INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING, *SERIES B*
Volume 3, Number 2, Pages 109–125

CRANK-NICOLSON FINITE ELEMENT FOR 2-D GROUNDWATER FLOW, ADVECTION-DISPERSION AND INTERPHASE MASS TRANSFER: I. MODEL DEVELOPMENT

MORRAKOT KHEBCHAREON

Abstract. Dense, non-aqueous phase liquids (DNAPLs) are common organic contaminants in subsurface environment. Once spilled or leaked underground, they slowly dissolved into groundwater and generated a plume of contaminants. In order to manage the contaminated site and predict the behavior of dissolved DNAPL in heterogeneous subsurface requires a comprehensive numerical model. In this work, the Crank-Nicolson finite-element Galerkin (CN-FEG) numerical scheme for solving a set coupled system of partial differential equations that describes fate and transport of dissolved organic compounds in two-dimensional domain was developed and implemented. Assumptions are made so that the code can be compared and verified with available analytical solutions.

Key words. Groundwater, Advection-Dispersi on, Crank-Nicolson, Finite Element Galerkin, Mass Transfer

1. Introduction

Non-aqueous phase liquids (NAPLs) are immiscible in water, representing another phase of concern in groundwater contamination problems. These liquids pose special problems for the hydrogeologists, regulators, and engineers because their fate and transport are difficult to simulate. Most NAPLs are health hazard and some are known to be carcinogens. Partial or full exposure to polluted groundwater results in a high risk for those who are located downstream of the DNAPL source zone. Although aqueous solubility of components in NAPLs is low, its concentration level is much higher than the regulated drinking water standards. Therefore, there is a need for immediate action to clean-up contaminated aquifers. In order to predict NAPL source's longevity or to estimate the clean-up duration of the selected remediation technologies, a validated numerical model is needed. Mathematical models are commonly used as a tool to evaluate DNAPL source zone longevity, cost/benefit of a selected remediation technology, and to predict the extent of groundwater contamination before and after remediation [1]. These models are developed using both finite-difference and finite-element methods and range from simple to sophisticated formulations. Unfortunately, available numerical models that deal with both groundwater flow and NAPL contamination are very limited. This is particularly due to the mathematical complexity of the multiphase flow and the dissolution of DNAPL in the heterogenous subsurface.

Numerical modeling of groundwater flow and contaminant transport has long been studied and their development have become relatively mature. Both analytical and numerical models have been proposed. Several numerical models are available

Received by the editors January 1, 2012 and, in revised form, March 22, 2012.
2000 *Mathematics Subject Classification.* 35R35, 49J40, 60G40.

for a wide range of applications related groundwater flow and contaminant transport [2, 3, 4, 5]. However, finite-element based computer code for solving this kind of problem in heterogeneous porous media is still at an early stage [6]. Relatively little effort has been made to develop a truly coupled model due to the complexity of the problem and the sophistication of the mathematical formulation as well as its numerical implementation. Traditional modeling exercise for the problem of this type assumes that the solute concentration does not affect the fluid density, viscosity, nor the soil's hydraulic conductivity. Based on these assumptions, groundwater modelers usually solve the two processes of groundwater flow and contaminant transport separately (i.e., uncoupled), thus, simplifying the model, its numerical implementation, and the computational power requirement. With an addition of the interphase mass transfer process to groundwater flow and solute transport, the model becomes more complicated and highly non-linear. Simple analytical solution to this problem does not exist unless simplifying assumptions are made. Available numerical models such as MODFLOW-MT3DMS suite [2, 3], SUTRA [4], and the finite-element groundwater flow/contaminant transport program by Istok [7] may not be able to handle this kind of problem, since these simulators do not capture processes occurring due to the presence of non-aqueous phase liquid. Delshad et al. [5] developed a multi-phase, multi-component compositional finite-difference model (called UTCHEM) to solve the migration and dissolution of the non-aqueous phase liquids. This model, however, has experienced some numerical difficulties and it can not simulate complex boundary conditions prevents it from widely acceptance.

Saenton et al. [8] and Saenton [9] have developed an *explicitly coupled* finite-difference mass transfer model based on existing groundwater flow program, MODFLOW [2], and reactive contaminant transport or RT3D [10] by adding the dissolution package (DSS) to the program module. They have successfully simulated the dissolution of entrapped tetrachloroethene (PCE) in the sandbox experiment under both normal and (surfactant-) enhanced conditions. However, these simulations required a very small time-step size in order to satisfy the stability criteria due to the use of a technique called operator splitting. This can cause excessively long execution time. The major limitation of the finite-difference model is that finite-difference grids do not conform to boundaries that are not parallel to the coordinate axes. Stair-step approximations to angular boundaries are inconvenient to specify and can cause local variations in the ground-water flow field or contaminant plume that are not realistic.

Khebchareon and Saenton [11] have recently developed a one-dimensional Crank Nicolson finite-element Galerkin numerical model to solve a coupled system of partial differential equations which include groundwater flow, advection-dispersion, and rate-limited dissolution of entrapped NAPL equations. They have also verified the code using analytical solution of a 1-D steady-state NAPL dissolution. Subsequently, the code is validated using experimental data obtained from soil column dissolution cell [12]. Although the developed program has successfully simulated the dissolution behavior of PCE in a soil column, it clearly needs further development and modifications in order to be used in real situations.

The present study, therefore, aims to develop a numerical code based on Crank-Nicolson scheme in time and finite element Galerkin method in spatial discretization