CFD modeling of contaminant transport in soils including the effect of chemical reactions

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Abstract The movement of chemicals through soils to the groundwater is a major cause of degradation of water resources. In many cases, serious human and stock health implications are associated with this form of pollution. In this work, a CFD model is presented for simulation of the flow of water and air and contaminant transport through unsaturated soils with the main focus being on the effects of chemical reactions. The governing equations of miscible contaminant transport including advection, dispersion–diffusion and adsorption effects together with the effect of chemical reactions are presented. The model is applied to the simulation of a real case study in-site of the oil production field in Libya involving transport of contaminants in a soil with particular reference to the effects of chemical reactions. Comparison of the results of the numerical model with the experimental results shows that the model is capable of predicting the effects of chemical reactions with very high accuracy.

Keywords: contaminant transport, unsaturated soil, chemical reaction, CFD.

1. Introduction

The production, processing, and storage of petroleum and its products are the main contributors to soil and groundwater contamination. The movement of chemicals through the soil to the groundwater or discharged to surface waters represents a degradation of these resources. In many cases, serious human and stock health implications are associated with this form of pollution.

Produced water is water trapped in underground formation that is brought to the surface along with oil or gas. It is by far the largest volume byproduct or waste stream associated with oil and gas production. Management of produced water and its environmental effects, present challenges to oil industry and environmental experts. The produced water contaminates the soil and causes the outright death of plants, and the consequent erosion of topsoil. Also, impacted soil serves to contaminate surface waters and shallow aquifers [1].

Therefore produced water is the principal source for hydrocarbon discharges from the petroleum sector to the environment. Total Petroleum Hydrocarbon (TPH) is constituent of produced water that receives the most attention. The soil suffers from high concentration of hydrocarbons constituents (crude oil base) which are accumulated due to direct disposing of produced water. Where a substantial amount of hydrocarbons free phase (crude oil) has being carried by produced water stream. Hydrocarbons effect and threaten wild life, soil biomass and groundwater resources [2].

CFD models are very useful in environmental assessments because measurements cannot be taken at all times and in all places with the intensity and focus needed to assess all environmental conditions. CFD models are thus needed to “fill in the gaps” as well as to extend the measurement data to characterize and evaluate an environmental problem or study [3]. The focus of this paper is the development, validation and application of a coupled transient CFD model for contaminant transport in unsaturated soils that incorporates the effects of chemical reactions on the contaminant transport.

2. CFD Modelling

The governing equations that describe fluid flow and contaminant transport in the unsaturated

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zone will be presented in this section. Richards' equation governs the saturated-unsaturated flow in the soil is [4]:

$$[C + Se.S]\frac{\partial H_p}{\partial t} + \nabla.\left[-K.k_r.\nabla\left(H_p + D\right)\right] = Q_s \quad (1)$$

where $\boldsymbol{C}$ denotes specific moisture capacity (m^{-1}); $\boldsymbol{Se}$ is the effective saturation of the soil; $\boldsymbol{S}$ is a storage coefficient (m^{-1}); $\boldsymbol{Hp}$ represents the dependent variable pressure head (m); $\boldsymbol{t}$ is time (d); $\boldsymbol{K}$ equals the hydraulic conductivity function (m/d); $\boldsymbol{kr}$ is the relative permeability of the soil; $\boldsymbol{D}$ is the coordinate (for example, x, y, or z) that represents vertical elevation, and $\boldsymbol{Qs}$ is a fluid source defined by volumetric flow rate per unit volume of soil (d^{-1}).

The governing equation for solute transport in the reaction model describes advection and dispersion of a sorbing, volatilizing, diffusion, adsorption and decaying solute in variably saturated soil:

$$\begin{aligned}&\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}\left(\rho_b c_p\right) + \frac{\partial}{\partial t}\left(a_v c_G\right) = \\ &= \nabla.\left[-\theta D_{LG}\nabla c + uc\right] = R_L + R_P + S_c\end{aligned} \quad (2)$$

where $\boldsymbol{\theta}$ is the volume fraction of fluid within the soil; $\boldsymbol{c}$ is the dissolved concentration (kg/m^3); $\boldsymbol{\rho_b}$ is the bulk density (kg/m^3); $\boldsymbol{c_p}$ is the mass of adsorbed contaminant per dry unit weight of solid (mg/kg); $\boldsymbol{a_v}$ is the air volume fraction; $\boldsymbol{c_G}$ is the solute concentration in air (kg/m^3); $\boldsymbol{D_{LG}}$ is the combination of hydrodynamic dispersion tensor for water and diffusion in air (m^2/d); **u** is the vector of directional velocities (m/d); $\boldsymbol{R_L}$ denotes reactions in water ($kg/m^3.d$); $\boldsymbol{R_P}$ equals reactions involving solutes attached to soil particles ($kg/m^3.d$); $\boldsymbol{S_c}$ is the quantity of solute added per unit volume of porous medium per unit time ($kg/m^3.d$).

The effects of chemical reactions on solute transport are generally incorporated in the advection, diffusion–dispersion, volatilization, and adsorption equation through additional terms. Consider a chemical reaction as;

$$aA + bB \leftrightarrow rR + sS \quad (3)$$

where $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{r}$ and $\boldsymbol{s}$ are the valences for ions. A general kinetic rate law for species $\boldsymbol{A}$ can be expressed as;

$$\frac{\partial c_A}{\partial t} = -\lambda c_A^{n1} c_B^{n2} + \gamma c_R^{m1} c_S^{m2} \quad (4)$$

where $\boldsymbol{c_A}$, $\boldsymbol{c_B}$, $\boldsymbol{c_R}$ and $\boldsymbol{c_S}$ are concentrations of reactant species $\boldsymbol{A}$ and $\boldsymbol{B}$ and resultant species $\boldsymbol{R}$ and $\boldsymbol{S}$, respectively; $\boldsymbol{\lambda}$ and $\boldsymbol{\gamma}$ are the rate constants for the forward and reverse reactions, respectively; **n1**, **n2** and **m1**, **m2** are empirical coefficients. The sum of **n1** and **n2** defines the order of the forward reaction while the sum of **m1** and **m2** defines the order of the reverse reaction. Equation (13) expresses the rate of change in species $\boldsymbol{A}$ as the sum of the rates at which it is being used in the forward reaction and generated in the reverse reaction.

The governing equations were discretized using a finite volume method and solved using the commercial computational fluid dynamics code COMSOL Multiphysics 3.2. Stringent numerical tests were performed to ensure that the solutions were independent of the grid size. The coupled set of equations was solved iteratively, and the solution was considered to be convergent when the relative error in each field between two consecutive iterations was less than 1.0×10^{-6}. The calculations presented here have all been obtained on a Pentium IV PC (3 GHz, 2GB RAM) using Windows XP operating system.

3. Results and discussions

The developed CFD model is validated by application to a contaminant transport problem in the laboratory. The model is then applied to a real case study (site-scale) to predict the transport of contaminant in a site.

The developed CFD model is applied to study contaminant transport through a column of sandy soil including the combined effect of advection and dispersion (Fig. 1). Produced water ponds in a ring seated on the ground of the soil column. The produced water moves through the bottom of the ring into the soil. The petroleum produced water in the ring contains a hydrocarbon, which moves with the water into the soil at constant concentration. The hydrocarbon enters the ground with the water and moves through the subsurface by advection and dispersion. Additionally, the hydrocarbon sorbs or attaches to solid surfaces, which reduces the aqueous concentrations and also slows hydrocarbon movement relative to the water. Microbial degradation also reduces both the liquid- and the solid-phase concentrations. At the ground surface outside the ring there is volatilization to the atmosphere.

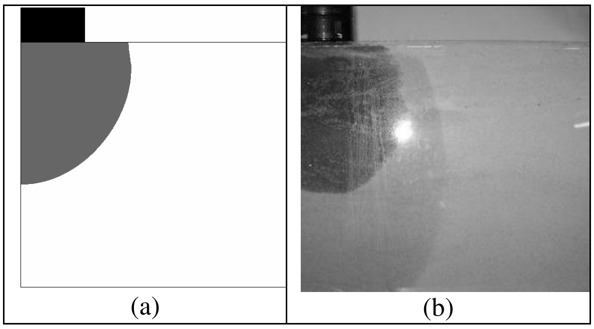

Fig.1. Contaminant transport through a column of sandy soil: (a) CFD model, and (b) laboratory prototype

The sorption, biodegradation, and volatilization proceed in linear proportion to the aqueous concentrations. Initially the soil is free of the hydrocarbon. The results of the CFD analysis are compared with experimental. Comparison of the results shows a very good agreement between the results of the numerical model and the experimental.

A contaminated soil around a disposal pit of produced water at a selected oilfield has been chosen as a case study area (Fig. 2).

Fig. 2. Pipe of produced water discharge to the pit.

The produced water is considered to be the main source of pollution, where many constituents are carried by it, especially hydrocarbons, which are presented in a significant concentration. Hydrocarbon content in the soil shows that the soil around the pit is suffering from high pollution by hydrocarbons, and this is an expected result due to accumulation of crude oil carried by produced water, on the soil. The validated CFD model has been applied to the present case study. Boundary conditions are specified from the experimental tested points as well as boundaries for various mass and scalar equations inside the computational domains.

The obtained results of TPH values from the experimental tests have been considered as boundary condition in CFD analysis to predict and investigate the spreading of crude oil inside the soil around the pit (see ref. [1] for detailed testes).

In order to follow up the vertical migration motion of the pollutants, and identify the extent of contamination at the studied area over the entire period of production and pollutants disposing activities, the most threaten pollutants have been selected was hydrocarbon content represented by Total Petroleum Hydrocarbon (TPH) to evaluate the dispersion profile in the impacted area. Fig. 3 shows the steps of hydrocarbons migration (TPH), through the soil at the bank of the pit.

4. Conclusions

Development, validation and application of a coupled transient CFD model for contaminant transport in unsaturated soils including the effect of chemical reactions has been presented. The model is then applied to predict the vertical migration transport of Total Petroleum Hydrocarbon (TPH) in the soil around a disposal pit of produced water at oilfield. The results showed that the contaminant transport model is capable of simulating various phenomena governing miscible contaminant transport in soils including advection, dispersion, diffusion, adsorption and chemical reaction effects.

The model performed well in predicting transport of contaminants through the soil. Comparison of the results of the model with the experimental results shows that the model is capable of predicting the effects of chemical reactions with very high accuracy.

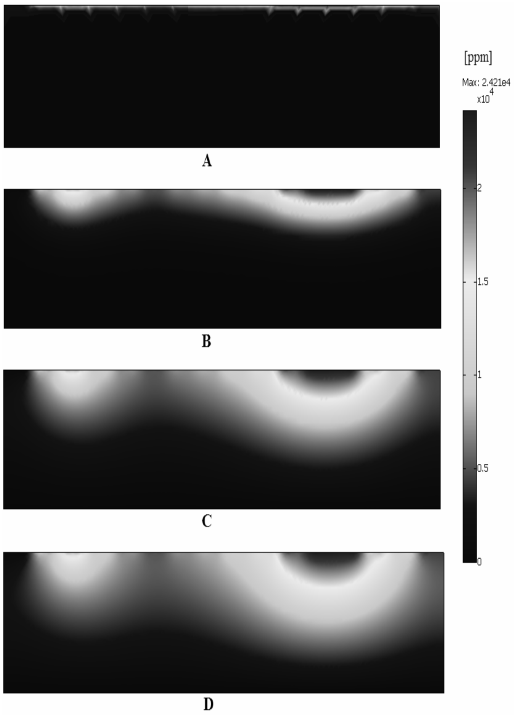

Fig. 3. Hydrocarbon migration steps over the entire period of production and pollutants disposing activities of the produced water: **A:** Initial, **B:** Concentrations at 1 year, **C:** Concentrations at 2 years, **D:** Concentrations at 3 years

The main conclusions which could be drawn from the case study are:

1. The employing of CFD technique in this research work was highly active due to the accurate outputs and prediction of the dispersal hydrocarbons that have been given.

2. CFD technique is effectively decreased the number of required samples, experiments, and the time.

3. The evaluation of dispersion profile of pollutants showed that the maximum dispersion rate is high at the beginning period of disposing, while the rate becomes slow in the most recent period, and that due to the blockage occurred in soil porous and decreasing of soil permeability.

4. High TPH values for soil indicate that the natural attenuation of petroleum hydrocarbons constituents in the soil can not be satisfied for soil remediation, so that complete plan of remediation has to be made.

5. References

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