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Project Summary

Kinematic Modeling of Multiphase Solute Transport in the Vadose Zone

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The goal of this research was the development of a computationally efficient simulation model for multiphase flow of organic hazardous waste constituents in the shallow soil environment. Such a model is appropriate for investigation of fate and transport of organic chemicals introduced to the soil through spills on the ground surface, leakage from surface impoundments or underground storage tanks, or land treatment of hazardous wastes. During the initial phases of a site investigation there usually does not exist sufficient data to support the application of comprehensive, computationally expensive numerical models. Simplified physically based models which can address the transport of an organic constituent experiencing volatilization, multiphase partitioning, biodegradation and migration may be preferred. Two models based on the kinematic theory of multiphase flow are developed and presented, along with a number of illustrative examples. The Kinematic Oily Pollutant Transport (KOPT) model assumes steady infiltration of water based on the expected annual infiltration rate; the Kinematic Rainfall and Oily Pollutant Transport (KROPT) model includes transient hydrologic phenomena (evaporation and infiltration) along with a model of stochastic generation of rainfall. The examples presented suggest that the KOPT model may be preferred for most applications.

This Project Summary was developed by EPA's Environmental Research Laboratory, Ada, Oklahoma, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The focus of this research has been on the fate and transport of organic hazardous waste constituents in the shallow soil environment. Organic hazardous waste constituents may be introduced into the soil by spills on the ground surface, leakage from surface impoundments or underground storage tanks, or land treatment of hazardous wastes. Oftentimes in these circumstances, an "oil" phase is present in addition to the water, air, and soil of the natural media, and the fate and transport characteristics are determined by the mobility of the water and oil, as well as by multiphase partitioning of the constituent between the air, water, oil and soil matrix. The emphasis of the research has been on development of simplified models for fate and transport of organic contaminants which may be appropriate for the initial screening or investigation of a site when the available data base does not warrant the application of more general models.

The primary objectives of this cooperative agreement have been to support RSKERL in their modeling studies of subsurface contamination from organic wastes, including hazardous waste land treatment operations, and to investigate the application of kinematic models for multiphase processes including the flow of water and oil, as well as multiphase-partitioning, volatilization, and biodegradation.

The Kinematic Oily Pollutant Transport (KOPT) and Kinematic Rainfall and Oily Pollutant Transport (KROPT) programs are implementations of a kinematic multiphase transport model that was developed as a part of this research. The KOPT program is a simplified implementation of the kinematic multiphase transport model, intended to be used as a screening tool for hydrocarbon spills or near-surface releases. It addresses the questions of how far an oil release might go into the soil and how soon it might get there. In the KOPT implementation, steady water infiltration is assumed to occur, and the specified water saturation is taken as representative of climatic conditions. The KROPT program is the full implementation of the kinematic multiphase transport model and includes modeling of transient hydrologic phenomena (evaporation and infiltration), along with a model for the stochastic generation of rainfall. This model handles multiple loadings or releases of oily wastes at or near the ground surface, multiple rainfall events, potential oil migration, sorption, volatilization, and biodegradation.

Research Background and Scope

The objective of this research was to apply kinematic modeling theory to fate and transport of hydrocarbons in the vadose zone for oil spills and land treatment sites. The purpose of the work was to provide a way to estimate the gross movement of pollutants in a multiphase system resulting from spills, leaks and at land treatment sites. In the case of land treatment systems, the long-term behavior of the site is of interest, so computationally efficient simulations are needed. This was the reason for using a simplified approach.

When placed in porous media, immiscible pollutants retain their unique properties. Although these pollutants are largely immiscible in water, they are capable of causing ground-water contamination by their dissolved constituents. Immiscibility leads to distinct bodies of pollutant in close contact with both air and water, where present. Above the water table, the addition of an immiscible pollutant causes the original two-phase water/air system to become a three-phase water/pollutant/air system. When flowing, the transport and fate of immiscible fluids are governed by a set of relationships which are, basically, expanded forms of the single phase governing equations. The former provides the theoretical framework for solving immiscible (or multiphase) flow problems in general. The specific application of the theory depends on the initial and boundary conditions imposed during pollutant migration as well as other features unique to pollution incidents.

Currently available analytic and semi-analytic multiphase flow models share the limitation that they rely on an assumed shape of the oil profile that is not based upon solution of the governing physically based equations. After an oil release ends, the oil is gradually replaced by air as it drains. A drainage profile, similar to those observed for water is expected, since the same forces that act on the water also act on the oil. Other phenomena outside the scope of these models are biodegradation, which also causes variable oil saturations, and simultaneous unsteady flow of the water. The latter is typical of actual time-varying conditions in the field.

Only a few numeric solutions of the multiphase flow equations have been presented for the specific problem of shallow aquifer contamination. A limitation of the numeric approach is that the models are computationally very intensive. To exploit fully their capacity for modeling geologic variability, a large amount of data is required. Because data is usually sparse, the full capacity of a numeric model may never be reached when applied to specific site investigations.

The analytic and semi-analytic flow models illustrate that if a constant amount of water is present in the pore space, only the mass conservation equation for the oil needs to be solved. A solution, that has not been used for this purpose, is the kinematic model for soil moisture transport. In addition to a solution for the duration of water application, this model gives a solution for the unsteady flow occurring in soils undergoing drainage (replacement of soil moisture by air). The solution is obtained by solving an approximate governing equation for the water by the method of characteristics (MOC). With the proper constitutive relationships for two-phase flow, the water solution is analytic. Adapting this solution for the oil phase gives a more realistic model than the analytic and semi-analytic models mentioned above, since the oil drainage profile is determined by solution of the governing equation. An analytic solution is not possible for the oil because the relative permeability function is too complicated and depends on the amount of water in the pore space. However, a semi-ana
solution for the oil phase can
achieved, allowing relatively low c
putation times to be achieved.

The following assumptions are
for the model formation. The m
equations are solved for one-dimensi
flow. This is one of the neces
assumptions to extend kinematic th
to multiphase flow. Lateral migra
however, reduces the amoun
pollutants and water that m
downward. The one-dimensional forn
tion is conservative as it will deter
the maximum amount of substances
will reach a given depth. A
component pollutant is assumed. Th
acts as an inert carrier for the diss
pollutant. Various transformations,
than biodegradation, that the oil
undergo are not modeled. Adve
transport is used to model the tran
of the constituent by oil and w
Equilibrium, linear partitioning rela
ships are used for sorption, dissol
into the water and for volatilization
the air phase. Volatilization is modele
applying the wet zone/dry zone m
To extend kinematic modeling to tl
phase, three more assumptions are
First, the flow of the air does not im
the flow of the liquids. Second, the
phase transport is dominated by gr
Lastly, the medium is assumed t
strongly wetted so that water will r
in the smallest pores, air in the la
and oil in the intermediate sized por

Under the conditions discussed
kinematic model can be applied 1)
unsteady flow of both the oil an
water and 2) to the fate and transp
the dissolved constituent. If onl
advective motion of the constitue
modeled, the resulting equation
compatible with the numerical app
taken for the oil equations.

Two separate implementations
created. The first (KOPT) was
kinematic model for the oil mig
only, with a constant amount of
present in the pore space. This mo
analogous to the simplified analyti
semi-analytic flow models noted
but with the capability to sim
degrading oil and the transport
dissolved constituent. In related re
this model was coupled with a mo
oil spread along the water table, wh
turn supplied input for a model of
transport in the saturated zone. He
overall model was intended
screening tool for oil spills. A
Guide for the KOPT model is pre
in Appendix A while the listing
code is presented in Appendix B.

The second implementation (KROPT) was a model to investigate the nteractions between incoming rainfall and oil moving within the profile. This model is suited for studying the effect of a series of rainfall events, irrigations and cultivations on a land treatment site. There are practical limitations to application of the KROPT model, and it is considered a research code at this time.

Discussion

This work has shown that kinematic heory can be applied to multiphase flow problems. Kinematic models have an advantage over traditional numeric models in that the kinematic models are well-suited for studying the hyperbolic or wave behavior of the multiphase flow equations. Inclusion of sharp fronts is atural to the kinematic models, while inite difference or finite element models ncounter difficulties when derivatives in he governing equations tend to become ndefined. Solution of the kinematic model shows how the oil and water fronts nteract. Thus, by simplifying the govrning equations, some of the fundamental behavior of the solution is clearly evealed. The effect of the neglected apillary pressure gradients are to crease the infiltration capacity of the oil and smear the fronts. Much of the mportant physics is retained, however, in he kinematic model.

Computationally, by reducing the riginal system of coupled partial ifferential equations to a system of rdinary differential equations, the ifficulty of finding a numerical solution is educed greatly. Resulting computer codes are well suited to solving problems where there is a constant amount of water in the pore space. Such a situation corresponds to a soil at the so-called field capacity and can represent typical conditions of the profile. The best perormance of the KOPT model is obtained when the oil is nondegrading and the oil characteristics are straight. Curving characteristics, due to biodegradation, inrease the computational effort.

The implementation of the more eneral model (KROPT) reveals the nteractions between the oil and water onts. The model is limited to situations where the initial water profile is uniform. Once again the best performance is btained when the oil characteristics are traight, since the characteristic equaons are not solved explicitly. Perormance is degraded where rainfalls xceed the kinematic capacity of the soil. Since the infiltration capacity is infinite initially, very large water fluxes are possible until runoff is produced. During this period small time steps are required.

This modeling work enhances understanding of multiphase flow through the results obtained from the example problems presented. Most important is the material concerning the oil banks. If incoming rainfalls displace oil, then the banks are created. Although this is a result of simplified modeling, the notion that incoming water displaces oil into a bank moving ahead of the water front is a more general result. In situations where the flow of the fluids is not kinematic, banks will also exist. In certain cases, the banks may be very pronounced, although short-lived. In others, the banks may persist for longer periods but would be virtually undetectable in the laboratory and the field or by numerical methods that are not based upon the kinematic model.

The kinematic model results indicate that the water displaces all of the mobile oil. This result was contrary to what was expected but was established through conservation of mass. Some displacement of oil would be expected, along with the creation of an oil bank, but the model result may or may not be confirmed by experiment.

The value of the residual oil saturation is critical for the results obtained from the model. This parameter could be easily manipulated to show that oil would spread over a smaller depth.

Biodegradation of the oil has only a small effect upon the ultimate depth attained by the oil. It does affect the mobility of the oil (reducing it). An interesting effect on the constituent is caused by biodegradation of the oil. Concentrations increase as the oil degrades because of the loss of solvent. If the constituent is also biodegradable, the shorter half life determines if the concentration will increase or not.

As in field cases where constituent concentrations in water are measured, a large mass of constituent may reside in the oil phase and not be detected. In one of the examples, concentrations in the oil are 50 times greater than in the water. If only the water phase concentrations are measured, most of mass in the soil is missed. This is particularly a problem if the oil is immobilized, since the oil cannot flow into an observation well (phenomena akin to end effects may prevent oil flow into wells even at higher saturations). The presence of the oil material is not detected by the observation wells; the core material itself must be analyzed.

Using a differential equation solver is well suited to solving the kinematic model, since the model equations can be written as a system of ordinary differential equations. The speed of the solver is degraded as more and more equations are added. For these situations, it might be advantageous to solve the method of characteristics portion of the solution by finite difference techniques instead of tracking the characteristics. The overhead associated with using the Runge-Kutta-Fehlberg solver may be comparable to that for the discretization methods. Also, the necessity to track sets of oil bank characteristics makes the program exceedingly complex. Extension of the model may not be practical because of this.

Conclusions and Recommendations

The results of this research found that kinematic theory was successfully applied to multiphase flow of water and oil. Kinematic models have an advantage over traditional numeric models in that the kinematic models are well-suited for studying the hyperbolic or wave behavior of the multiphase flow equations. Inclusion of sharp fronts is natural to the kinematic models, while finite difference or finite element models encounter difficulties when derivatives in the governing equations tend to become undefined. The kinematic model simplifies the governing equations revealing some of the fundamental behavior of the solution and showing how the oil and water fronts interact. Solution of the kinematic model indicates that the incoming water must displace all of the mobile oil for mass to be conserved. Another important result is that oil banks are formed when the incoming water displaces the oil that is present. The main limitation to the kinematic model is that displacement of oil by water may be unstable depending on the fluid properties of the oil and the speed of the incoming water.

The two computer codes written to implement two versions of the kinematic model, KOPT and KROPT, run in a computationally efficient manner and may be used to estimate the vertical migration of oil and a dissolved constituent within the soil profile, including the effects of volatilization and biodegradation. Running these codes showed that the amount of residual oil saturation strongly affects the total depth over which the oil will be predicted to spread.

In light of the success of kinematic models for multiphase flow problems, further development of the KOPT and KROPT programs is recommended. Specifically, the following recommendations are suggested:

- Generalize KOPT and KROPT models for use in simulation of facilitated transport. Such an application could look at the use of solvents (such as heptane) for flushing a soil profile to remove low mobility organic hazardous wastes and then model the much more rapid volatilization and degradation of the solvent.
- Development and implementation of user-friendly versions of the KOPT and KROPT programs.
- Expand KROPT program to handle unstable displacements of oil by water, thereby eliminating the main limitation of the model and enabling the use of randomly generated rainfalls that may exceed the kinematic rate. This program enhancement would also handle cases where oil is the displacing fluid, instead of water, such as for when the oil loading rate exceeds the kinematic capacity of an initially nonuniform water profile.
- Expand KROPT to handle lay systems, where the effects of fluids crossing into media of diff intrinsic permeabilities and pore distributions can have an impo effect on their migration.
- Modify KROPT to have the opti use other oil relative permea models, in addition to the Br Corey approach.
- Modify KROPT to handle depth time variability in oil resi saturations.

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***John E. Matthews** is the EPA Project Officer (see below).*
The complete report, entitled "Kinematic Modeling of Multiphase Solute Transport in the Vadose Zone," (Order No. PB 89-207 948/AS; Cost: $21.95, subject to change) will be available only from:

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