17 shows the pollutant transport process in the soil assuming different time steps for a period of (0 to 120 step 5) min. The simulation was achieved with the help of the CFD simulated model taking in a count the same entry original laboratory values for ( $n = 0.32$ ,  $V_o = 0.0065$  m/s ,  $C_0 = 25.09$  mg /l ,  $K_d = 0.003$  m<sup>3</sup> / kg and temperature = 300k). The times range from the start of pumping the contaminant into the soil to the middle and until the end of the tube. It is observed that the transition in the sample is homogeneous in the transverse direction or along the radius of the sample, that is, the y and x axes. Where the concentrations are equal at any point in the section perpendicular to the direction of flow (z axis) as shown in the Fig.17. The pollutant arrives at the ends of the 3-meter pipe, but at a low concentrations compared to the concentrations at the first points. The Concentrations have the

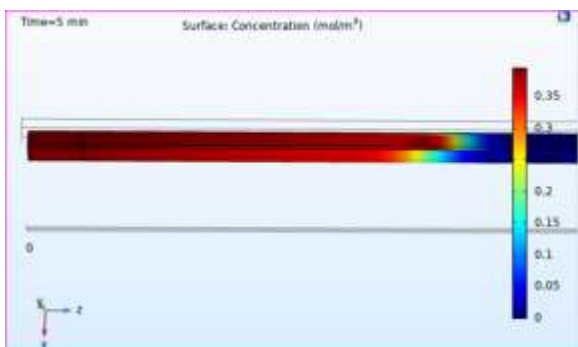
highest value at the first point of the pipe and the pollutant is distributed to the rest of the soil, with an increase in the time of passage of the pollutant on it. It is important to note from the Fig. 18 that the simulation of the transition reach to the case of steady state at a time of 40 minutes. After that and moving to the end time (120 s), the curve is relatively constant until the end of the run. This is due to the reason of saturation soil particles with copper and their inability to absorb greater amounts of pollutants passing on them after about 60 minute reaching to the steady state case.



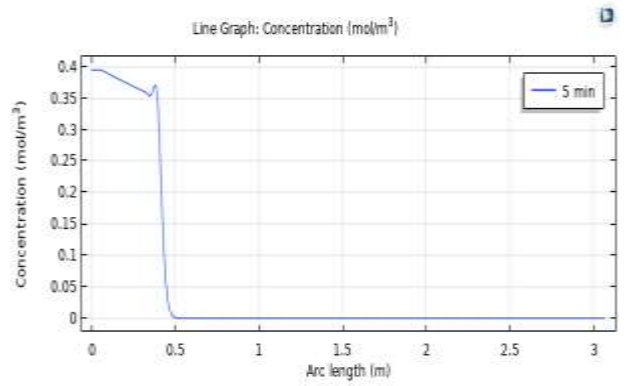
(a)



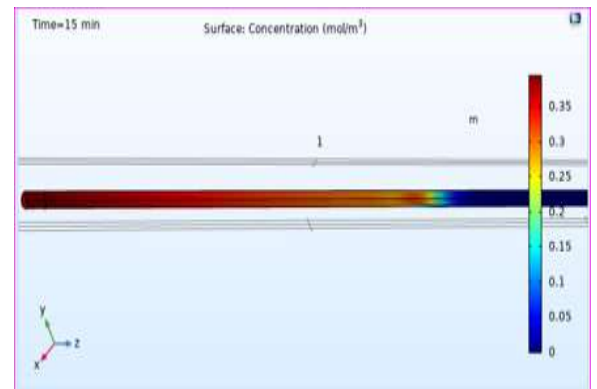
(b)



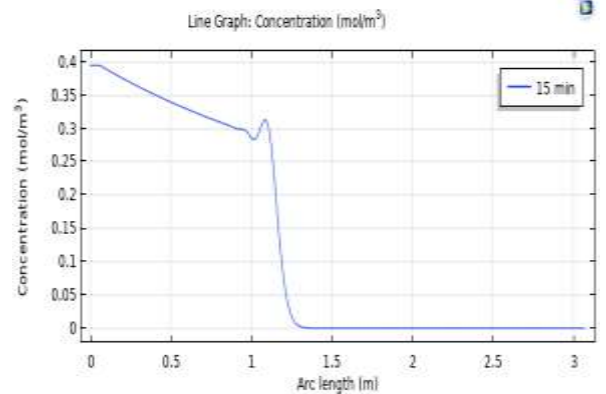
(c)



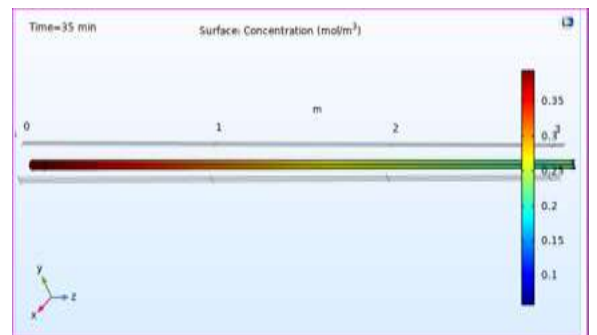
(d)



(e)

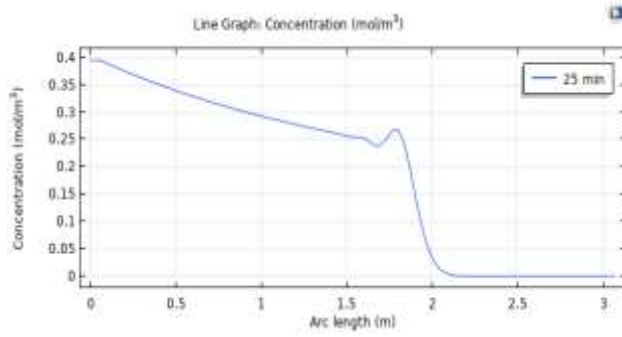


(f)

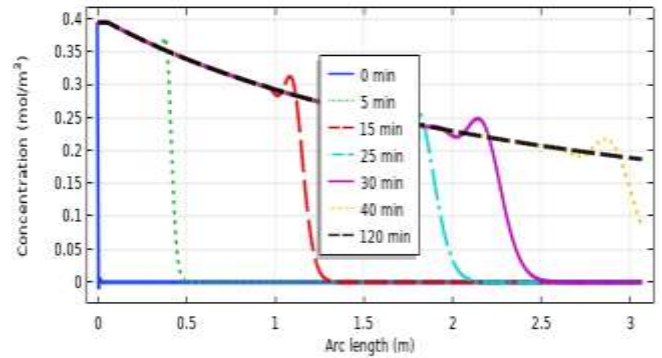


(g)

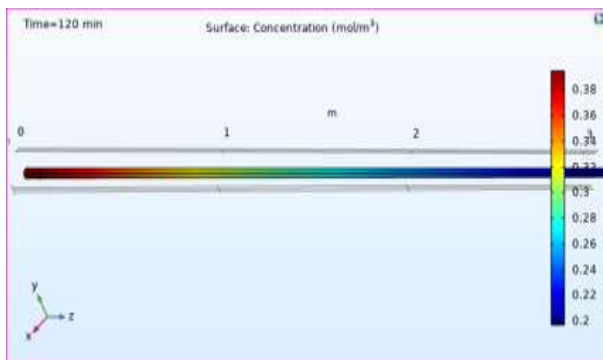




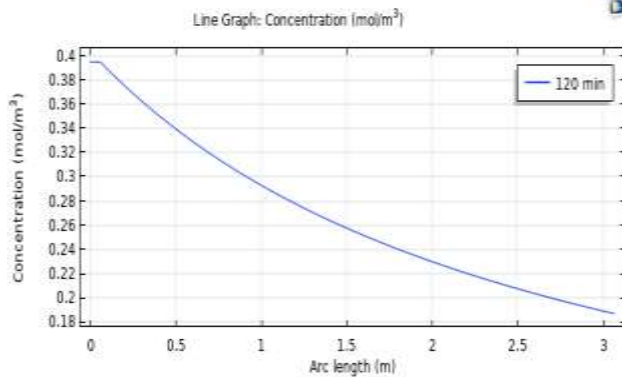
(H)



**Figure 18.** Length - Ce relationship for simulation of transient pollutants transport through porous media along the time.



(I)



(J)

**Figure 18.** Simulation of movement's transient for contaminant's spot through the porous media

### 5. Conclusion

From the results and analyzes mentioned, the following points can be found numerical results presented by the imitation CFD model showed great harmony with the empirical work of All the tested cases. Thus, CFD technology is able to examine the current trouble, keeping In mind the passable mistake rate. As the length of the pollutant flow path through the porous medium rise the concentrations in the porous medium decrease result from the adsorption of the pollutants by soil particles. The center of the study that is physical represented by (porosity and adsorption coffin) have obvious influence on the concentration distribution. An increase in the velocity of the flow leads to an increase in the concentrations from the entry points because the pollutants go through a specific time which is not allowed to fully interact with the medium and allow them to adsorption or ion exchange. The results showed that the effect of changing the temperature is imperceptible on the concentration of pollutants whose concentration is observed in the clouds An increase in the value of the adsorption coefficient by 50% led to an increase in the absorption of pollutants by soil particles, and thus a decrease in the

concentrations computed from the set points, and a decrease in the adsorption coefficient leads to an increase in the concentrations computed from the drawing points. Whereas, an increase in the porosity leads to an increase in the calculated concentrations from The points are a result of decreasing surface area for soil particles used. The rat of adsorption Has a significant impact on focus as the concentration decreases at slow speeds and the time required to reach the highest point value is relatively short. The lack of adsorption plays a main role in reducing the concentration And transport of pollutants. The results also showed that the transport o0f pollutants is gradual over time, homogeneous for the longitudinal axis of the tube, in a gradual spreading manner, and also in a homogeneous manner in the cross section of the tube as shown. Based on some statistical criteria, we can use a CFD simulation model using COMSOL 5.4 to demonstrate the transport through sandy gravel soils and it is well matched. With the results of work on the physical sample in the development of simulated pollutant transport processes.

## 6. Acknowledgments

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## 7. Conflict of Interest

There is no conflict of interest.

## Abbreviations

C	Concentration of contaminants
C <sub>f</sub>	Friction coefficient, Dimensionless

(cm <sup>-1</sup> )	The mean measured concentration
C <sub>m</sub>	Measured concentration
c <sub>s</sub>	Simulated Concentration
D= D <sub>x</sub> =D <sub>y</sub>	Diffusion Coefficient
e	Error
H	Up stream water head
k	Intrinsic permeability
K <sub>d</sub>	Adsorption isotherm
MAE	Mean absolute error
MSE	Mean squared error
n	The Porosity
r	Average of engender
R	Retardation of adsorption
RSE	Relative squared Error
RMSE	Root Mean Squared error
s	External source values, function of
u	Velocity field in the x-axis
v	Velocity field in the y- axis
ρ	Density
μ	Dynamic Viscosity

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