3rd International Conference on Green Energy and Environmental Engineering (GEEE-2016)

Proceedings of Engineering & Technology (PET)
pp. 54-57

Modeling of Benzene Transport in Soil

Nora. Boukhalfa[1*], Wafa. Kerboub[2]

[1,2] Department of Chemistry
University of Batna 1
Batna, 05000. Algeria.
[*]boukhalfa_nora@yahoo.fr

Abstract—**Release of petroleum hydrocarbons in the environment is a widespread occurrence. One particular concern is the contamination of drinking water sources by the toxic, water soluble, and mobile petroleum components such as benzene. The migration of the contaminant through a soil is modeled using the convection-dispersion equation. The solution is obtained analytically using Laplace Transform technique. The results are illustrated graphically. This work may helpful to predict the concentration of the contaminant in the aquifer at futur times and to assess the risk associated with such releases.**

***Keywords*— Benzene; transport; soil; Laplace transform; model.**

I. Introduction

Light aromatic hydrocarbons such as benzene, toluene, ethylbenzene and xylene (BTEX) are present in virtually every type of crude oil. They are also soluble in water and their aqueous solubilities increase with increasing temperature and pressure [1].

Contamination of groundwater due to surface spill or subsurface leakage of such petroleum products has been of concern to many industries and governments. Evaluation of its potential impact on public health is a key component in studying this type of contamination problem. All these BTEX compounds are toxic and have noticeable adverse health effects at high concentrations. Most studies have been done on benzene, which is the only proven carcinogen. Upon exposure to benzene, the benzene will move into the blood stream, it can then get into fatty tissues where it can undergo reactions that produce phenol which is an even more serious carcinogen than benzene [2].

Accidental releases of these petroleum hydrocarbons to the subsurface environment through leakage or spills may cause environmental problems, including the migration through the subsurface to ground water. To evaluate the risk associated with such releases, it is necessary to be able to predict the concentration of the pollutant in the aquifer at future times.

Modeling transport of petroleum hydrocarbons in soil requires an understanding of the physical and chemical properties of the compounds wich will control their different rates of migration. Solute transport in the soil and the groundwater is affected by a large number of physical, and chemical processes; and the properties of the media. In many practical situations, one needs to predict the time behaviour of a contaminated groundwater layer. Most of the groundwater contaminants are reactive in nature and they infiltrate through the soil, reach the water-table; and continue to migrate in the direction of groundwater flow. Therefore, it is essential to understand the transport process of contaminants through the subsurface porous media.

Several mathematical models have been developed in the literature, an overview of them is given in [3]. This overview provides the information of various approaches that can be applied for modelling of contaminant transport.

The search for analytical solutions to model solute transport in soil continues to be of scientific interest. The objective of this work is to obtain the analytical solution using the Lapace transform technique.

II. Mathematical model

A. List of Symbols

c	pollutant concentration (mg/l)
t	time since release of the solute (s)
x	the longitudinal distance (m)
D	the longitudinal dispersion coefficient (m^2/s)
v	the average flow velocity (m/s)
c_0	the initial concentration (mg/l)
s	Laplace domain
C	pollutant concentration in s-domain.
L	Laplace transform
erfc	the complementary error function.

B. The convection-dispersion model

The transport of the pollutant through a soil involves mainly two processes, convection and dispersion. The mathematical model which describes theses processes in a one dimensionnal soil profile is [4] :

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \quad (1)$$

The initial and boundary conditions are :

Initial condition:

$c(x,0) = 0$ for $x \geq 0$.

Boundary conditions :

$c(0,t) = c_0$ for $t \geq 0$

$c(\infty,t) = 0$ for $t \geq 0$

ISSN: 2356-5608

The governing equation can be solved analytically using Laplace transforms.

C. Analytical Solution

The mathematical model is a partial differential equation. To solve it, we use Laplace transform technique [5]. The solution is presented here briefly.

Applying Laplace transform to both sides of equation (1) on the variable t,

$$L\left\{\frac{\partial c}{\partial t}+v\frac{\partial c}{\partial x}\right\}=L\left\{D\frac{\partial^2 c}{\partial x^2}\right\} \quad (2)$$

$$sC(x,s)-c(x,0)+v\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2} \quad (3)$$

Where $L\left[c(x,t)\right]=C(x,s)$

Since the initial concentration is zero, c(x,0)=0, equation (3) becomes:

$$D\frac{\partial^2 C(x,s)}{\partial x^2}-v\frac{\partial C(x,s)}{\partial x}-sC(x,s)=0 \quad (4)$$

The equation (4) is a homogeneous differential equation, linear and with constant coefficients.

The solution is in the form :

$$C(x,s)=A(s)e^{\lambda_1(s)x}+B(s)e^{\lambda_2(s)x} \quad (5)$$

Where: $\lambda_1(s)$ and $\lambda_2(s)$ are the roots of the caraceristic equation:

$$D\lambda^2-v\lambda-s=0 \quad (6)$$

$$\lambda_1(s)=\frac{v+\sqrt{v^2+4Ds}}{2D}\succ 0$$

$$\lambda_2(s)=\frac{v-\sqrt{v^2+4Ds}}{2D}\prec 0 \quad (7)$$

The coefficients A(s) and B(s) are obtained using the boundary conditions.

When $x\to\infty$, we have $\lim_{x\to\infty}C(x,s)=0$ and A(s) =0.

Hence, equation (5) reduces to :

$$C(x,s)=B(s)e^{\lambda_2(s)x} \quad (8)$$

At x=0, the initial concentration is c_0, then

$$C(0,s)=L\{c(0,t)\}=L\{c_0\}=\frac{c_0}{s}$$

Substituting in equation (8) gives :

$$C(0,s)=B(s)=\frac{c_0}{s}$$

Equation (8) becomes:

$$C(x,s)=\frac{c_0}{s}e^{\frac{v-\sqrt{v^2+4Ds}}{2D}x} \quad (9)$$

The solution obtained in the *s*-domain is transformed back into the *t*-domain.

By applying the inverse Laplace transform to equation (9) and using Laplace transform tables and after several steps, the solution obtained is written as :

$$c(x,t)=\frac{c_0}{2}\left[erfc\left(\frac{x-vt}{2\sqrt{Dt}}\right)+e^{\frac{vx}{D}}erfc\left(\frac{x+vt}{2\sqrt{Dt}}\right)\right] \quad (10)$$

Where, erfc is the complementary error function.

We find again the analytical solution proposed by Ogata and Banks [6].

The presented analytical solution is exact. This solution is programmed in FORTRAN language in order to generate the solute concentration.

III. ILLUSTRATION

The concentration profile of solute in the soil is determined without iterative steps commonly used in numerical methods. The input requirement for analytical simulation includes: dispersion coefficient and soulte infiltration velocity.

The solubility of benzene in water is about 1780 mg/l, therfore, it has a high mobility [4].

The application of equation (10) is illustrated in figures 1 and 2. The impact of velocity on pollutant infiltration in soil is presented in figure1. As illustrated in figure 1, benzene can migrate at far distances with higher velocity.

The distribution of benzene concentration at different times (1year, 2years, 3 years and 5 years) is presented in figure 2. As illustrad in figure 2, more migration of the pollutant in soil is observed when time increases.

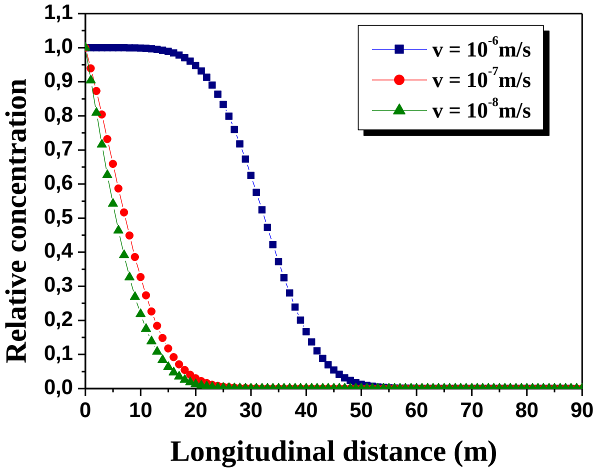

Fig.1. İnfluence of velocity on pollutant infiltration in soil.

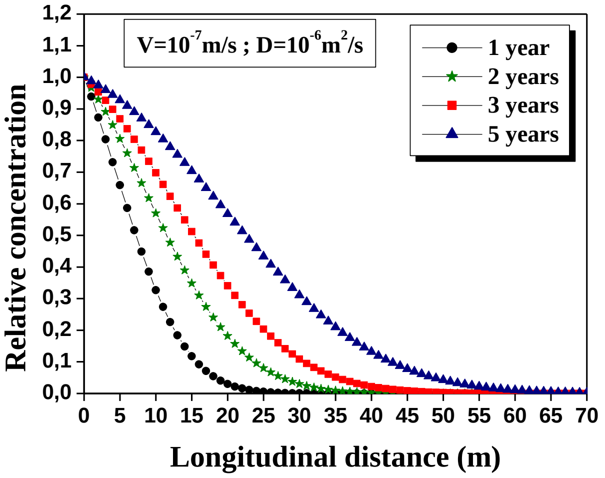

Fig.2. Distribution of pollutant concentration at different times.

IV. CONCLUSION

The migration of benzene through a soil is modeled using the convection- dispersion equation. The solution is obtained analytically using Laplace transforms.

The presented analytical solution is exact and the solute concentration is easily programmed and generated.

This work may helpful to predict the concentration of the contaminant in the soil and groundwater at futur times and to evaluate the risk associated with releases of such contaminants.

REFERENCES

[1] Y. Zhang, M. Person, E. Merino,“ Hydrologic and geochemical controls on soluble benzene migration in sedimentary basins,” Geofluids, vol. 5, pp. 83–105, 2005.

[2] Z. Chen, G.H. Huang, A. Chakma,“ Risk assessment of a petroleum-contaminated site through a multi-phase and multi-component modeling approach, ” Journal of Petroleum Science and Engineering , vol. 26, pp. 273–281, 2000.

[3] S.B. Patil, H.S. Chore, “Contaminant transport through porous media: An overview of experimental and numerical studies,” Advances in Environmental Research, vol. 3, pp. 45-69, 2014.

[4] C.W. Fetter. Applied hydrogeology, 4th ed, USA, Prentice Hall, 2001, pp. 400- 414.

[5] R. J. Beerends, H. G. ter Morsche, J. C. van den Berg and E. M. van de Vrie. Fourier and Laplace Transforms, 1st ed, Cambridge University Press, 2003, pp. 330-332.

[6] A. Ogata, R.B. Banks,“A solution of the differential equation of longitudinal dispersion in porous media,” US Geological survey professional paper 411 A , ” pp. 1-7, 1961.