

A NOVEL HYBRID MODEL DEVELOPMENT FOR THE ESTIMATION OF PLUME LENGTH

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**A NOVEL HYBRID MODEL DEVELOPMENT
FOR THE ESTIMATION OF PLUME LENGTH**

by

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Submitted

In the fulfilment of the requirements of the degree of Doctor of Philosophy

to the



**INDIAN INSTITUTE OF TECHNOLOGY DELHI
OCTOBER 2022**

Dedicated

To

My Parents

CERTIFICATE

This is to certify that the thesis entitled “**A Novel Hybrid Model Development for the Estimation of Plume length**” being submitted by Ms. Sandhya Birla to the Indian Institute of Technology Delhi for the award of the degree of ‘Doctor of Philosophy’ in the Department of Civil Engineering is a record of the bonafide research work carried out by her under our supervision and guidance. She has fulfilled the requirements for the submission of this thesis, which to the best of our knowledge, has reached the requisite standard. The material contained in the thesis has not been submitted in part or full to any other University or Institute for the award of any other degree or diploma, except where due acknowledgment has been made in the text.



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"If I have seen further, it is by standing on the shoulders of giants." – Isaac Newton

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Sandhya Birla

Abstract

There are millions of potentially contaminated and contaminated sites in India and abroad. Field and experimental data on the characterization of such sites are available in the literature. The focus of this thesis work is to study the processes and parameters of contaminated sites in detail and assess and develop mathematical models that can aid in the initial assessment of contaminated sites. The analytical models available in the literature along with the field data of contamination sites have been compiled and analyzed. Descriptive statistical analysis of the various field parameters at contamination sites, and data analysis primarily focused on the steady-state plume lengths (L_{max}) have also been performed. This study provides multiple scenarios for various analytical models, consisting of several necessary assumed parameters including dispersivity parameter. Liedl et al. (2005) and Maier and Grathwohl (2006) have been found to estimate better for shallow aquifers, leading to smaller ratios of estimated to field plume lengths. Alternative methods such as Liedl et al. (2011), BIOSCREEN-AT models, and simplified numerical modeling are recommended for highly estimated cases, as well as the concept modification/ development of analytical models.

Also, the transverse dispersivity, which is among the most critical parameter for solute transport has always been found to be missing from the sites database. The parameter has been studied extensively and a detailed table that encompasses values of the transverse dispersivity and other parameters has been presented. Further analysis of dependencies of the transverse dispersivity has been made, and an empirical relationship has also been proposed for the estimation of the transverse dispersivity using the Peclet number. Contamination Assessment and Site-management Tool (CAST), a graphical user interface for the initial assessment using simple models has been

developed and hosted on IIT Delhi website, along with the contaminant site data and transverse dispersivity data

The present investigation also proposes a novel solution, i.e., a hybrid model for estimating steady-state plume lengths in 2D and 3D scenarios, including the influence of recharge rates and source geometry. A hybrid analytical-empirical solution has been developed by the superimposition of analytical models and empirical models. For that, a large number of simulations from a numerical model (using MODFLOW, MT3D) have been run to obtain $L_{max, num}$ with varying recharge and source geometry parameters. The simulated results have been analysed through plots and consequently an empirical function has been hypothesized. The MATLAB[®] Curve Fitting Toolbox[™] has been used to fit the custom equation on the simulated data for evaluating $L_{max, hyb}$ using $L_{max, ana}$. The empirical function takes care of the additional complexity not considered by the analytical model. The hybrid model provides a relationship between L_{max} and recharge rate, with all the other assumptions still valid, as stated in the analytical development of L_{max} in the base model.

The performance of the proposed hybrid model has been evaluated by comparison with the field data. The proposed hybrid model improves the estimation of the field L_{max} significantly. While the proposed hybrid model improves the estimation of the field L_{max} significantly, it is essential to consider its limitation and applicability. These include the two-dimensional, homogeneous isotropic domain with only horizontal groundwater flow. Besides, the reaction system in the domain is limited to an instantaneous bi-molecular reaction that may only be very suitable for very rapidly reacting contaminants. Furthermore, the role of dispersivity has not been assessed in the current study. The selection of a base analytical model should be done more rigorously. However,

in this work, analytical model of Liedl et al. (2005, 2011) have been used as base model due to its simplicity, requirement of less data and being vertically oriented model.

The proposed models can be used for the pre-assessment of contaminated sites as the accuracy for estimation is found to be higher in comparison to the analytical solution, thus making them more relevant. Given that hybrid models are being proposed for aiding risk management tools, minor overestimations can be overlooked.

सार

भारत और विदेशों में लाखों संभावित-दूषित और दूषित स्थल हैं। ऐसे स्थलों के लक्षण वर्णन पर क्षेत्र और प्रयोगात्मक जानकारी साहित्य में उपलब्ध हैं। इस शोध कार्य का उद्देश्य दूषित स्थलों की प्रक्रियाओं और मापदंडों का विस्तार से अध्ययन करना और गणितीय मॉडल का आकलन और विकास करना है जो दूषित साइटों के प्रारंभिक मूल्यांकन में सहायता कर सकते हैं। साहित्य में उपलब्ध विश्लेषणात्मक मॉडलों के साथ-साथ संदूषण स्थलों के क्षेत्र डाटा को संकलित और विश्लेषण किया गया है। संदूषण स्थलों पर विभिन्न क्षेत्र मापदंडों का वर्णनात्मक सांख्यिकीय विश्लेषण, और मुख्य रूप से स्थिर-राज्य प्लूम लंबाई (L_{max}) पर केंद्रित विश्लेषण भी किया गया है। यह अध्ययन विभिन्न विश्लेषणात्मक मॉडलों के लिए कई परिदृश्य प्रदान करता है, जिसमें फैलाव प्राचल सहित कई आवश्यक कल्पित प्राचल शामिल हैं। लिडल और अन्य (2005) और मायर और ग्राथवोहल (2006) को उथले जलभृतों के लिए बेहतर अनुमान लगाने के लिए पाया गया है, जिससे क्षेत्र के प्लूम लंबाई के अनुमानित अनुपात में कमी आई है। वैकल्पिक तरीके जैसे लिडल और अन्य (2011), बायोस्क्रीन-एटी मॉडल, और सरलीकृत संख्यात्मक मॉडलिंग की सिफारिश अत्यधिक अनुमानित मामलों के साथ-साथ विश्लेषणात्मक मॉडल के अवधारणा संशोधन / विकास के लिए की जाती है।

इसके अलावा, अनुप्रस्थ फैलाव, जो विलेय परिवहन के लिए सबसे महत्वपूर्ण प्राचलों में से एक है, हमेशा स्थल आंकड़ाकोष से गायब पाया गया है। प्रचालों का बड़े पैमाने पर अध्ययन किया गया है और एक विस्तृत तालिका जिसमें अनुप्रस्थ फैलाव और अन्य मापदंडों के मूल्यों को शामिल किया गया है, प्रस्तुत किया गया है। अनुप्रस्थ फैलाव की निर्भरता का और विश्लेषण किया गया है, और पेकलेट संख्या का उपयोग करके अनुप्रस्थ फैलाव के आकलन के लिए एक अनुभवजन्य संबंध भी प्रस्तावित किया गया है। संदूषण आकलन और स्थल-प्रबंधन उपकरण (सीएएसटी), सरल मॉडल का उपयोग करके प्रारंभिक मूल्यांकन के लिए एक चित्रात्मक प्रयोक्ता इंटरफ़ेस विकसित किया गया है और इसे आईआईटी दिल्ली वेबसाइट पर दूषित साइट डाटा और अनुप्रस्थ फैलाव डाटा के साथ दिया गया है।

वर्तमान जांच में पुनर्भरण दरों और स्रोत ज्यामिति के प्रभाव सहित द्विविमीय और त्रिआयामी परिदृश्यों में स्थिर-राज्य प्लूम लंबाई का अनुमान लगाने के लिए एक नया समाधान, यानी एक संकर मॉडल का भी प्रस्ताव है। विश्लेषणात्मक मॉडल और अनुभवजन्य मॉडल के संयुक्त द्वारा एक संकर विश्लेषणात्मक-अनुभवजन्य समाधान विकसित किया गया है। उसके लिए, एक संख्यात्मक मॉडल (MODFLOW, MT3D का उपयोग करके) से बड़ी संख्या में अनुरूपण को $L_{max, num}$ को अलग-अलग रिचार्ज और स्रोत ज्यामिति मापदंडों के साथ प्राप्त करने के लिए चलाया गया है। अनुरूपणीय परिणामों का विश्लेषण भूखंडों के माध्यम से किया गया है और परिणामस्वरूप एक अनुभवजन्य कार्य की परिकल्पना की गई है। MATLAB® कर्व फिटिंग टूलबॉक्स™ का उपयोग $L_{max, hyb}$ का उपयोग करके $L_{max, num}$ का मूल्यांकन करने के लिए अनुकारित डाटा पर समीकरण उपयुक्त करने के लिए किया गया है। अनुभवजन्य कार्य विश्लेषणात्मक मॉडल द्वारा विचार नहीं की गई अतिरिक्त जटिलता का ख्याल रखता है। संकर मॉडल L_{max} और रिचार्ज दर के बीच संबंध प्रदान करता है, अन्य सभी धारणाएं अभी भी मान्य हैं, जैसा कि आधार मॉडल में L_{max} के विश्लेषणात्मक विकास में कहा गया है।

क्षेत्र डाटा के साथ तुलना करके प्रस्तावित संकर मॉडल के प्रदर्शन का मूल्यांकन किया गया है। प्रस्तावित संकर मॉडल L_{max} क्षेत्र के अनुमान में काफी सुधार करता है। जबकि प्रस्तावित संकर मॉडल L_{max} क्षेत्र के अनुमान में काफी सुधार करता है, इसकी सीमा और प्रयोज्यता पर विचार करना आवश्यक है। इनमें केवल क्षैतिज भूजल प्रवाह के साथ द्वि-आयामी, सजातीय समस्थानिक अनुच्छेत्र शामिल हैं। इसके अलावा अनुच्छेत्र में प्रतिक्रिया प्रणाली एक तात्कालिक द्वि-आणविक प्रतिक्रिया तक सीमित है जो केवल बहुत तेजी से प्रतिक्रिया करने वाले दूषित पदार्थों के लिए बहुत उपयुक्त हो सकती है। इसके अलावा वर्तमान अध्ययन में फैलाव की भूमिका का आकलन नहीं किया गया है। एक आधार विश्लेषणात्मक मॉडल का चयन अधिक सख्ती से किया जाना चाहिए। हालाँकि, इस काम में, लिडल और अन्य (2005, 2011) का विश्लेषणात्मक मॉडल को इसकी कम डाटा की आवश्यकता और लंबवत उन्मुख मॉडल होने के कारण आधार मॉडल के रूप में उपयोग किया गया है।

प्रस्तावित मॉडलों का उपयोग दूषित साइटों के पूर्व-मूल्यांकन के लिए किया जा सकता है क्योंकि अनुमान के लिए सटीकता विश्लेषणात्मक समाधान की तुलना में अधिक पाई जाती है, इस प्रकार उन्हें अधिक प्रासंगिक बना देती है। यह देखते हुए कि जोखिम प्रबंधन उपकरणों की सहायता के लिए संकर मॉडल प्रस्तावित किए जा रहे हैं, मामूली अतिप्राक्लन की अनदेखी की जा सकती है।

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List of Symbols

α_L, α_{Th} and α_{Tv}	Dispersivity in Longitudinal, Transverse Horizontal and Transverse Vertical Directions [L]
$C_{A,0}$	Ambient Oxygen Concentration in the Groundwater [LT ⁻³]
$C_{D,0}$	Initial Organic Concentration [LT ⁻³]
C_D^{Thres}	Threshold Concentration [ML ⁻³]
C_{EA}	Initial Reactant Partner Concentrations of Electron Acceptor [ML ⁻³]
C_{ED}	Initial Reactant Partner Concentrations of Electron Donor [ML ⁻³]
D_A	Effective Molecular Diffusion Coefficient of the Oxygen [L ² T ⁻¹]
$D_{S,A}$	Dispersion Term of Oxygen in the Moving Aqueous Phase [L ² T ⁻¹]
D'_x, D'_y and D'_z	Dispersion Coefficient [LT ⁻²]
L_{max}	Maximum Plume Length [L]
q_0	Specific Discharge in X-Direction at $X = 0$ [LT ⁻¹]
v	Groundwater Velocity [LT ⁻¹]
α_L	Transverse Dispersivity[L]
λ_{EFF}	Decay Factor [T ⁻¹] – BIOSCREEN- AT
A	Source Area [L ²]
d	Grain Size [L]
D_{mech}	Mechanical Dispersion [L ² /T],,
D_p	Pore Diffusion [L ² /T]
D_t	Hydrodynamic Dispersion [L ² /T]

F_A	Utilization Factor [-]
H	Depth of Source Penetration [L] – BIOSCREEN- AT
i	Hydraulic Gradient [-]
k	Hydraulic Conductivity [L]
L_{field}	Field Plume Length[L]
$L_{max, ana}; L_{ana}$	Analytically Estimated Maximum Plume Length [L]
$L_{max, hyb}; L_{hyb}$	Hybrid Model Maximum Plume Length [L]
$L_{max, num}; L_{num}$	Numerically Estimated Maximum Plume Length [L]
M	Aquifer Thickness [L]
M_S	Source Thickness [L]
n	Porosity [-]
P	Source Perimeter[L]
Q	Injection Flow Rate [L ² T ⁻¹]
q	Specific Discharge [LT ⁻¹]
R	Recharge Rate [LT ⁻¹]
v	Groundwater Velocity [LT ⁻¹]
W	Source Width [L]
x, y, z	Cartesian Co-Ordinates [L]
γ	Utilization Factor [-]
γ'	Source Decay Coefficient [-] – BIOSCREEN- AT
ε	Bio-Utilization Concentration [ML ⁻³]

List of Abbreviations

ADE	Advection-Dispersion Equation
AFCEE	Air Force Center For Engineering and the Environment
BMBF	Bundesministerium für Bildung und Forschung German Federal Ministry of Education and Research
BTEX	Benzene, Toluene, Ethylbenzene And Xylenes
CAST	Contamination Assessment and Site-Management Tool
CS	Contaminated Sites
DNAPL	Dense Non Aqueous Phase Liquid
EA	Electron Acceptor
ED	Electron Donor
EDA	Exploratory Data Analysis
EEA	European Environment Agency
EU	European Union
GDP	Gross Domestic Product
KORA	Kontrollierter Natürlicher Rückhalt Und Abbau Von Schadstoffen Bei Der Sanierung Kontaminierter Böden Und Grundwässer
LNAPL	Light Non Aqueous Phase Liquid
MNA	Monitored Natural Attenuation
MT3DMS	Modular Three-Dimensional Multi- Species Solute Transport Mode
MTBE	Methyl Tert-Butyl Ether

NA	Natural Attenuation
NAPL	Non Aqueous Phase Liquid
PAH	Polycyclic Aromatic Hydrocarbons
PCE	Tetrachloroethylene
PCS	Potentially Contaminated Sites
RMSE	Root Mean Squared Error
SD	Standard Deviation
TCE	Trichloroethylene
TMB	1,2,4-Trimethyl Benzene
WWAP	World Water Assessment Programme