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RESEARCH ARTICLE

Modeling gasoline dispersion and risks in soil after the 2019 spill in Tlahuelilpan, Hidalgo, using the HSSM and ChemCAN software

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ABSTRACT

The dispersion of gasoline from the spill due to illegal fuel extraction activities from pipelines that occurred in Tlahuelilpan, Hidalgo, in 2019, was modelled. We used the HSSM software (vertical profile of gasoline saturation, profiles in the vadose zone, and radial profile of the light non-aqueous phase liquid lens), and prediction of its concentration in different media was obtained using the ChemCAN program. Gasoline infiltration would reach 7.5 meters deep at a rate of 0.30 mg/day in 10 days. Assuming that the vadose zone was at 10 m, the underground body of water would not be reached by the hydrocarbon. It was estimated that the maximum concentration of gasoline for the light fraction present in the soil was 2,200 mg/kg, ten times above the maximum permissible regulated limits. Benzene, a characteristic compound of gasoline, was studied in air-water-soil-sediment system, and it was observed that it would preferably accumulate in the sediments (84.9%) and the soil (11.8%), being the systems in greater contact with gasoline. The greatest risk due to the spillage during three subsequent years was related to the surface of the soil, affecting the flora, fauna, and population with exposure by inhalation and dermal contact, and the flammable danger of gasoline.

Keywords: gasoline spill; HSSM software; ChemCAN software; infiltration model; risk assessment

1. Introduction

Hydrocarbons are raw materials used extensively throughout the world and, when not properly managed, they offer both environmental and health risks, due to their content of toxic and dangerous substances. Extraction, conduction, refinement, and transportation of petroleum-based products can cause serious pollution problems[1,2]. In Mexico, a recognized petroleum producer, there are extensive areas contaminated due to gasoline and diesel spills. There have been 13,832 clandestine taps for fuel theft, 4,509 of them generated pollution of the sites due to gasoline spills[3]. This represents a serious risk to life and integrity of near-by communities, as it occurred in 2019 in the town of San Primitivo, municipality of Tlahuelilpan, Hidalgo, when after gasoline escaped uncontrollably for several hours, culminating in an explosion at a clandestine intake in the Tuxpan-Tula pipeline, 137 people died, and irreversible ecological damage was generated[4] (**Figure 1**).

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Figure 1. San Primitivo, Tlahuelilpan, a day after the explosion of the spill at the clandestine intake[5].

Spilled hydrocarbons infiltrate into different strata, depending on the porosity and structure of the soil. A fraction of the contaminant material is retained in the solid phase, but the liquid can be conducted into groundwater, forming a layer known as a contamination lens. Light non-aqueous phase liquid lenses (LNAPL) are less dense and immiscible accumulations of liquid hydrocarbons found in groundwater and shallow soils; they are a persistent source of pollutants[6].

Conceptual modeling of oil spills in a soil-aquifer system describes the transport process and can help to predict environmental risks and hazards. Among the best-known models are the HSSM (Hydrocarbon Spill Screening Model) that simulates flow and transport of a chemical constituent of the LNAPL from the surface to the water table; radial spreading of the LNAPL at the water table, and dissolution and aquifer transport of the chemical constituent[7]. In addition, the ChemCAN model is designed to estimate average concentrations in air, fresh surface water, fish, sediments, soils, and vegetation, and is intended to assist in human exposure assessment[8]. The HSSM model has been successfully applied in countries such as Canada[9], and China[10]. For instance, Kawamoto *et al*.[11] have reported the application of ChemCAN in the description of the fate of 68 pollutants in Japan.

This work aimed to model the possible dispersion in the soil of gasoline from the spill that occurred in Tlahuelilpan, Hidalgo, using the version 1.20a HSSM free software. It also intended to predict its concentration in air, water, soil, and sediments using the version 6.00 ChemCAN program.

2. Methodology

2.1. Study area

The municipality of Tlahuelilpan is located in the state of Hidalgo (20°07'47" north latitude, 99°13'43" west longitude, 2040 masl)[12] (**Figure 2**). The town of San Primitivo (20°07'25" north latitude, 99°13'38" west longitude), is located 5.4 km southeast of the Juandhó gasoline pumping station and half a kilometer east of the Tuxpan-Tula pipeline that runs parallel to the municipal highway. The territory consists of 80% vertisol plains. Its climate is moderate with rainfall from June to September, with an average annual temperature of 17 ° C, and total rainfall of 675 millimeters/year[12].

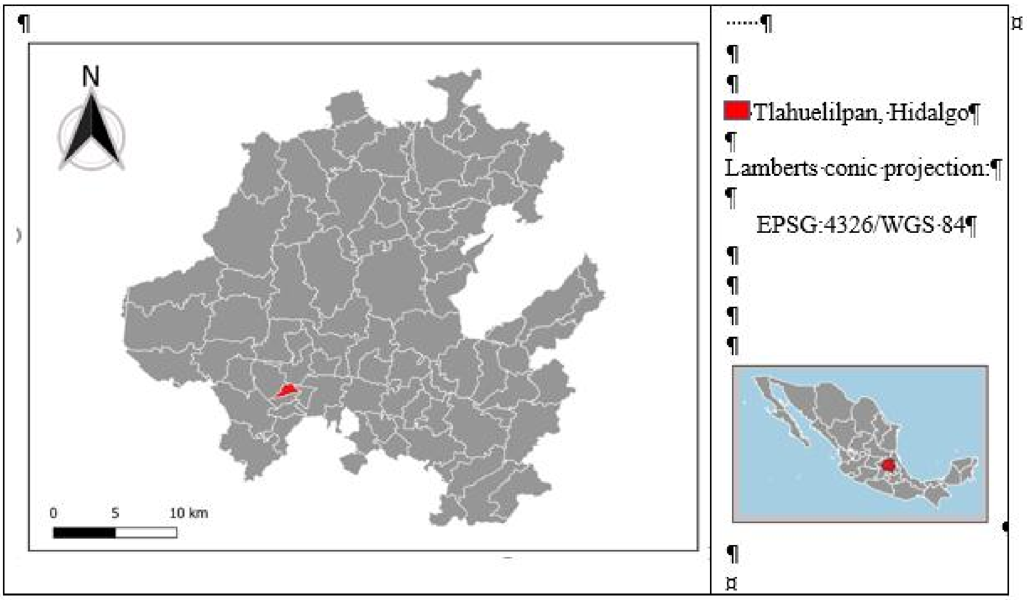

Figure 2. Geographical location of the municipality of Tlahuelilpan, Hidalgo (Own elaboration with data retrieved from INEGI[13]).

2.2. Evaluation model

The simulation of the spill was performed with the version 1.20a HSSM free software[7], based on the Hydrocarbon Spill Screening Model[14]. To obtain the specific model of San Primitivo, Tlahuelilpan, the parameters corresponding to the study site and the physical and chemical properties of the pollutant were entered (**Table 1**). The likely plume of contamination and associated risk were estimated based on the presence of nearby water bodies, the soil type of Tlahuelilpan, the amount of gasoline spilled, and the health effects of the contaminants present. The aquifer of the Mezquital Valley was taken as a reference with static depth between 10 and 40 m. The shallowest values (10 m) corresponded to the Endhó Dam[15]. The soil type selected for the model was vertisol[12].

Table 1. Parameters applied in HSSM software.

Parameter		
Soil bulk density (g cm^{-3})	2.500	[16]
Gasoline density (g cm^{-3})	0.750	
Dynamic viscosity of gasoline (cp)	0.450	[10]
Surface tension gasoline (dina cm^{-1})	26.00	
Porosity (f)	0.400	[17]
Soil-water partition coefficient (L kg^{-1})	80.000	[16]
Hydraulic conductivity (m d^{-1})	1.280	[18]
Residual water saturation	0.200	
Residual saturation of gasoline in the vadose zone	0.100	
Gasoline-water partition coefficient (L kg^{-1})	312.000	[10]
Maximum gasoline saturation in the lens	0.326	

The simulation of the spill from the surface to the water table was carried out using the Kinematic Transport of the Oily Pollutant (KOPT) module and the HSSM Module for the movement of the LNAPL lens and the Gaussian Type Transient Source Plume (TSGPLUME) Module. To estimate the possible health risks related to gasoline, its average concentration in air, soil, sediment, and surface fresh water was calculated, using the ChemCAN free software. Benzene was specified as a representative substance of the components of gasoline, since its characteristics of low solubility in water and toxicity, allow determining the risk with acceptable safety margins in scenarios of environmental relevance[19].

3. Results and discussion

The water saturation zone and the vertical saturation profiles up to the water table, obtained with the one-dimensional KOPT model (**Figure 3**), show a constant saturation and gasoline migration rate during the first 18 h of the spill. After 24 h, gasoline saturation and migration velocity decreased rapidly; 5.5 days after the spill, the net fraction of gasoline in the vadose zone was calculated at 0.2.

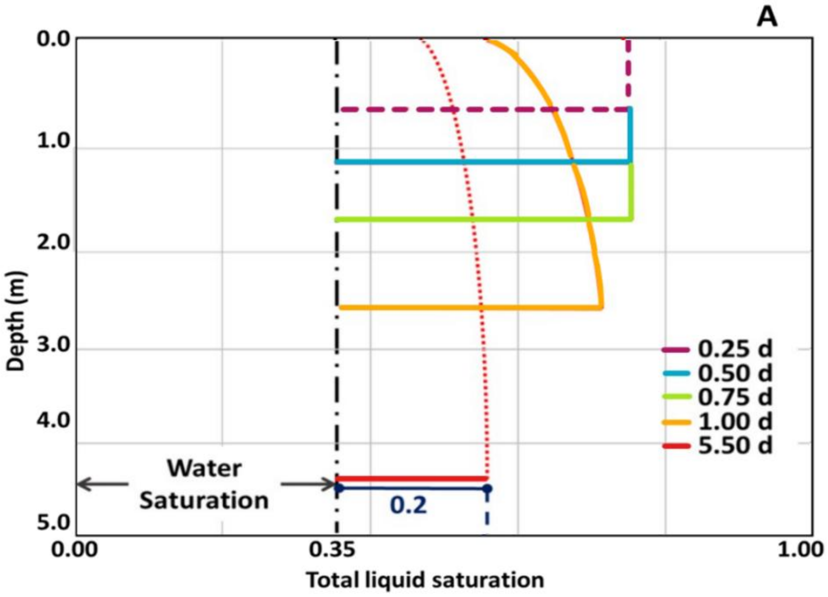

Figure 3. Vertical profile of gasoline saturation in Tlahuelilpan, obtained with HSSM software.

The relationship between depth (y) and time (x) was established according to equation:

$$y = 1.25ln(x) + 2.22 \ (R^2 = 0.963),$$

from which it could be estimated that the pollutant front would reach the water table in 9.3 days. The ratio of saturation fraction (z) and time (x) is represented by the equation: $z = 0.1748x^{-5.13}, (R^2 = 0.997)$, with a gasoline net saturation fraction (gasoline volume/porosity volume) of 0.17. The saturation of the water with a constant value of 0.54, was fixed up to 8 m deep, with a margin of error of 2 m with respect to the water table[15]. The net saturation fraction in the vadose zone was 0.24, and it was reached ten days after the spill and at 4.25 m depth (**Figure 4**). This distance is considered the minimum depth of infiltration of the spill, beyond which the saturation fraction decreases at the rate of 0.03 per meter.

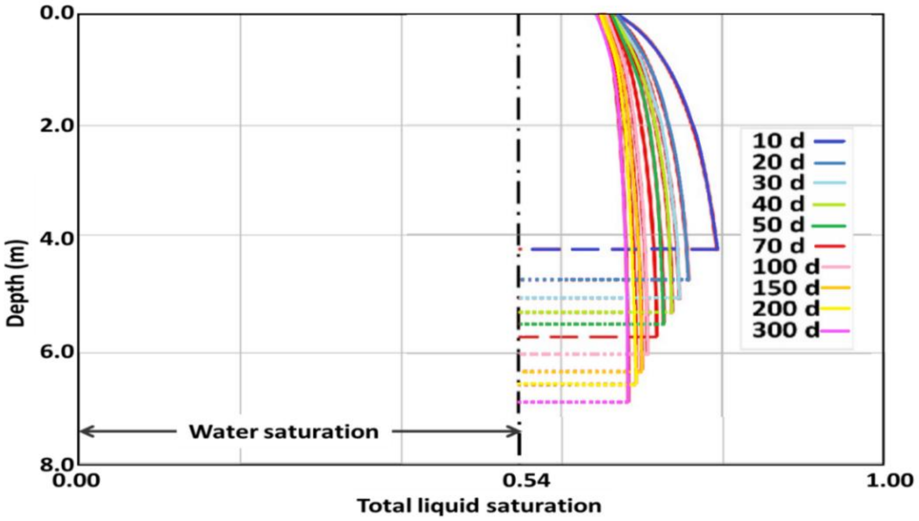

Figure 4. Gasoline saturation profiles in the vadose zone of the spill occurred in Tlahuelilpan (Own elaboration with the HSSM software).

Fuel transport was modelled up to 300 days after the start of the spill, when the infiltration front would reach a net saturation fraction of 0.14. The net saturation fraction of gasoline would be 0.03 when it met the water table. The projection of the historical position of the LNAPL front of the spill (**Figure 5**) shows that in the first days gasoline would reach 4 m deep. Six months later, it would be 6.5 m deep, and 3 years later it would reach 7.5 m. LNAPL was projected to peak its radius at 7.5 m depth near the first 20 days after the spill, while by then, the maximum radius of benzene would be present at a depth of 7 m.

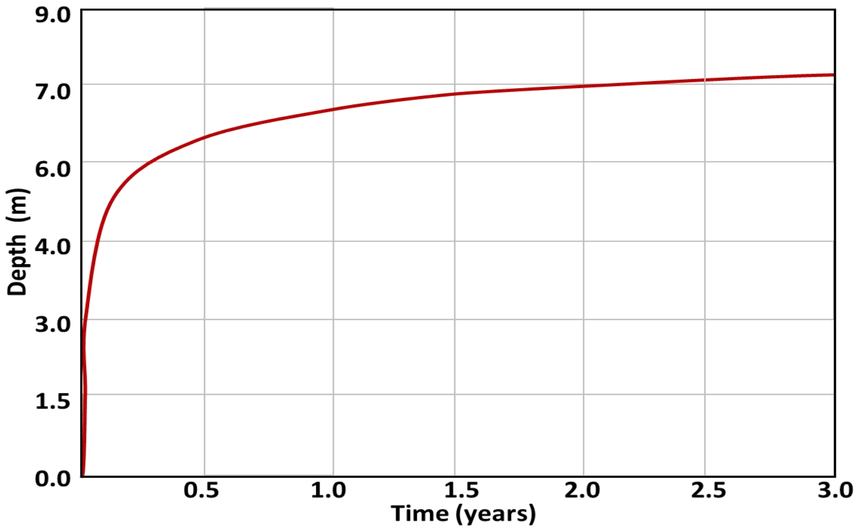

Figure 5. History of the position of the LNAPL front of the spill that occurred in Tlahuelilpan (Own elaboration with the HSSM software).

The maximum concentration of the total mass of LNAPL was calculated for the first 3 days of the event, as 2,250 mg/kg soil. Experimentally, the maximum concentration of the light fraction of total petroleum hydrocarbons in 27 samples from the spill area was 3,219 mg/kg soil[4]. The maximum limit allowed in Mexican legislation for this fraction is 500 mg/kg dry industrial soil[20]. Both concentrations, theoretical and experimental, exceeded this limit by more than an order of magnitude. Considering this fact, the maximum vertical migration rate of the pollutant was 0.3 mg/d, and 10 days after the spill the velocity gradually decreased until the vertical movement ceased after 2 months. It can be estimated that during the period of greatest transport, the pollutant only reached depths between 0 and 3 meters. The vertical movement of the LNAPL through the vadose zone would stop at 6 m, preventing the contact of gasoline with the aquifer.

The model revealed that the greatest risk of spillage during three subsequent years would be found on the soil surface, suggesting the affectation to flora, fauna, and human population with exposure by inhalation and dermal contact, including the flammable hazard of gasoline[21].

The probable plume of modelled contamination up to 300 days would reach in a cross-section of the LNAPL lens of 8 m radius and a depth of 7.9 m (**Figure 6**). Considering the reference water table at 10 m depth, it was estimated that it would not be affected by the gasoline spill.

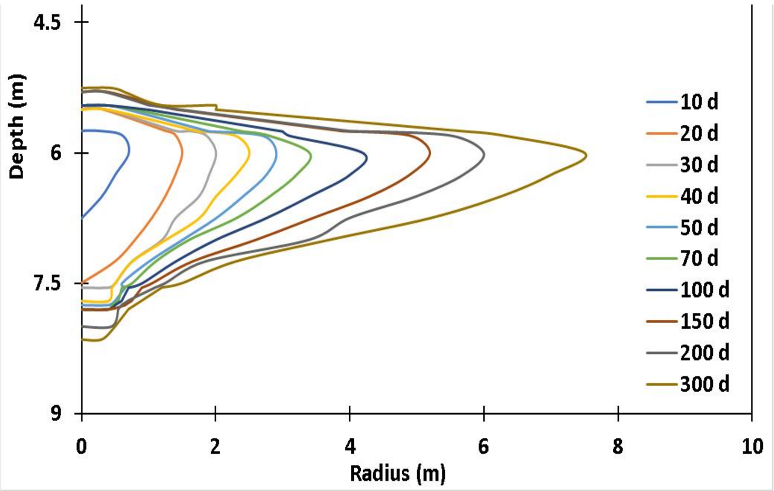

Figure 6. Radial profile of the LNAPL at different times from the start of the spill (own elaboration using the HSSM software, 2022).

The balance performed with the ChemCAN program estimated that a total mass of benzene of 1,480 kg entered the ecosystem at the time of the spill and that it would have a residence time of 4,301 days due to the slow degradation of the compound in the soil. An emission rate of 2.7 kg/d in water, air, and soil was calculated. Transport flows indicated that the net transfer from air to soil would be 1.2 x 10^{6} m^3/h, from water to sediment 1.0 x 10^5 m^3/h, and from water to air, 3.8 x 10^4 m^3/h. It can also be observed that soil and sediment represented a containment barrier for the transport of the contaminant over long distances from the spill site. The most affected systems would be sediments (1,256 kg) and soil (174 kg) due to their ability to retain gasoline (**Figure 7**).

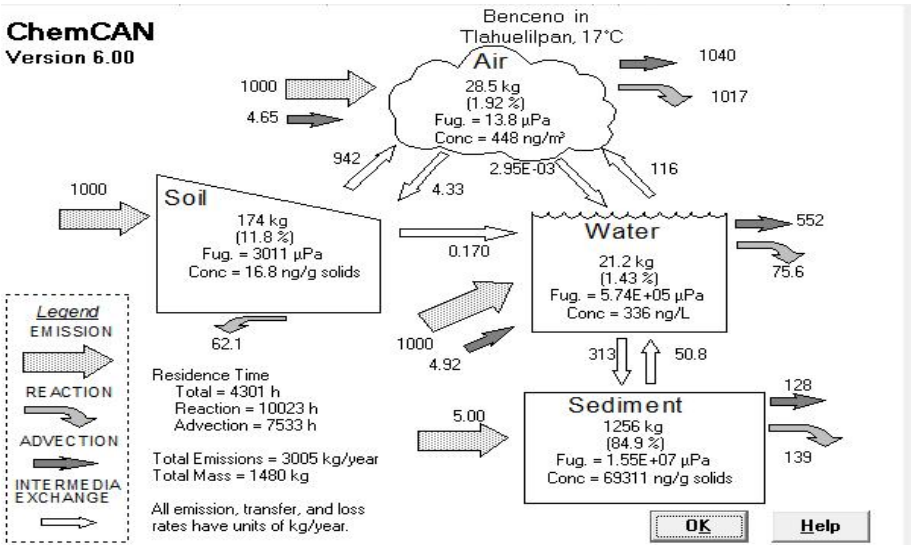

Figure 7. Diagram of benzene transport model between water, air, soil, and sediment systems, obtained with ChemCAN.

The polluted open field site in Tlahuelilpan suffered extensive impacts and the estimations in this study and field samplings indicate high risks that should be attended. These would require the application of *in-situ* bioremediation techniques such as biostimulation or bioaugmentation which have economical and technical advantages[22]. In the former method, native microorganisms are stimulated to grow with the addition of nutrients like phosphorus and nitrogen, and sometimes, oxidating agents to reduce the presence of organic contaminants. On the other hand, bioaugmentation consists in the addition of previously selected microbial species to support oil degradation, could be very effective, considering that the gasoline spill and explosion affected the native microorganisms capable to degrade the pollutants.

4. Conclusion

This work used the *HSSM* and ChemCAN programs to model the dispersion of hydrocarbons and the possible health risks, derived from the gasoline spill that occurred in Tlahuelilpan, Hidalgo on January 18, 2019, due to illegal fuel extraction activities from pipelines.

It was observed that gasoline infiltration would reach 7.5 meters deep at a maximum infiltration flow of 0.30 mg/day in the first 10 days. Assuming that the vadose zone were 10 meters deep, the underground body of water would not be affected by the released hydrocarbon.

With the HSSM software it was estimated that the maximum concentration of gasoline for the light fraction present in the soil would be approximately 2,200 mg/kg, ten times above the maximum permissible limits regulated. The probable plume of contamination was defined, observing that the first 40 days the radial growth of the LNAPL would be carried out slowly, with an increase of 0.5 meters after 10 days and 2.3 meters in 40 days. The gasoline spill would reach a radial length of approximately 7.5 meters.

The transport and reaction of benzene, as a characteristic compound of gasoline, in an air-water-soil-sediment system was studied, and it was observed that the media where this pollutant would be found in a greater percentage are the solid phase of the sediment (84.9%) and the soil (11.8%), being the systems in greater contact with gasoline. The greatest risk due to the spillage during three subsequent years would be related to the surface of the soil, affecting the flora, fauna, and human population with exposure by inhalation and dermal contact, and the flammable danger of gasoline.

Conflict of interest

Authors declare that there is no conflict of interest.

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