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A 3D Numerical Environmental Modeling Approach for Assessing Transport of Spilled Oil in Porous Beach Conditions under a Meso-Scale Tank Design

J. X. Dong, C. J. An, Z. Chen, E. H. Owens, M. C. Boufadel, E. Taylor, K. Lee

***Abstract*—**Shorelines are vulnerable to significant environmental impacts from oil spills. Stranded oil can cause potential short- to long-term detrimental effects along beaches that include injuries to ecosystem, socio-economic and cultural resources. In this study, a three-dimensional (3D) numerical modeling approach is developed to evaluate the fate and transport of spilled oil for hypothetical oiled shoreline cases under various combinations of beach geomorphology and environmental conditions. The developed model estimates the spatial and temporal distribution of spilled oil for the various test conditions, using the finite volume method and considering the physical transport (dispersion and advection), sinks, and sorption processes. The model includes a user-friendly interface for data input on variables such as beach properties, environmental conditions, and physical-chemical properties of spilled oil. An experimental meso-scale tank design was used to test the developed model for dissolved petroleum hydrocarbon within shorelines. The simulated results for effects of different sediment substrates, oil types, and shoreline features for the transport of spilled oil are comparable to that obtained with a commercially available model. Results show that the properties of substrates and the oil removal by shoreline effects have significant impacts on oil transport in the beach area. Sensitivity analysis, through the application of the one-step-at-a-time method (OAT), for the 3D model identified hydraulic conductivity as the most sensitive parameter. The 3D numerical model allows users to examine the behavior of oil on and within beaches, assess potential environmental impacts, and provide technical support for decisions related to shoreline clean-up operations.

***Keywords*—**Dissolved petroleum hydrocarbons, environmental multimedia model, finite volume method, FVM, sensitivity analysis, total petroleum hydrocarbons, TPH.

I. Introduction

BEACHES that support a multitude of ecosystem functions (e.g., shoreline buffering, maintenance of biological diversity, and support of natural processes) are frequently impacted by oil spills which have the potential to cause mass mortality and contamination of aquatic organisms (including invertebrates and macrobenthos) and interrupt the food chain [1], [2]. To evaluate the potential risk of spilled oil, environmental modeling approaches are useful tools [3] for describing the fate and transport of chemicals and providing reliable exposure assessment coupled with monitoring data [4].

Many numerical oil spill fate and transport models have been developed for the simulation of spilled oil in coastal areas and marine environment [5]-[7]. For instance, Guo and Wang developed a hybrid particle tracking/Eulerian-Lagrangian approach which is coupled with the 3D free-surface hydrodynamics model and the wave model to obtain accurate environment information [5]. A number of studies have been focused on the transport of the spilled hydrocarbons in porous media (e.g., unsaturated and saturated zones) [8]-[10]. The BIOMARUN model considered biodegration [11] and bioremediation [12] of residual hydrocarbons in beaches. Of residual hydrocarbons in beaches, the MODFLOW-SURFACT groundwater transport model evaluated the effectiveness of potential of remediation scenarios to select the optimal treatment strategy for contaminated areas [9]. To improve our predictive capability, further studies are needed to assess the fate and transport of spilled oil in the shoreline environment.

Our team developed an extended 1D environmental multimedia modeling system for organic contaminants, which includes source, air, soil, and groundwater modules. These modules are solved within the entire framework [13]. Afterward, based on this modeling system, a 2D numerical environment multimedia model was developed to evaluate the behavior of organic pollutants in a contaminated site with complex conditions under non-uniform and unsteady conditions [14]. It can address the contaminant transport and serve as a risk assessment tool to provide spatial and temporal risk assessment. Based on these previous works, it is potential to develop a 3D numerical environment model for comprehensively evaluating the spilled oil exposures.

This study proposes a 3D numerical environmental modeling approach to simulate the spilled oil distribution in the shoreline area with a focus on dissolved phase in shoreline porous media. A hypothetical case based on a meso-scale tank design is applied to demonstrate its effectiveness and the results from MODFLOW method are used to make a comparison. Moreover, the effects of different substrates, oil types, and oil removal of shoreline are evaluated. The OAT method is conducted to rank and quantified the sensitivities of input parameters.

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II. Methodology

A. 3D Numerical Environmental Modeling Method

Fig. 1 illustrates the distribution of dissolved hydrocarbon in a typical beach area as applied in the conceptual model. Dissolved hydrocarbon migration into the surrounding media, including unsaturated and saturated zones, and into the water column are processes of oil translocation.

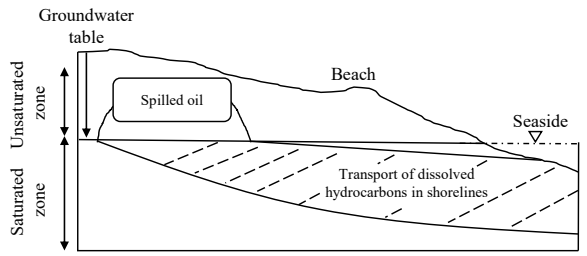

Fig. 1 The conceptual model of the proposed model

The multimedia model is formulated first by considering physical transport, sink, and sorption processes. The governing equation is given by [13], [15].

$$\frac{\partial C^k}{\partial t}=\frac{1}{R^k}\left(D_x^k\frac{\partial^2 C^k}{\partial x^2}+D_y^k\frac{\partial^2 C^k}{\partial y^2}+D_z^k\frac{\partial^2 C^k}{\partial z^2}-V_x^k\frac{\partial C^k}{\partial x}-V_y^k\frac{\partial C^k}{\partial y}-V_z^k\frac{\partial C^k}{\partial z}\right)-\mu C^k+S^k \tag{1}$$

$$R=1+K_d\frac{\rho}{\theta} \tag{2}$$

where C_α^k is the concentration of the α component of the dissolved hydrocarbon in the k zone (g/m^3), subscript x and z are the x- and z-direction, V is the effective solute velocity (m/h), D is the effective diffusion coefficient (m^2/h), μ is the degradation rate (1/h), S is concentration fluxes (g/m^3 h) due to emission and deposition, R is the retardation factor, ρ is the bulk density of the soil (g/m^3), K_d is the distribution coefficient (m^3/g) and θ is the volumetric moisture content of the soil.

i. Flux Transfer between Each Module

The mass transport of spilled oil can be expressed as flux. At the boundary of the domain, we set the dissolved hydrocarbon flux percolating through this section as F_t into the aquifer:

$$F_t=-\frac{D_i}{R}\frac{\partial C}{\partial x_i}+\frac{V_i}{R}C \tag{3}$$

where i means different direction, and the others are detailed in the former paragraph.

ii. Finite Volume Method (FVM)

The FVM is one of the most widely used for the solution of the advection-diffusion equations [16]. The 3D pollutant transport model is numerically solved based on FVM. The governing equation of 3D numerical environmental model (1) is discretized through the central control volume method with flexible mesh. Control volumes are established around the interior nodes with six control volume faces as shown in Fig. 2. The ends of the domain are considered as the boundary control volumes, in which the ghost points are applied based on boundary conditions.

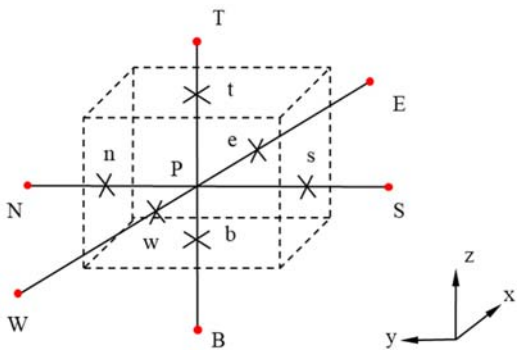

Fig. 2 Control volume for an interior node

Integration of (1) in the control volume $N_{i,j,k}$ gives:

$$\int_t^{t+\Delta t}\int_{\Delta V}\frac{\partial C}{\partial t}dVdt=\int_t^{t+\Delta t}\int_{\Delta V}D\frac{\partial^2 C}{\partial x_i^2}dVdt-\int_t^{t+\Delta t}\int_{\Delta V}V\frac{\partial C}{\partial x_i}dVdt-\int_t^{t+\Delta t}\int_{\Delta V}(\mu C+S)dVdt \tag{4}$$

The diffusion derivatives can be approximated with the central difference. An upwind approximation is used for the advection derivatives. Taking diffusion and advection approximation in x-direction as an example, the equation is shown as:

$$\int_t^{t+\Delta t}\int_{\Delta V}D\frac{\partial^2 C}{\partial x_i^2}dVdt\approx\int_t^{t+\Delta t}\left(AD_e\frac{C_E-C_P}{\Delta x_{PE}}\right)-\left(AD_w\frac{C_P-C_W}{\Delta x_{WP}}\right)dt \tag{5}$$

$$\int_t^{t+\Delta t}\int_{\Delta V}V\frac{\partial C}{\partial x_i}dVdt\approx\int_t^{t+\Delta t}A(V_eC_P-V_wC_W)dt,\ V_e>0,\ V_w>0 \tag{6}$$

$$\int_t^{t+\Delta t}\int_{\Delta V}V\frac{\partial C}{\partial x_i}dVdt\approx\int_t^{t+\Delta t}A(V_eC_E-V_wC_P)dt,\ V_e\le 0,\ V_w\le 0 \tag{7}$$

where, subscript e and w mean the face e and w, subscript E, P and W mean the node E, P, and W. A is the area of faces, Δx means the length of two interior nodes. The other parameters are mentioned in the previous section.

The time discretization of (1) is performed by a forward approximation. Combing the previous expression, the FVM solution to the governing equation for n+1 time is obtained:

$$a_pC_P=a_eC_E+a_wC_W+a_sC_S+a_nC_N+a_bC_B+a_tC_T+a_{p0}C_P^n+S-F \tag{8}$$

where,

$$a_p=\frac{1}{\Delta t}+\frac{(D_e+D_w)}{\Delta x^2}+\frac{V_e}{\Delta x}+\frac{(D_n+D_s)}{\Delta y^2}+\frac{V_n}{\Delta y}+\frac{(D_t+D_b)}{\Delta z^2}+\frac{V_t}{\Delta z}+\mu \tag{9}$$

$$a_w=\frac{D_w}{\Delta x^2}+\frac{V_w}{\Delta x},a_s=\frac{D_s}{\Delta y^2}+\frac{V_s}{\Delta y},a_b=\frac{D_b}{\Delta z^2}+\frac{V_b}{\Delta z} \tag{10}$$

$$a_e = \frac{D_e}{\Delta x^2}, a_n = \frac{D_n}{\Delta y^2}, a_t = \frac{D_t}{\Delta z^2} \tag{11}$$

$$a_{p0} = \frac{1}{\Delta t} \tag{12}$$

After generating the mesh, (8) is applied in each node, and a matrix including variables in the nodes can be established. Then the initial conditions and boundary conditions are applied to solve the matrix. Finally, the value of concentrations in the nodes for n+1 time are obtained. These processes are repeated during the simulation period.

iii. User-Friendly Interface

The proposed numerical model is established by using the Python language. Fig. 3 shows the graphical user interface that is developed to manage data inputs and run the model. The required input data are directly entered or imported as Excel files through the graphical interface. All equations are solved in the Pycharm, and then the output can be imported to Excel as .xls format.

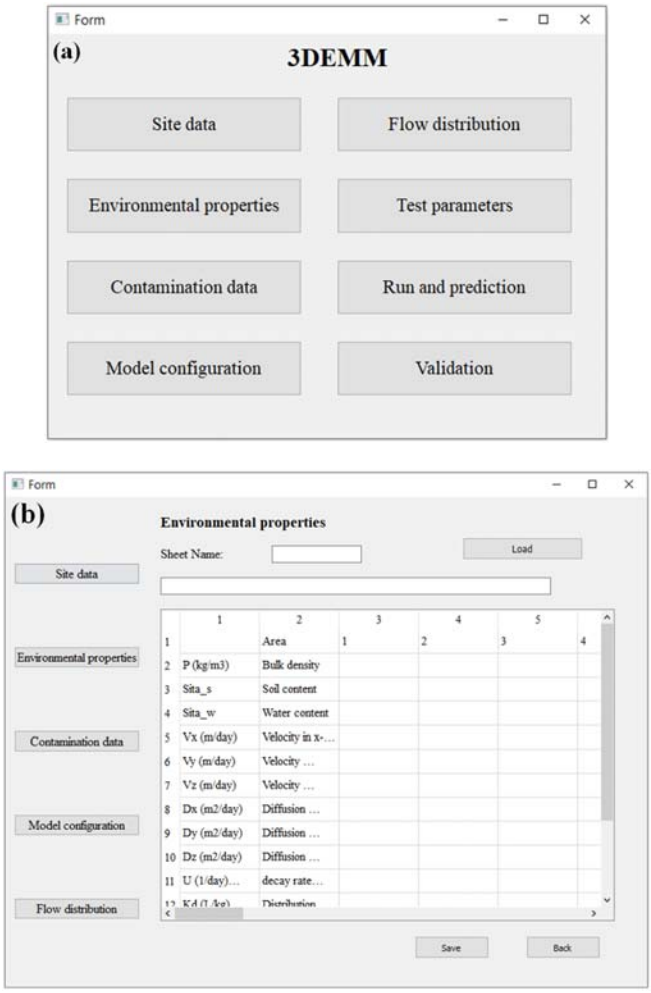

Fig. 3 The graphical user interface of the developed model

The required data can be classified into different parts: site data, environmental properties, contamination properties, model configuration, and flow distribution. As shown in Fig. 3 (b), it allows the user to directly input the related parameters or import the environment properties by the excel file. Then the Excel sheet shows the imported information related to the variables. All of the input data are saved in the database by clicking "Save". After inputting the required data, these data can be linked to the developed model and run the simulation processes by clicking the button "Run and validation" as shown in Fig. 3 (a).

B. MODFLOW Method

The MODFLOW from the USGS (United States Geological Survey) is a widely used model relying on a 3D block-centered finite difference method for layered aquifer systems, in which water flow is based on Darcy's law [17]. MODFLOW can simulate both steady and unsteady states and may represent a wide variety of aquifer conditions. MODFLOW was coupled herein with the MT3DMS available from the USGS, which is developed to evaluate the fate and transport of pollutants in the groundwater. MT3DMS uses cell-by-cell flow data provided by MODFLOW to predict solute fate and transport. The basic processes considered in this model include advection, dispersion, source/sink, and decay reaction [18]. The model output provides the predicted contaminant concentration for some specified time steps. Therefore, MODFLOW and MT3DMS are applied to the study case for validation of the 3D numerical environmental modeling approach.

C. Sensitivity Analysis Methods

Sensitivity is a measurement of the effect of change in one factor on another factor. The OAT method is one of the most frequently applied approaches [19]. The sensitivity coefficient is usually defined by computing partial derivatives of the output functions concerning the parameters. The sensitivity of the input parameter k is calculated by:

$$X_k = \frac{\partial E_k / E_k}{\partial k / k} \approx \frac{E(k+\Delta k) - E(k)}{E_k \times \Delta k / k} \tag{13}$$

where E is the output variable after the parameter perturbation. The sensitivity coefficient for any given parameter is in the same unit as the dependent variable. The high X_k value means that this parameter has a great impact on the output.

D. Estimation of Sediment Substrates Properties

Sand and gravel beaches are widespread around the world. Their properties highly depend on the component sand and gravel. She et al. and Bobo et al. provide a number of equations for estimating the porosity, density, and hydraulic conductivity of a mixed sand-gravel sediment [20], [21]. The porosity (n) can be represented by:

$$\begin{cases} n = \dfrac{n_g - \lambda}{1-\lambda} & (\lambda \le \lambda_c) \\ n = \dfrac{\lambda n_g}{1 - n_s(1-\lambda)} & (\lambda > \lambda_c) \end{cases} \tag{14}$$

$$\lambda_c = \frac{n_g(1-n_s)}{1-n_g n_s} \tag{15}$$

where λ is the percentage of the sand by weight. The porosity of the pure gravel is n_g and the pure sand has a value of n_s.

For simplicity, the same density ρ_s is assumed for both sand and gravel.

$$\begin{cases} \dfrac{\rho_{bulk}}{\rho_s} = \dfrac{1-n_g}{1-\lambda} & (\lambda \le \lambda_c) \\ \dfrac{\rho_{bulk}}{\rho_s} = \dfrac{1-n_s}{1-n_s(1-\lambda)} & (\lambda > \lambda_c) \end{cases} \tag{16}$$

Furthermore, the hydraulic conductivity of a mixed sand-gravel media may be estimated by:

$$\begin{cases} k = k_g(1-\xi)^2 + k_s n_g \xi & (\lambda \le \lambda_c) \\ k = \dfrac{k_s \lambda}{\lambda + (1-n_s)(1-\lambda)} & (\lambda > \lambda_c) \end{cases} \tag{17}$$

$$\xi = \frac{(1-n_g)\lambda}{\lambda + (1-n_s)(1-\lambda)} \tag{18}$$

E. Method for Estimating the Effect of Shoreline

The phase of the initial oil removal from a shoreline can result in the transfer of bulk and mobile oil on the porous substrate to the adjacent water column [22]. To evaluate the removal rate of oil from a shoreline segment, Shen et al. proposed the volume of oil remaining on the beach can be related to its original volume by [23]:

$$\frac{\Delta V_b}{V_b} = 1 - 0.5^{\Delta t/\lambda} \tag{19}$$

where ΔV_b is the volume of the beached oil re-entrained into the sea during each time step, V_b is the volume of oil on the beach; and λ is the half-life. The "half-life" of the sand-gravel beach is estimated as 24 h [23]. Equation (19) will be used to estimate the removal rate of spilled oil in the tank case and coupled to the developed model. Afterward, the simulated results with/ without applying it will be compared and discussed in the next section.

III. Case Study

A. Model Verification with MODFLOW/MT3DMS

The proposed numerical model is tested against MODFLOW/MT3DMS in predicting the dissolved petroleum hydrocarbon concentrations in a meso-scale tank, conducted for 3D flow for the hypothetical situations described in Fig. 4. The inland tank contains a mixed sand-gravel substrate and its width is 0.7 m. It assumes that at the initial period, the dissolved petroleum hydrocarbon stays in the left part of the substrate as shown in the red area, where the length is 0.2 m. It assumes that 2 L typical light crude oil (the properties are modified from the crude oil from Algeria) spilled into the tank, of which the density is 804.5 kg/m^3 [24] and thus, the API gravity is estimated as 44.3. Total petroleum hydrocarbons (TPH) include a broad family of several hundred compounds originally present in crude oil which have carbon ranges between ≥ C5 and ≤ C40 [25]. In the crude oil from Algeria, the percentage of products that the boiling ranges are from 150 □ to 500 □ is 88.5% [24]. The carbon ranges of these products are similar to that of TPH. Moreover, the percentage of dissolved petroleum hydrocarbon in TPH is set as 3%. Thus, the initial concentration of dissolved petroleum hydrocarbon in the red zone can be estimated as 508.6 g/m^3.

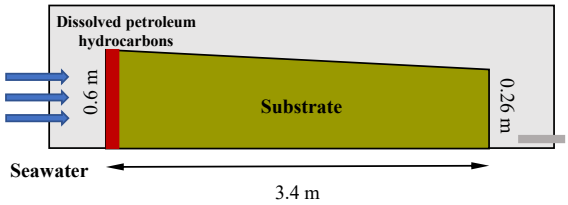

Fig. 4 2D side view of the tank

The properties of a typical sandy beach are adapted from the sandy beach in the coast of Valdivia, Chile and selected as the substrate in the tank, which here is considered as Case 1. The average percentages of gravel and sand in this substrate are 9.6% and 90.4%, respectively [26]. According to the previous researches, the porosity and the hydraulic conductivity of sand are set as 40% and 8.0×10^{-4} m/s (2.88 m/h), respectively [27], [28]. The porosity, hydraulic conductivity, and density of gravel are estimated as 0.45, 3.0×10^{-4} m/s, and 1600 kg/m^3, respectively [20], [29]. Based on (14)-(18), the bulk density, porosity, and hydraulic conductivity of this substrate are estimated as 1000 kg/m^3, 0.35, and 7.5×10^{-4} m/s (2.70 m/h). Afterward, Darcy's law is applied to calculate the average velocity of the fluid, and the average velocities in x-direction and z-direction are estimated as 0.78 and 0.078 m/h. The diffusion coefficient of oil in water is estimated as a function of temperature T in Celsius: $D = 4.13\times10^{-3}\times T^{1.53}$ [30]. The temperature is set as 20 □ and the diffusion coefficient is estimated as 4.04×10^{-5} m^2/h. The organic carbon partition coefficient of TPH is 0.347 m^3/kg [31], which is applied for dissolved petroleum hydrocarbon, and the organic carbon fraction in the substrates is set as 0.05. The properties of the tank case are summarized in Table I.

TABLE I
THE MODEL PROPERTIES IN CASE 1

Parameters	Value	Parameters	Value
Velocity in x-direction (m/h)	0.78	Length (m)	3.4
Velocity in y-direction (m/h)	0	Width (m)	0.7
Velocity in z-direction (m/h)	0.078	Height (m)	0.6
Longitudinal diffusion coefficient (m^2/h)^a	4.04E-5	Porosity	0.346
Transverse diffusion coefficient (m^2/h)^a	4.04E-6	Bulk density (kg/m^3)	1000
Organic carbon partition coefficient (m^3/kg)^b	0.347	Organic carbon fraction	0.005

Note: a Data calculated from [30]; b Data from [31]

The spatial distributions of dissolved petroleum hydrocarbon in the tank after 10, 20, 30, and 40 hours are provided in Fig. 5.

It indicates that the dissolved petroleum hydrocarbon transports through x-direction due to the flow effect. After 10 hours, the majority of the hydrocarbons moves to the middle of the tank and the peak concentration is about 64.7 g/m^3. Then, with time increasing, the contaminants continue to move to the right side of the tank and the peak concentration is also decreasing. After 40 hours, most of dissolved petroleum hydrocarbon is out of the tank and the highest concentration is 8.0 g/m^3 at the right boundary.

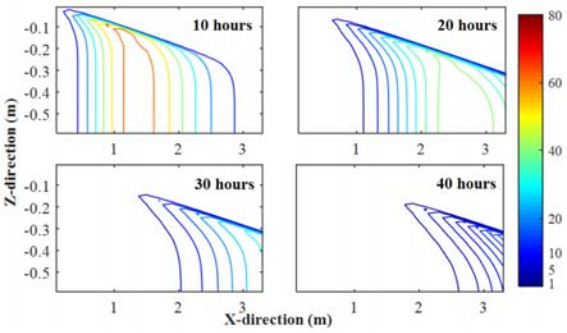

Fig. 5 Spatial distribution of dissolved petroleum hydrocarbon in the tank from 10 to 40 hours (g/m^3)

Fig. 6 provides the temporal variance of dissolved petroleum hydrocarbon concentrations at the outlet. The comparison between results sis imulated by the proposed model and MODFLOW package is conducted, which indicates similar results. The concentrations of outlets reach their peak at the 24th hour, while the peak concentration from MODFLOW method (52.9 g/m^3) is higher than that from the developed model (37.9 g/m^3). Moreover, the tendency of concentration decreasing after 40 hours is also different. The possible reason is that based on the boundary conditions (constant head), MODFLOW methods simulate the water flow distribution in the study area, while this distribution in the 3D numerical model is simplified as discussed in the previous section. Additionally, the Massachusetts groundwater standard for TPH (5 mg/L) is applied to evaluate the outflow of tanks [32]. It shows that possibly during the time between the 11th and 46th hour, effluent from the tank may contain dissolved petroleum hydrocarbon with some concern. After that, the outflow has no risk in the tank effluent.

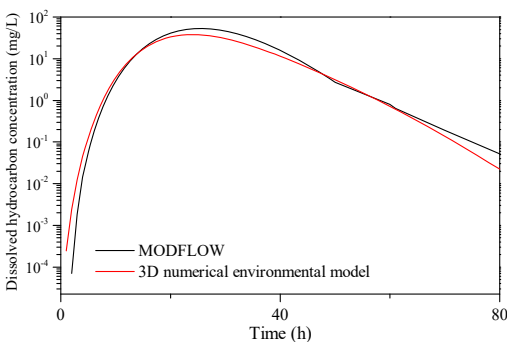

Fig. 6 The comparison between results from the 3D numerical environmental model and MODFLOW

B. The Effect of Sediment Substrates and Oil Types

To evaluate the impacts of substrates and oil types on spilled oil transport, another substrate from Isle of Sheppey, England, is considered as Case 2, which is less sandy compared to the substrate applied in Case 1. Crude oil from Daqing, China, with a density of 866.6 kg/m^3, or API gravity of 31.7, [24] is selected as a typical medium oil. The percentages of sand and gravel in the substrate from Sheppey are 14% and 86%, respectively [33]. According to (14)-(18), the density, porosity, and hydraulic conductivity of this substrate can be estimated as 1023 kg/m^3, 0.36, and 1.46×10^{-3} m/s (5.25 m/h), respectively. In the crude oil from Daqing, the percentage of products that the boiling ranges are from 150 □ to 500 □ is 56.1% [24] and the proportion of dissolved petroleum hydrocarbon is set as 1%. Thus, the initial concentration of dissolved petroleum hydrocarbon in the red zone (Fig. 4) is estimated as 115.7 g/m^3.

For the two mentioned cases involving two different substrates and two different crude oils, there are four different combinations, which are marked as Chile-Algeria, Chile-Daqing, Sheppey-Algeria, and Sheppey-Daqing. Fig. 7 provides the temporal variance of the dissolved petroleum hydrocarbon concentrations and mass flux in the outlet under these scenarios. The results indicate that, regardless of oil types (i.e., light and medium crudes), the properties of substrates have significant impacts on oil transport in beach area: when the substrate is less sandy with more gravels as tank Case 2, the spilled oil transport rapidly and the concentrations reach the peak at the 13th hour. This is because this substrate is dominated by gravel and its hydraulic conductivity is much higher than the other substrate; on the other hand, when the substrate is more sandy but with less gravel as tank Case 1, the concentrations reach the peak at the 24th hour.

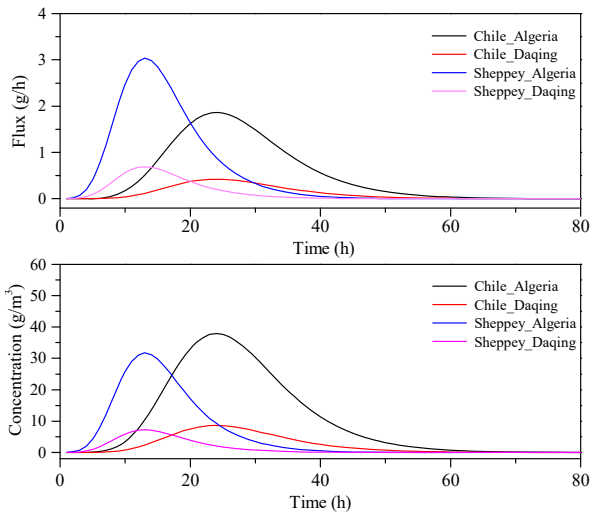

Fig. 7 The temporal variance of the dissolved petroleum hydrocarbon concentrations and mass fluxes in the outlet under these scenarios

The initial mass/concentration of dissolved petroleum hydrocarbon as marked red in Fig. 4, is a critical input to the model, such initial mass/concentration of dissolved petroleum hydrocarbon is largely affected by oil types, which

subsequently affects the spatial distribution of concentrations in the beach area (or tank here is this study). For the shoreline oil spill modeling studies, the oil types also affect other important model parameters such as the diffusion coefficient in (1). In this study, the method provided by [30] is examined to estimate the diffusion coefficient. In general, different approaches should be used to estimate the diffusion coefficient as it is affected by oil types.

C. The Effect of Shoreline

To evaluate the shoreline effect, (19) is applied and coupled to the developed model. Case 1 and Case 2 that combinations include Chile-Algeria and Sheppey-Algeria are applied to evaluate the effect of shoreline. Fig. 8 shows the temporal variance of dissolved petroleum hydrocarbon concentrations in the outlet with/without applying (19). It indicates that the oil removal of shoreline has significant influences on the concentrations in the outlet. This is because the "half-life" of oil in the sand-gravel beach is estimated as 24 h [23], which means the dissolved petroleum hydrocarbon concentrations will be reduced to 50% of the initial values after 24 hours. Moreover, the shoreline does not affect the speed of spilled oil transport, since the dissolved petroleum hydrocarbon concentrations reach the peak at a similar time when applying the same combination. It shows that under the scenarios (Chile_Algeria_shoreline and Sheppey_Algeria_shoreline), effluent from the tank exceeds Massachusetts groundwater standard during the 13th-39th hour and 3rd-24th hour, respectively.

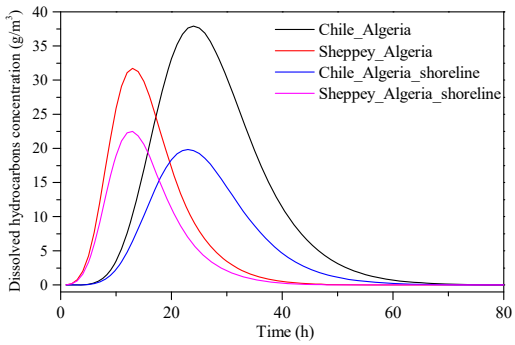

Fig. 8 Temporal variance of dissolved petroleum hydrocarbon concentrations with/without considering the effect of shoreline

IV. Sensitivity Analysis

The fate of dissolved petroleum hydrocarbon simulated by this system highly depends on environmental properties. Sensitivity analysis is applied to explain the relationship and identify the parameters estimated from the references, which are listed in Table I. The chosen parameters are the retardation factor, diffusion coefficient, and hydraulic conductivity. These parameters were adjusted by factors of 50%, 75%, 125%, and 150% (of the values used in the model). In this case study, the sensitivity of given parameters is calculated by using OAT as shown in Fig. 9. The sensitivity coefficient of the hydraulic conductivity changes from -5.19% to 14.85%, meaning that altering the retardation factor has the most significant impact on the model output. The negative value means that the concentration decreases as the retardation factor increases. The other parameters are less sensitive than the hydraulic conductivity. The results indicate that the diffusion coefficient has a negligible influence on the transport of dissolved petroleum hydrocarbon pollution and the variance of the sensitivity coefficient due to changes in diffusion coefficient is tiny (from -1.18×10^{-3} to 1.19×10^{-3}).

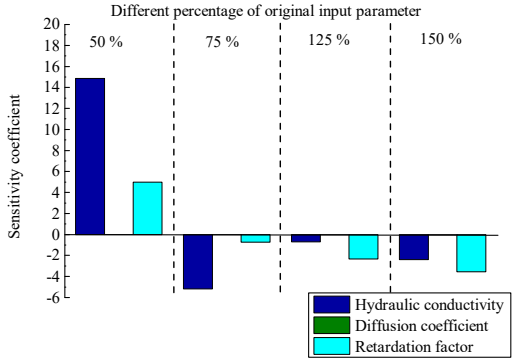

Fig. 9 Sensitivity analysis for parameters

V. Discussion

A. Dissolved Petroleum Hydrocarbon in Oil Spill Modeling Study

Oil spill modeling simulates the fate and transport of oil and its components in the environment including soil, groundwater, lakes, rivers, shorelines, and open seawater. The simulation can focus on oil components such as BTEX, or free phase oil (e.g., NAPL and oil droplets). This study focuses on dissolved oil and uses dissolved petroleum hydrocarbon to represent oil concentrations in the porous shoreline site, as the developed modeling approach mainly considers dissolved species in the environment. For example, these studies employ similar modeling methods to assess the spilled oil transport in porous media based on TPH concentrations [8], [9]. Further studies can include free phase oil or residual oil in shoreline sites.

B. Environmental Guideline for Shoreline Sites

There are few TPH guidelines for shorelines [34]. TPH guidelines can be found for freshwater supplies, which is generally much more stringent than the guideline for shoreline or open seawater. For example, in North America, the Massachusetts guideline for TPH is for fresh groundwater [32], here we use this as a reference TPH guideline to show the maximum possible adverse effects.

In western Canada, the BC oil and gas waste guideline is found for extractable petroleum hydrocarbons (EPH), with a regulated value of 15 mg/L [35]. Afterward, the simulated results of dissolved petroleum hydrocarbon as shown in Fig. 6 are compared to the BC guideline for EPH. It indicates that the dissolved petroleum hydrocarbon concentrations may be above the regulatory threshold from the 15th to the 37th hour (at maximum) of an experiment without considering tide and wave effects. Furthermore, the simulated results considering shoreline effects (i.e., Chile_Algeria_shoreline) are also

compared to the BC guideline for EPH, the results show that the effluent may exceed the limitation from the 18th to the 29th hour. Although it will be diluted right away below the permissible EPH level once the tank effluent is discharged to the massive coastal waterbody, monitoring and water treatment measures including a filter using oil absorbents have been included in the tank design to ensure zero risk to the receiving coastal water.

C. Ongoing Future Studies

This study achieves a comparable modeling result with the commercial model package on dissolved petroleum hydrocarbon concentrations and particularly takes the effects of shoreline and oil types into consideration. Our ongoing studies include: 1) extended modeling of the hydrodynamic flow field with moving boundary conditions considering the tidal cycle and other meteorological effects; 2) further investigation of model parameters, for example, the diffusion coefficient of spilled oil estimated in this study here is only tested based on the crude oil (API 28) [30], other oil types can be considered based on the developed model; and 3) incorporation of free phase non-aqueous phase liquid (NAPL) in the developed model to further address the retention, penetration, and biodegradation of spilled oil in shorelines.

VI. Conclusion

The 3D numerical environmental modeling approach is developed to deal with problems concerning the fate and transport of dissolved petroleum hydrocarbon and its components in typical contaminated shoreline sites with various beach conditions. The advection-dispersion equations are applied to evaluate the physical transport (dispersion and advection), sink, and sorption processes, and the FVM is used to solve these equations. Furthermore, the developed 3D numerical model comes with a user-friendly interface for controlling the required input data like beach properties, spill source information, and physical-chemical properties of spilled oil. The study cases based on a meso-scale tank design with four combinations (i.e., Chile-Algeria, Chile-Daqing, Sheppey-Algeria, and Sheppey-Daqing) are studied to test the developed model, and MODFLOW method is used for model verification. According to the comparison, this model can provide results that match well with those from the commercial modeling package. There are some differences due to the methods used by these two models to estimate the flow distribution. The specific case of a planned meso-scale tank test study indicates that, at the tank discharge port, the EPH concentrations may be above the regulatory threshold from the 15th to the 37th hour (at maximum) of a 2-liter spill experiment, however, this discharge contains a very small amount oil which will be diluted right away below the permissible EPH level once the tank effluent is discharged to the massive coastal waterbody. Additionally, the effluent dissolved petroleum hydrocarbon results have not considered the hydrodynamic and biodegradation effects, which further significantly reduces oil and its dissolved petroleum hydrocarbon levels in the discharges.

The effects of different substrates and oil types on the transport of spilled oil are further examined. The properties of substrates have significant impacts on oil transport in the beach area: when the substrate is less sandy with more gravels as tank Case 2, the spilled oil transport rapidly and the concentrations reach the peak at the 13t hour; on the other hand, when the substrate is more sandy but with less gravel as tank Case 1, the concentrations reach the peak at the 24th hour. The initial mass/ concentration of dissolved petroleum hydrocarbon is largely affected by oil types, which subsequently affects the spatial distribution of dissolved petroleum hydrocarbon in the beach area. Sensitivity analysis is conducted by performing OAT to test the applicability and performance of the developed model. The most sensitive parameter in the study area is found as hydraulic conductivity. Additionally, the effect of shoreline is evaluated through an empirical method, which shows that it largely affects the dissolved petroleum hydrocarbon concentrations at the discharge point to the open seawater, and can be further investigated in the future considering the influence of tidal cycle, the effect of oil types on input parameters, and the transport processes of free phase oil or droplets. Nevertheless, this developed 3D numerical modeling approach can be used to consider other substrates and oil types under both experimental or real field scale studies, to forecast the fate and transport of spilled oil, and to provide technical support for the risk assessment and clean of the spilled oil.

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