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SUBSURFACE FLOW MODELING OF A BIOREMEDIATION LABORATORY TEST TANK

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***Abstract*—**Bioremediation of soil is an important topic of sustainable waste management where specific kinds of bacteria are used to clean soils from oil or other pollutants. Even if this topic is mainly related to biology research, there are aspects as subsurface flow, which are first of all an engineering problem. Modeling the flow of water, pollutants and liquid bacterial compounds can be made using state of the art FEA software. This model helps researchers to optimize bacterial injection timing and quantities which are necessary to remove pollutants from the soil.

***Keywords*—**subsurface flow modeling, Darcy's law, bioremediation, finite element analysis.

I. INTRODUCTION

BIOREMEDIATION is the use of microorganism metabolism to remove pollutants. Technologies can be generally classified as in situ or ex situ. In situ bioremediation involves treating the contaminated material at the site, while ex situ involves the removal of the contaminated material to be treated elsewhere. Some examples of bioremediation technologies are phytoremediation, bioventing, bioleaching, farming, bioreactor, composting, augmentation, rhizo-filtration, and bio-stimulation.

There are numerous advantages to bioremediation. First and foremost, it is ecologically sound. It is one of the most environmentally responsible ways to treat contamination. Secondly, it allows the treatment of areas that are difficult to reach, including underground and deep sea. It is also less expensive than traditional cleanup techniques which often require excavation, incineration and mechanisms for pumping. Lastly, it is safer than traditional techniques and does not place humans in danger.To insert images in *Word,* position the cursor at the insertion point and either use Insert | Picture | From File or copy the image to the Windows clipboard and then Edit | Paste Special | Picture (with "Float over text" unchecked).

In order to optimize the bioremediation process studies and analyzes must be made on how the pollutants and microbial solutions used for bioremediation are carried under the soil by underground waters and efficient can be the bioremediation in this conditions. The state of the bacteria must be also studied under different conditions.

II. BIOREMEDIATION LABORATORY

The bioremediation laboratory, in our case is composed by two test tanks filled with soil through which water is conducted to create a subsurface flow. Then different kinds of pollutants are added together with a solution that contains bacteria which presumably will feed on this pollutant. In this process it is very important to study the subsurface flow, pressure conditions and speed of flow of different liquids in different kind of soils. Flow parameters are very hard to be measured precisely without modifying the flow conditions, so numerical simulation of subsurface flow can produce important results which can support experimental analysis. That is the reason why the laboratory had to be equipped with modeling capabilities to simulate the subsurface flow. This was made by integrating the experimental laboratory with the modeling facility as it is shown in figure 1. This platform was developed in the framework of cross-border cooperation program CBC-HURO, 0802/100_AF,acronym "Micromodel" project.

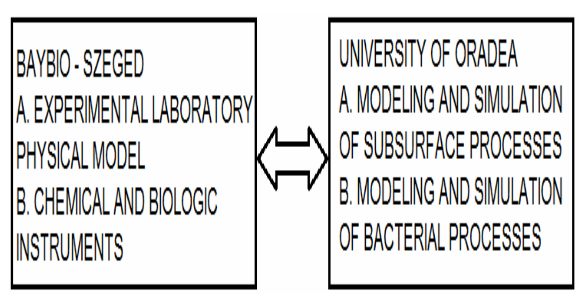

Fig.1. Structure of the research platform.

Fig.2. Test tanks in the experimental laboratory.

III. Modeling of Subsurface Flow Considering the Laboratory Test Tank Geometry

From a microscopic point of view, in a porous media, there is a very complicated flow which depends on the media geometry. Therefore, in this kind of flow, a mean velocity is introduced, which is defined as the velocity of a liquid which flows through a tube with the area section Sa, filled with a porous material.

We can define the porous media flow system having the following elements: the porous media, one or more liquid phases and air.

Saturated flow – when the porosity is fully occupied by the liquid;

1) *Non saturated flow* – when porosity is partially filled with liquid and the rest is filled with air;

2) Partially saturated flow (variable saturation) – when more saturated and non-saturated zones can co-exist;

3) *Homogeneous flow* – when the porous media is completely saturated with a single phase;

4) *Heterogeneous flow* – when the porous media is saturated with at least two phases. This includes the situation, otherwise frequent, when in the porous media more phases are present even if only one of them flows and the others are stationary. If that happens it does not mean that it is a homogenous flow;

1D flow or one dimensional flow (one directional) – the velocity of the fluid can be described by two spatial variables;

2D flow or bidirectional (plane or axisymmetric) – the velocity of the fluid is described by three spatial variables;

3D flow or tridimensional flow (spatial) - the velocity is described by a single spatial variable;

3D saturated variable flow at constant density – in this case there are two phases: air and liquid variably saturated. The effect of air movement is negligible so the problem is reduced to a mono-phasic flow. This approximation is valid when the air phase is connected to the atmosphere.

The flow phenomenon in porous media is a very complex one and can be analyzed only indirectly, on models or by measuring some macroscopic quantities which describe the flow. The flow can be seen in two modes: at micro and macro scale.

In the case of non-Newtonian fluids (heavy oils or polymer solutions), the behavior in micro spaces is very different of that in macro spaces. Regarding the flow mode we can say that hydrocarbon flow velocity is very slow.

In the one dimensional case for a laminar flow, Darcy has established the specific flow rate q=Q/S also called as flow flux or Darcy velocity and the hydraulic load:

$$\vec{q} = \vec{U} = k\frac{\Delta H}{L} \tag{1}$$

The intrinsic mean velocity can be also defined as:

$$\vec{q}_f = \frac{1}{V_f}\int_{V_f}\vec{q}dV \tag{2}$$

Because the porous media is saturated with fluid $V_f = V_p$ and considering the definition of porosity (n), the relation between Darcy velocity and intrinsic velocity can be obtained. This is called the Dupuit-Forchheimer relation and is given by:

$$\vec{q}_f = \frac{\vec{q}_V}{n} \tag{3}$$

In case of a tilted tube, Darcy's law can be written in the vector formulation as:

$$\vec{q} = -\frac{K}{\mu}grad(p + \rho\vec{g}h) = -K grad\ p + \rho\vec{g} \tag{4}$$

Where: $K = \frac{k\mu}{\rho g}$ is the permeability;

μ – is the dynamic viscosity of the fluid;

As the importance of subsurface flow had grown during time the researchers had developed more mathematical models to cope with different flow situations. The models which are mostly used today, are as follows:

- The Brinkman equation - for high velocity flows in porous media;
- Darcy's law – for slow velocity flows in porous media;
- Richards equation for variable saturated flow.

These models are completed with different soil models like those presented in [1], for example:

- van Genuchten;
- Brooks–Corey
- Clapp–Hornberger

At present, the existing software offer is based on this type of model.

There are different approaches in this type of study.

Statistic approach – natural porous media (subsurface) has a great degree of n0n homogeneity and its characteristics cannot be established in a deterministic way. Evaluation of these characteristics will be made using statistic methods applied to multi-support measures: point, linear, on surface, on interfaces. In order to obtain the numeric model of the soil interpolation methods can be used.

Black box approach – in this case the so called neural network technique which uses a set of input data and a set of observed outputs and which learns the relationship between these quantities This relation is further applied to a model under study. The modeling is reduced, in fact, to the simplest possible relation, without phenomenological or geometrical relations or boundary conditions. After the model calibration, this can be used to process another sets of input data for the applied system. This type of modeling is not used yet for subsurface flow due to the large number of experimental parameters which are needed for model calibration.

The stochastic approach – physical and mechanical properties of a porous media presents large variability in time and space inducing a high variability of studied parameters, in order to describe pollutant transport phenomena.

A stochastic modeling is necessary when one or more parameters of the domain are treated as random variables, a stochastic process or a random field in space. For example soil permittivity can be considered as a random field, the boundary conditions can be described as stochastic processes (precipitations, water levels, and so on). Transport phenomena and pollutant transfer in porous media are considered to be quantifiable by stochastic modeling.

With the development of computational power these methods had been rewritten as numeric algorithms and implemented through finite element or other methods in order to be able to solve subsurface flow problems for different geometries and porous media parameters.

Such an implementation had been made in the COMSOL Multiphysics environment which is able to solve complex problems, coupling subsurface flow with thermal and fluid dynamic physics [2], [3], [4].

As a first step for modeling the processes which take place in the test tank our purpose, presented in this paper, is to model the subsurface flow in the tank and to extend, in future works, the model to more complex phenomena, including variable saturated flow, subsurface flow of multiple fluids coupled with thermal analysis, to study the flow around obstacles with different geometries and eventually to integrate all these physics with bacterial growth models.

The present paper describes our studies on subsurface flow based on the Darcy’s law model.

In order to develop the subsurface flow model the COMSOL Multiphysics® software was used.

The first step to develop the model was to establish the 3D geometric model. This was made by using the SolidWork CAD software and then the geometric model had been imported as a parasolid file. The geometric model strictly follows the geometry and dimensions of the laboratory test tank. The geometric model is shown in figure 3.

After having completed the geometry model, the materials properties have to be defined. Considering the materials which are currently used in the test tank, the property values chosen for the model are presented in table 1.

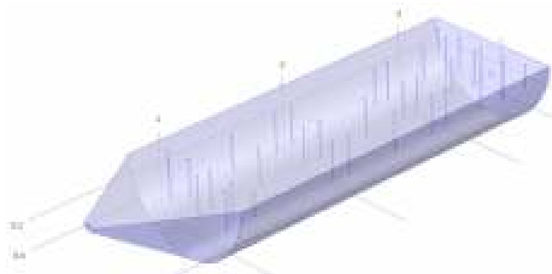

Fig.3. The 3D geometric model of the test tank.

TABLE I.
MATERIAL PROPERTIES OF THE MODEL

Description	Value
Density	1000
Dynamic viscosity	1e-3
Permeability	{{1e-11, 0, 0}, {0, 1e-11, 0}, {0, 0, 1e-11}}
Porosity	0.3
Compressibility of fluid	4.4e-10[1/Pa]
Effective compressibility of matrix	1e-8[1/Pa]

The next step in model development is to generate the mesh. This can be made automatically or defining user values. In the first case the user can set predefined sizes of the elements which best suites the geometry. Usually Tetrahedral elements are used for solids and triangular elements are used for surface boundaries.

TABLE II.
ELEMENT SETTINGS

Property	Value
Minimum element quality	0.1021
Average element quality	0.7083
Tetrahedral elements	225153
Triangular elements	14066
Edge elements	1787
Vertex elements	150

TABLE III.
MESH STATISTICS

Name	Value
Maximum element size	0.178
Minimum element size	0.013
Resolution of curvature	0.4

Resolution of narrow regions	0.7
Maximum element growth rate	1.4
Predefined size	Finer

The generated mesh is shown in figure 4.

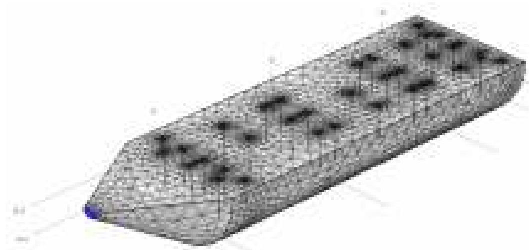

Fig. 4. Diagram of the generated mesh for the test tank model.

Once the mesh is generated, we can proceed to define the boundary conditions. All the surfaces of the model are declared in no flow condition except the Inlet and Outlet boundaries shown in figure 5. The values of pressure for Inlet and Outlet boundaries are given in table 4.

TABLE IV.
BOUNDARY PRESSURE VALUES

Pressure	**Value**
Outlet Pressure	p0= 101325[Pa]
Inlet Pressure	p0=10000[Pa]

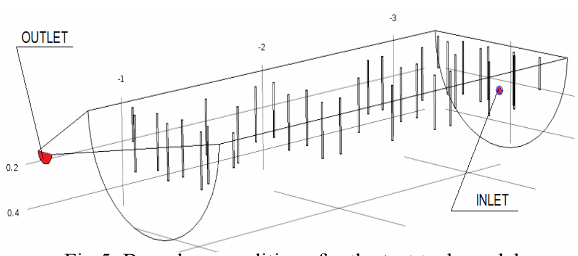

Fig.5. Boundary conditions for the test tank model.

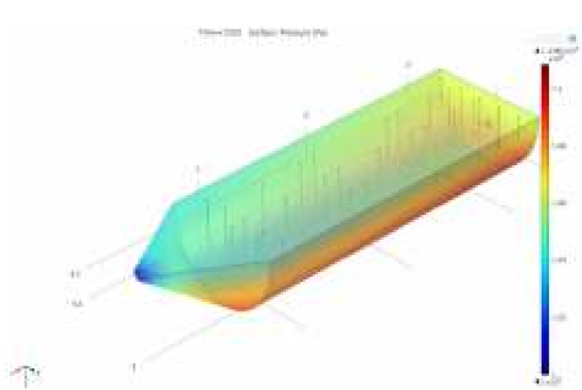

Fig.6. Simulation results showing pressure distribution in the test tank model.

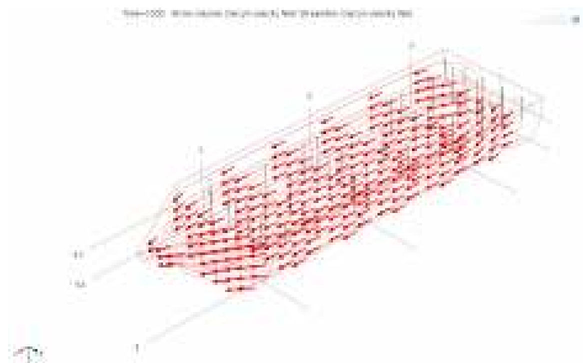

Fig.7. Simulation results showing subsurface flow velocity vector field.

IV. CONCLUSION

The development of test tank subsurface flow model is an important step in the study of bioremediation processes giving experimental researchers a substantial support. Due to the multiphysics capabilities of the COMSOL software, the developed model can be to study further complex situations like coupled flow and thermal analysis, two-phase flow and heat transfer and also covers a wide range of studies regarding soil and liquid parameters. The developed models can use as experimentally obtained input values linking experimental and simulation studies.

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REFERENCES

[1] H. J. Morel-Seytoux, P. D. Meyer, M. Nachabe, J. Touma, M. T. van Genuchten, R. J. Lenhard, *Parameter equivalence for the Brooks-Corey and van Genuchten soil characteristics: Preserving the effective capillary drive*, Water Resources Research, vol. 32;no. 5, pages 1251-1258, May 1996.

[2] H.A. Akhlaghi Amiri, A.A. Hamouda, *Pore-scale Simulation of Coupled Two-phase Flow and Heat Transfer through Dual-Permeability Porous Medium*, Proceedings of 2012 COMSOL Conference in Milan.

[3] A. Thoraval, Y. Guglielmi, F. Cappa, *3D simulations of an injection test done into an unsaturated porous and fractured limestone*, Proceedings of 2012 COMSOL Conference in Milan.

[4] K. K. Singh, *Two-phase Flow and Multiphysics Simulations in Comsol*, 3rd November 2012, COMSOL Conference Bangalore.

[5] R. W. Lucky, "Automatic equalization for digital communication," *Bell Syst. Tech. J.*, vol. 44, no. 4, pp. 547–588, Apr. 1965.