3D NUMERICAL SIMULATION OF THE TRANSPORT OF EXPLOSIVES FROM UXO's AND LANDMINES

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ABSTRACT

The transport of explosives from buried mines in a three-dimensional (3D) array has been numerically modeled using the finite-volume technique. Compounds such as trinitrotoluene, dinitrotoluene, and their degradation products, are semi volatile and somewhat soluble in water. Furthermore, they can strongly adsorb to the soil and undergo chemical and biological degradation. Consequently, the spatial and temporal concentration distributions of such chemicals depend mainly on the mobility of the water and gaseous phases, their molecular and mechanical diffusion, adsorption characteristics, soil water content, compaction, and environmental factors affecting water content or its transport. A 3D approach is used in this work since two-dimensional (2D) symmetry may easily fade due to terrain topography: non-flat surfaces, soil heterogeneity, or underground fractures. The spatial and temporal distribution of explosives, in an inclined grid has been obtained. The fact that the chemicals may migrate horizontally, giving higher surface concentrations at positions not directly on top of the objects, emphasizes the need for understanding the transport mechanism of explosives when a chemical detector is used. Deformation in the concentration contours after rainfall is observed in the inclined surface and is attributed to both: the advective flux, and to the water flux at the surface caused by the slope. The analysis of the displacements in the position of the maximum concentrations at the surface, respect to the actual location of the mine, in an inclined system, is presented.

Keywords: Numerical simulation, transport, landmines, chemical detection.

1. INTRODUCTION

The goal of detecting and removing landmines is a great challenge for the scientific community. The presence of these artifacts in many regions of the world causes an environmental hazard as well as an important humanitarian concern. Several approaches are used to deal with this situation, being the most common ones those based in metals detection. Most anti-personal and anti-tanks devices, however, have little or none metal on them, and are essentially made of plastic compounds with the exception of parts of the fuse and activation mechanism. This forces the use of very sensitive devices resulting on a high frequency of false-positives.

Chemical detection has been implemented by the use of dogs, and their success lies on the quality of training and the personnel skills. On the other hand, spectroscopic techniques may be tuned to allow the detection of small traces of specific energetic compounds, and may serve as a basis for the development of more reliable chemical detectors. The main concern with this approach has to do with the fate and transport of the chemicals releases into the ground. Thus, factors affecting the fate and transport (like environmental and soil parameters) will also affect the process of locating the exact position of the buried object. Environmental factors (temperature, relative humidity, rainfall precipitation, wind, sun irradiation, pressure, etc.) as well as soil characteristics (water content, compaction, porosity, chemical composition, particle size distribution, topography, vegetation, etc), have a direct impact in the fate and transport of the chemicals released from a landmine. Chemicals like TNT, DNT, and their degradation products, are semi-volatile, and somewhat soluble in water. Also they may strongly adsorb at the soil particles, and are susceptible to degradation by microorganism, light, or chemical agents. Thus, transport may occur on the three phases, by multiple coupled mechanisms. Phelan and Webb, (2002), reported that the transport associated to water fluxes (advection) is usually the dominant transport mechanism [1].

In most cases, only vapor and solutes move through soils. The main processes contributing to chemical transport in soils are diffusion and convection (advection). As water evaporates from the soil; the chemicals are carried up and deposited at the ground surface. During rainfall, solutes are dissolved and migrate downward. Figure 1 pictures the factors affecting the fate and transport of chemicals from landmines. The large number of variables needed in a numerical modeling of this phenomenon as well as and the complexity of the transport equations may be perceived when observing this sketch.

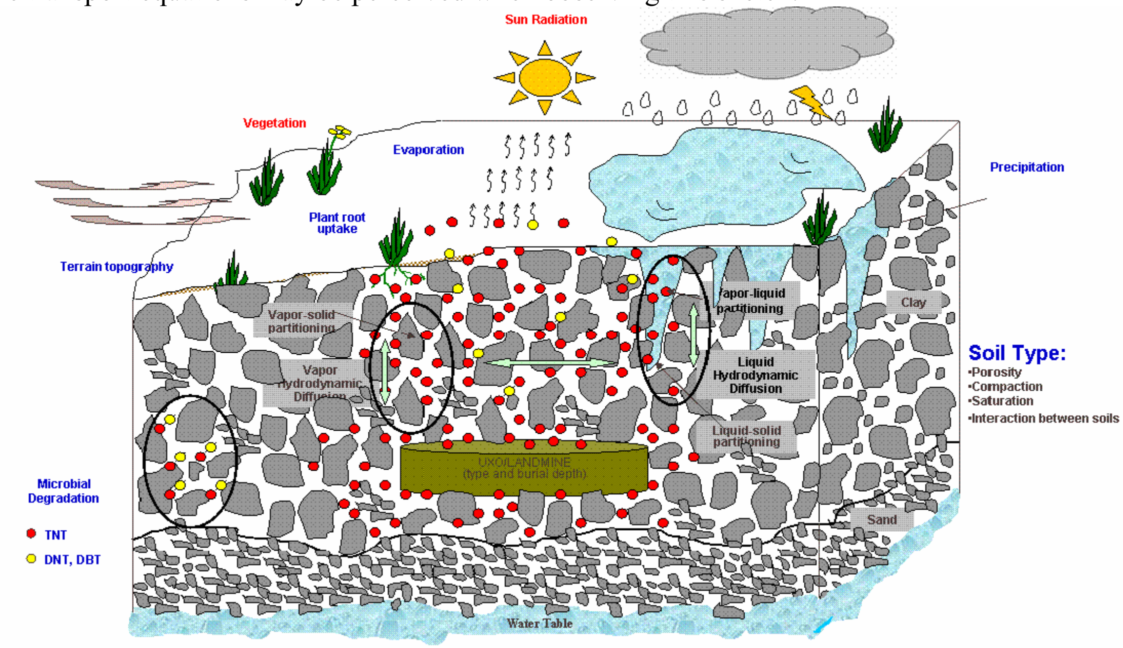

Figure 1: Variables and transport mechanisms in the fate and transport of chemicals released from landmines.

The actual modeling of this transport problem, requires a three dimensional approach. The symmetry implicit in two dimensional models, may be incorrect due to terrain heterogeneity, topography, inclined surfaces, etc. The code used by Sandia's group T2TNT [2] based on finite differences is adequate to study the vertical transport of contaminants and for modeling systems under controlled environments. For a more complex situation, one requiring a 3-D approach, a code based on finite elements is needed. In this preliminary work, we have based our simulations on FEHM, a code developed at Los Alamos Natl. Labs which allows the simulation of the energy and mass transport of multiple solutes in porous media for saturated and unsaturated systems. This program was developed in the early 1980's to simulate and solve geothermal and hot dry rock reservoirs. The most important application of this tool was in the Nuclear Waste and Management Program at Yucca Mountain. One of the most challenging aspects of these numerical simulations has to do with discretization of the system, namely, the generation of the simulation grid. Special attention must be given to the connection of the homogeneous grid (used for the underground) to the heterogeneous elements at the surface. In this task we have used as a staring point, the code LaGrit, also developed at LANL. In this work, we model the transport of the chemical species release from a landmine, subjected to soil and environmental factors. Since the chemical may migrate on all directions, we will focus our analysis on locating the point of maximum concentration at the surface, and its relation to the actual position of the object.

2.1. Simulation parameters

Over 80% of landmines are composed essentially of TNT [3]. Military grade TNT contains about 99% of 2,4,6-trinitrotoluene [4] [5]. The signature compounds released from landmines [6], in addition to their degradation complexes are: 2,4,6-TNT, 2,4-DNT, and 1,3-DNB. Some of the physical properties of these compounds have been reported. Table 1, summarized the properties of 2,4,6-TNT and 2, 4-DNT [7].
Capillarity characteristics are one of the most important soil properties affecting the water transport underground. The equations developed by van Genuchten describe the water flux induced by capillarity. Table 1 and 2, display the basic explosive-soil parameters as reported by [7] for a typical soil from Ft. Leonard Wood, Missouri, USA.

Table 1: Chemical Properties*

Definition	Parameter	2,4-TNT	2,4-DNT
Liquid-gas partition coefficient (Henry constant)	K_H(25°C)	8.2E-7	1.0E-5
Soil-liquid partition coefficient	K_d	5.7	2.9
Soil-gas partition coefficient [KSG]	$A_0(\log_{10}K_d'(w=0))$	15.3	13.1
	α	51.2	43.5
Liquid diffusion	D_l(cm^2/day)	0.580	0.632
Gas diffusion	D_g(cm^2/day)	5530	5790
Molecular Weight	MW	227.13	182.14

*Phelan and Webb, 2003

Table 2: Soil Parameters**

Property	Value	Units
Permeability	8.4 x 10^{-12}	m
Porosity	0.43	--
Fully-saturated conditions	0.999	--
Liquid Residual Saturation	0.1046	--
Matching Saturation	0.1105	--
Air Entry Pressure Parameter ($1/\alpha_{vG}$)	676	Pa
van Genuchten fitting parameters (n)	2.68	--
Bulk soil density (ρ_b)	1.5	g/cm^3

**Phelan and Webb, 2003

Average degradation rates for TNT and DNT [8] (half life) varies from hours to months, depending on the environmental conditions. For the matter of this preliminary work, we assumed half-life values of one year for TNT and DNT and a first order degradation model.
The driving force for water transport is strongly affected by the boundary layer humidity, and thickness. The boundary layer thickness is affected by atmospheric and soil-surface conditions [1], [7]. For the purposes of this study, a boundary layer thickness of 0.5 cm was chosen [9].

2.2. Simulation model

The system under study has dimensions of .72 m x 0.72 m x 10 m with a surface slope of 5.7°. A mesh consisting of 146,987 nodes and 836,471 elements in a 3D tetrahedral grid was generated. To increase the resolution in the areas of interest, elements of different size were used. Close to the surface (up to 20 cm of depth), the mesh spacing of 1cm in all directions was used. From 20 cm to 24 cm of depth, the mesh spacing increases to 2 cm. For depth higher than 21 cm, we chose a mesh of 7.2 cm into the X and Y directions, and of 9 cm into the Z direction.

In figure 2 we sketch the system. Notice that a water table located 10 meters under the surface has been imposed. In addition the 5.7° of slope, makes the surface declined from 10.07 m to 10 m (Δz=0.07 m).

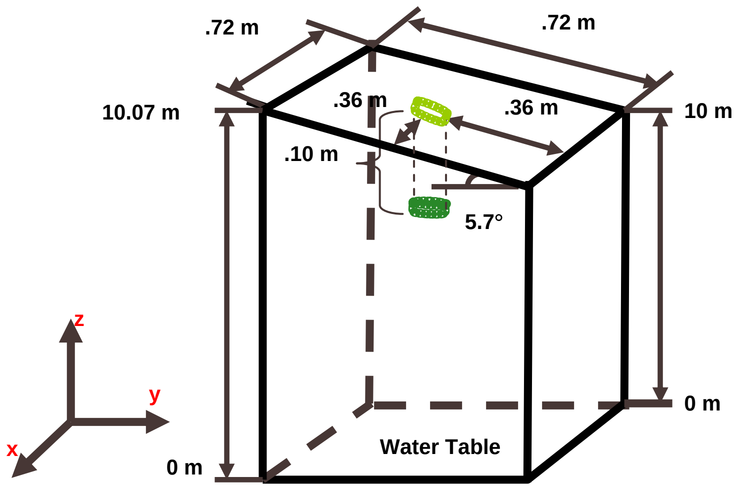

Figure 2: System dimensions and landmine location.

Non-flux boundaries are imposed around the system and water saturation is assumed at the bottom. At the surface, a convective boundary condition is imposed which depends on the relative humidity and the thickness of the laminar layer. The bottom boundary conditions, represented by the water table, are constant pressure and saturation, while the top air boundary layer conditions are constant pressure (0.1MPa), temperature (25°C), and relative humidity (50% RH). The weather conditions (pressure, temperature, wind, radiation, etc.) are coupled through the boundary layer thickness. The source of chemicals is modeled as one point of constant concentration located 10 cm below the surface, at the center of the system. This source point, which may be associated to a crack in the mine case, is equivalent to a solid with concentrations of 80% TNT and 20 % DNT in a weight base.

The simulation was divided into 4 phases. During the first stage, the system (without landmine) is allowed to achieve a steady state water profile. Simulation equivalent to 10 years, no precipitation, and initial soil saturation of 0.46, give a good starting point for the transport process. During this initialization phase a capillary fringe forms above the water table described by the van Genuchten model and influenced by the following surface boundary conditions: 0.1Mpa, 25°C, and 50%RH. The second stage with the TNT-DNT source 10 cm under the surface was run for 180 days, and may be described as an evaporation period since no precipitation was imposed. The third phase may be characterized as a rainfall period with precipitation at a rate of 2 cm/day, for three consecutive days. During this period, the surface relative humidity increased from 50% to 99%. The fourth phase consisted in a dry 2 days period.

3. SIMULATION RESULTS

The first stage permit the development of steady humidity profiles required as a starting point for the simulation. Homogeneous and isotropic properties for the soil are assumed, porosity, compaction, permeability, etc. are constant through the system. The following plots represent the contours of the concentration profiles of TNT and DNT at the surface. The coordinate origin, indicate the position of the chemical source which is placed 10 cm under the surface. The incline surface has slope into the y- direction, with the maximum elevation at the top of the chart.

Figures 3a and 3b, shows TNT + DNT concentration contours at the inclined surface after the second stage of the simulation (180 days of evaporation), in [μg/cm^3 soil water] and [μg/cm^3 soil], respectively.

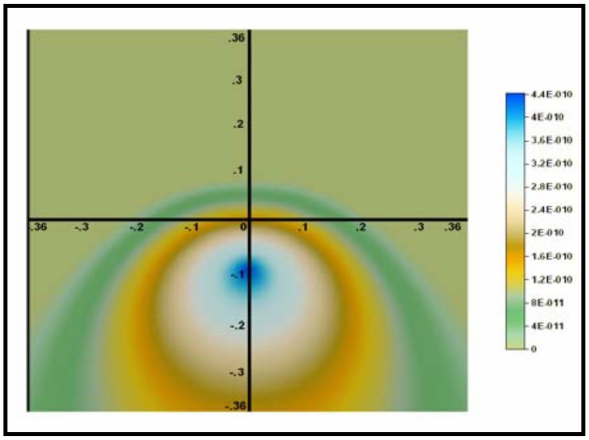

Figure 3a: Concentration contour of TNT + DNT in the liquid phase [μg/cm^3 soil water]

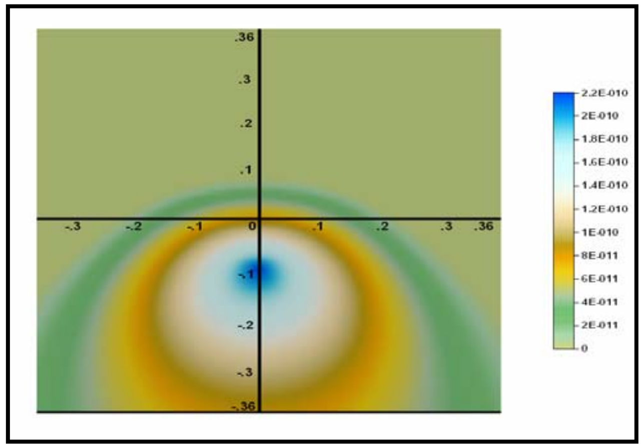

Figure 3b: Concentration contour of TNT + DNT in the solid phase [μg/cm^3 soil]

In both cases, it is possible to appreciate displacements of about 10 cm in the positions of the maximum concentrations, respect to the actual location of the buried object. Maximum concentrations of 4.4E-10 [μg/cm^3 soil water] and 2.2E-10 [μg/cm^3 soil], are appreciated for the liquid phase and solid phase, respectively. Figures 3c and 3d, shows the TNT + DNT concentration contours at the inclined surface after the third stage (3 days of rainfall), in [μg/cm^3 soil water] and [μg/cm^3 soil], respectively.

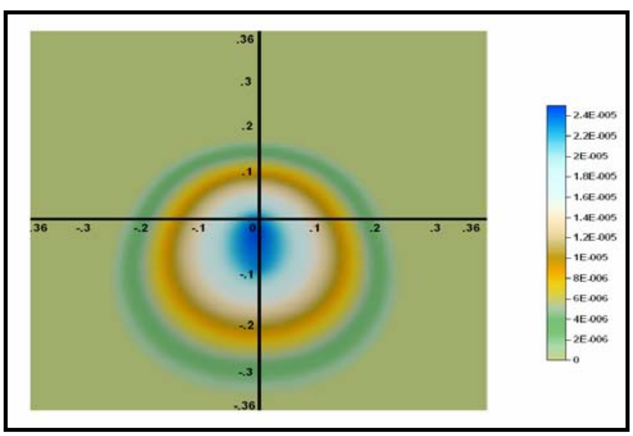

Figure 3c: Concentration contour of TNT + DNT in the liquid phase [μg/cm^3 soil water]

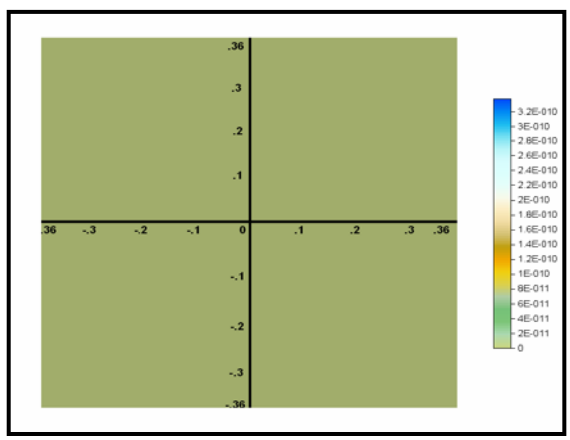

Figure 3d: Concentration contour of TNT + DNT in the solid phase [μg/cm^3 soil]

Precipitation washed down the surface and saturates the system. After this rainfall stage, concentration at the solid surface is close to zero (the chemicals are re-dissolved and carried away). When the system is saturated, the main transport mechanism is diffusion through the liquid phase, and the point of larger concentration move closer to the center of the figure (actual source position). The deformation of the concentration profile is evident as was also reported by [10]. The maximum concentration of TNT + DNT at the surface (in the liquid phase), is several orders of magnitude larger than in the second stage where only evaporation took place. This is in agreement with the report by Phelan, J. and Webb S., 2002 [1], who emphasized the importance of the water in the transport of landmines explosives

Figures 3e and 3f, shows the TNT + DNT concentration contours at the inclined surface after the fourth stage of the simulation (2 days of evaporation), in [μg/cm^3 soil water] and [μg/cm^3 soil], respectively.

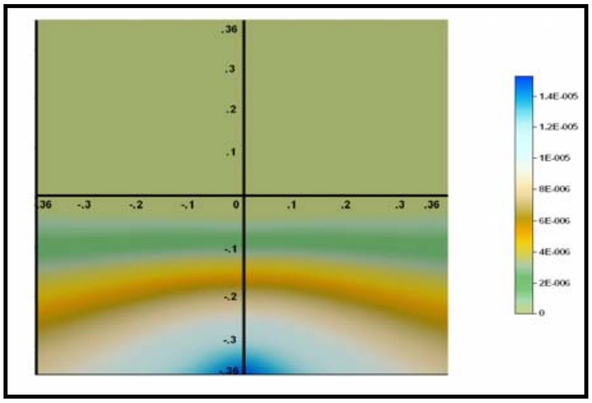

Figure 2a: Concentration contour of TNT + DNT in the liquid phase [μg/cm^3 soil water]

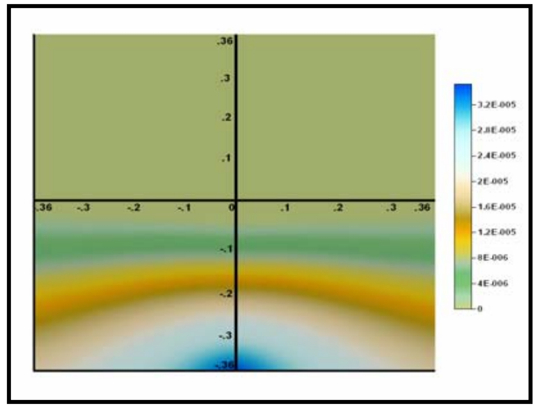

Figure 2b: Concentration contour of TNT + DNT in the solid phase [μg/cm^3 soil]

After this second dry period, media is partially saturated and advection and diffusion mechanisms are in competition. The horizontal component of the advective flux, move the point of maximum concentration following the terrain slope. A displacement in the position of the maximum concentration of more than 30 cm from the center is appreciated in both phases.

4. CONCLUSIONS

Numerical simulations are being used to study the characteristics of explosives chemical signatures transport in soils, and the spatial and temporal concentration contours at the surface above the buried object. A small slope on the terrain topography has a large effect on the displacement of the point of maximum concentration at the surface respect to the actual position of the source. Thus, chemical detection must be accompanied by some transport analysis; otherwise the actual position of the object may be missed.

Deformation in the concentrations contours at the inclined surface is observed and it is attributed mainly to the advective flux in the vertical direction, and the flux parallel to the surface. Spatial and temporal concentration distributions from the numerical model must be validated by comparison to actual results from experimentation. Experimental data is necessary to complete the process of model validation and obtain parametric equations by integrating simulations and experiments.

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