Computer Simulation of Heated Soil Vapor Extraction System for Effective Remediation

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ABSTRACT

Soil remediation using Heated Soil Vapor Extraction System has gained a significant attention in recent years. The process, developed by Advanced Remedial Technology, comprises of a heat well (heat source) and an extraction well (sink). These wells are pipes, which are implanted in the soil. Heating is accomplished by circulating hot oil through the heat exchange units in heat well. The extraction well has a blower, which sucks the air, and other volatile gases that are evaporated due to heating. An analysis aimed at improving the predictability of the process using numerical tools has been carried out. The key parameters in the process can be identified as the distance between the wells, the temperature that has to be maintained in the heat well and the time required vaporizing the gases and taking them off the soil. These parameters are strongly dependent on the properties of the soil and properties of the chemical pollutants present in the soil. An attempt has been made to model the real process of heating the soil and vaporizing the chemicals in the soil. Such comprehensive analysis is very much helpful in predicting the different parameters as discussed above and result in increase in effectiveness and efficiency of the process.

KEY WORDS: Heating technology, Remedial process, species transport, discrete phase, modeling

NOMENCLATURE

\[ D \text{ diameter of the particle (m)} \\
F \text{ force (N)} \\
J \text{ diffusive mass flux (kg/m}^2\text{)} \\
R \text{ mass rate of creation or depletion of the chemical (kg/sec)} \\
S \text{ mass rate of addition (kg/sec)} \\
T \text{ temperature (K)} \\
g \text{ Gravitational acceleration (m/sec}^2\text{)} \\
t \text{ time (sec)} \\
u \text{ velocity (m/s)} \\
m \text{ mass (kg)} \]

Greek symbols
\[ p \text{ mass density (kg/m}^3\text{)} \\
\mu \text{ molecular viscosity (N-S/m}^2\text{)} \]

Subscripts
\[ p \text{ particle} \\
x \text{ co-ordinate axis} \\
z \text{ co-ordinate axis} \]

Superscripts
\[ 1 \text{ species} \]
\[ D \text{ drag} \]

INTRODUCTION

The Soil Remediation Process has gained an enormous attention for the last decade in order to make the surroundings environmentally friendly. The areas around chemical companies or waste disposal sites have been seriously contaminated from the chemicals and other polluting materials that are disposed off. The present research effort is concentrated on modeling the Heated Vapor Extraction System, which is a very efficient and a cost effective process. Different remediation processes like venting [1] for soil contaminants like diesel, solvent washing of soil [2] for contaminants like Pentachlorophenol (PCP), which is a wood preserving agent have been studied and used for the purpose. The present research analysis focuses on the Heated Soil Vapor Extraction (HSVE) [3] process, which is a remediation process primarily used to strip the soil off pollutants like organic compounds that include solvents, fuels and Para-Nuclear Aromatics (PNA). Previous research work on this process by the authors [4,5] has proved the feasibility and the effectiveness of the process. Application of this process in real-life case has shown that, in the soil contaminated with fuel like diesel, the levels of diesel after the process have been reduced to as low as 1 PPM. Soil contaminated with organic substances can be remediated to either non-detect level or below acceptable Government standards.

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Heated Soil Vapor Extraction (HSVE) system essentially consists of a heating source pipe and the extraction well embedded in the soil. The number of heat source pipes and the extraction wells depends on the type of soil, the type of pollutants and the size of the area to be cleaned. The heat source heats the soil, which is transported in the soil by means of conduction and convection. This heating of soil results in vaporization of the gases, which are then driven out of the soil by the extraction well. The extraction well consists of the blower which would suck the vaporized gases out of the system.

HSVE cleans contaminated soil (biological and organic) by a thermally enhanced recovery method. It has been successfully used to treat toluene, xylene, chlorinated solvents, total petroleum hydrocarbons, polyaromatic hydrocarbons and very high numbers of diesel fuels. Key points of the HSVE technology include:

- Utilizes a closed-loop system that is:
  - Welded
  - Pressure tested, and
  - Enclosed with outside barrier piping.
- Circulates hot oil/water into the piping grid between injection and extraction wells,
- Transfers heat through conduction as well as convection.
- Treats organic constituents in-situ
- No excavation of the contaminated soil, and
- Removes any organic concentration of contaminants.

HSVE has following proven benefits:

- Reduces clean-up time from years to weeks,
- Minimally disrupts the contaminated area,
- Suitable for installation under existing structures,
- Uniform efficiency throughout the year, and
- Utilizes a small area for its equipment.

**HSVE System**

Figure 1 shows the schematic of a typical HSVE system used in this study. The extraction process is accelerated by the heating system as shown in Fig. 1. This system is interposed between re-injection and extraction (recovery) wells to heat sub-surface soil 20 by means of thermal conduction and convection. Fluids such as oil, water, steam or ethylene glycol are heated with a boiler, or other heat exchange techniques and then pumped through piping 22 to heat exchange devices 24 inserted in thermal contact with the subsurface soil 20. Due to the isolation of the heated fluid from the soil, no increase in contamination is caused by this heating technique. Additionally due to high heat obtainable (approximately 700 degrees F) contaminants, such as gasoline, can be stripped out of the soil in approximately 2-4 weeks.

The simulation model that is used to carry out the analysis is based on the fact that the system of the pipes that perform the heating and suction operations are arranged in a symmetrical manner as shown in Figure 2. Thus a quarter-symmetrical model has been chosen for the analysis. The geometry used for the analysis is shown in Fig. 3 with the dimension 5'×5'×10'. Both the heating pipe and suction pipe extend 7.5' depth into the soil.
computational fluid dynamics (CFD) for discretizing and modeling fluid flow and heat transfer in complex geometries. With the other products, FLUENT package mostly includes solving the domain. and initial conditions, defining fluid properties, executing the creating the geometry and mesh. Once the meshed geometry dimensional geometries in variety of conditions. It can be used have been imported into the software, all remaining operations are performed in the solver. These include setting boundary and initial conditions, defining fluid properties, executing the solution, refining the grid and viewing and post processing the results. This software is capable of simulating two and three-dimensional geometries in variety of conditions. It can be used for steady or transient analysis of convective, coupled or radiative heat transfer. Mixing, reactions of chemical species and vaporization can also be modeled in this software. Earlier analysis [4] carried out was more concentrated on proving the effectiveness of the whole system. Further, after demonstrating the effectiveness, an attempt has been made to understand the physics of the system in greater details. Thus, effect of convection coupled with multiple species analysis and change in phase analysis has been carried out in the present study.

Species transport Analysis.
In this analysis, three different species are assumed to be present in the soil, namely: benzene, toluene, and water vapor. Conservation of mass equations were solved and the mass fraction of each component was predicted using the convection-diffusion equation. FLUENT predicts the local mass fraction of each species, $m_i$, through the solution of a convection-diffusion equation for the $i$th species. This conservation equation takes the following general form:

$$\frac{\partial}{\partial t}(\rho m_i) + \frac{\partial}{\partial x_j}(\rho u_j m_i) = \frac{\partial}{\partial x_j} J_{i,j} + R_i + S_i \quad \text{Eq 1}$$

where $R_i$ is the mass rate of creation or depletion by chemical reaction and $S_i$ is the rate of creation by addition from the dispersed phase plus any user-defined sources. An equation of this form will be solved for N-1 species where N is the total number of fluid phase chemical species present in the system.

Discrete Phase Modeling.
To simulate the evaporation of chemicals, discrete phase modeling in a Lagrangian frame of reference is used. With the trajectory of a particle, Fluent always keeps track of the heat, mass and momentum gained or lost by the particle stream that follows that trajectory and these quantities are incorporated in the subsequent continuous phase calculations. Thus, the continuous phase always impacts the discrete phase and one can incorporate the effect of the discrete phase trajectories on the continuum. This two-way coupling is accomplished by alternately solving the discrete and continuous phase equations until the solutions in both phases have stopped changing. The second phase consists of spherical particles (which may be taken to represent droplets or bubbles) dispersed in the continuous phase. The trajectories of these discrete phase entities as well as heat and mass transfer to/from them are computed.

FLUENT predicts the trajectory of a discrete phase particle (or droplet or bubble) by integrating the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written (for the $x$ direction in Cartesian coordinates) as:

$$\frac{du_p}{dt} = F_D (u - u_p) + g_i (\rho_p - \rho) / \rho_p + F_1 \quad \text{Eq 2}$$

where $F_D (u - u_p)$ is the drag force per unit particle mass and

$$F_D = \frac{18 \mu}{\rho_p D_p^2} C_D \frac{24}{Re} \quad \text{Eq 3}$$

Here, $u$ is the fluid phase velocity, $u_p$ is the particle velocity, $\mu$ is the molecular viscosity of the fluid, $\rho$ is the fluid density, $\rho_p$ is the density of the particle, and $D_p$ is the particle diameter. $Re$ is the relative Reynolds number, which is defined as

$$Re = \frac{\rho D_p |u - u_p|}{\mu} \quad \text{Eq 4}$$

Boiling of Droplet Particles.
In this study we assumed that the contaminants are present in the droplet particles form. The convective boiling of the droplet starts when the temperature of the droplet reaches its boiling temperature, $T_{bp}$, and while the mass of the droplet exceeds the non-volatile fraction, $1 - L_0$.

The equation of the boiling rate is given by equation 5.
\[
\frac{dQ}{dt} = 4k_w \rho c_w D_p \left[1 + 23(Re_p) \ln \left(1 + \frac{c_w(T_w - T_p)}{h_p} \right) \right] \quad \text{Eq5}
\]

where:
- \( c_w \) = heat capacity of the contaminants in vapor phase (J/kg-K).
- \( \rho_p \) = droplet density (kg/m³).
- \( k_w \) = thermal conductivity of the contaminants in vapor phase (W/mK).

The general procedure adopted in solving for discrete phase quantities is:
1. Solve for continuous phase.
2. Create discrete phase injections.
3. Solve the coupled flow.
4. Track the discrete phase injections.

The flow chart used for the simulation is shown in figure 4.

**Boundary Conditions.**

Appropriate boundary conditions were chosen to represent the actual physics of the process involving soil remediation. The boundary conditions used here have been closely matched against the experimental data obtained from the field.

According to figure 3, in the pipe region (B) where blower sucks away the gaseous chemicals, a velocity of 0.32 m/s is assumed (from blower and pipe specifications). On top surface of the soil (A), pressure is assumed to be atmospheric since it is exposed to ambient conditions. On the side surfaces (D), no-slip boundary condition (from symmetry) is applied.

For thermal analysis, the heating side of the system (C) is considered to be at a constant temperature of 477 K, and the region from where the gaseous chemicals are withdrawn from the system (B), a temperature of 322 K is assumed. On top surface (A) ambient temperature of 300 K is assumed. On side surfaces (D), insulated (zero heat-flux) boundary condition (from symmetry) is applied. At the bottom surface, (E) it is assumed that the waterbed exists from the given geographic configuration and since it is a faraway boundary, a temperature of 300 K is assumed.

For discrete phase modeling, escape boundary condition for particles is applied in the region (B) where suction is applied. On top surface (A), again, escape boundary condition is applied since the particles can escape to the atmosphere as they rise after being heated. On all other side surfaces (D) and (C) zero diffusive flux boundary condition is applied due to symmetry. On the bottom surface (E), it is assumed that all the species exist at equal mass fractions (0.33), and the concentration of each species is assumed to be 100% here.

**RESULTS AND DISCUSSIONS**

In this study, we considered the waterbed at 10' depth from the top surface. It is important that the depth of waterbed from the soil surface and the concentration of chemicals should be known as correctly as possible. Excess amount of water in soil decreases the performance of HSVE, since in the saturated zone it is difficult to remove chemicals. To see the effect of moisture in the soil we took only three kind of droplet particles in our present simulation i.e. benzene, toluene and water vapor. The steady state temperature distribution is shown in Fig. 5. Initial temperature in the hot and cold well was 477 K and 322 K, respectively. After simulation we find that the temperature varies between 455 K and 300 K. Since the top surface is exposed to atmosphere it will always remain constant at 300 K. In the interior region of the soil heat diffuses by conduction of the soil and convection of the droplet particles. Depending on the soil conductivity and soil permeability the heat diffusion rate changes. Here, in our simulation we considered soil conductivity as 0.16 W/mK and soil permeability as 1×10⁻¹⁰ m².
Presence of the water vapor increases the time for effective remediation. This soil vapor extraction system will be more effective if the soil is dry and waterbed is far below the top surface.

Figure 8 shows the distribution of toluene concentration in the soil. As it evaporates from the bottom and interior of the soil it is sucked by the suction well. So the concentration of toluene increases near the suction well.

Figure 9 shows the benzene concentration in the soil. This distribution is similar to the toluene distribution as shown in Fig. 8. Since toluene and benzene are similar kind of chemicals, they vaporize almost at the same rate. Both of these toluene and benzene concentration is higher near the bottom surface. This can be attributed to the fact that we applied zero diffusive flux to all other surfaces except the bottom one. Also because of the presence of the waterbed at 10' depth, the temperature does not vary near the bottom surface.
CONCLUSIONS

The previous work by Jadhav, et al. [4,5] considered only the dry soil mixed with hazardous chemicals. In this present study we included water vapor in our chemical mixture. Though we excluded other hazardous chemicals like ethylacetate-benzene, xylene and other petroleum hydrocarbons, this analysis is more realistic one. Because more or less soil itself has some water content which makes the process more difficult and expensive. Also, applying the waterbed at a certain depth is a new concept in this case. Instead of applying zero diffusive flux, we applied constant source moisture and other chemicals at the bottom boundary. This has affected the performance of the remediation process. This is a very comprehensive model, which incorporated the species transport of the different chemicals in the process. Discrete phase model was used to model the phase change of the chemicals. Future work will be directed towards the transient analysis of the same phenomena. The transient analysis can actually show the time requirement for complete remediation process. The transient behavior of different chemicals can be predicted from the transient analysis. This will give us more insight to the physical phenomena and serve as a numerical predictive tool for more efficient process.

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