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PARALLEL FINITE ELEMENT METHOD FOR COUPLED CHLORIDE MOISTURE DIFFUSION IN CONCRETE

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Abstract. Penetration of chloride ions into concrete and diffusion of moisture in concrete are important factors responsible for the corrosion of steel in concrete. The two diffusion processes are coupled. This paper deals with the analysis and simulation of coupled chloride penetration and moisture diffusion in concrete. Of particular interest is the parallel programming in finite element method for solving the coupled diffusion problem. Parallel computing technology has been advantageous for solving computationally intensive problems. It has become quite mature technology and more affordable for general application. Our approach to solve the parallel programming problem is to use available libraries, i.e. Portable, Extensible Toolkit for Scientific Computation (PETSc) and The Message Passing Interface (MPI) standard. The formulation of the coupled diffusion problem, the material models involved in the differential equations, the details of parallel domain decomposition technique in the finite element algorithm are presented. The advantages of parallel programming are demonstrated by a numerical example.

Key Words. Chloride, moisture, humidity, diffusion, parallel computing, finite element, concrete.

1. Introduction

Reinforced concrete structures are often exposed to deicing salts, salt splashes, salt spray, or seawater, resulting in penetration of chloride ions into concrete. The chloride ions in the concrete will eventually reach the embedded reinforcement bars (rebar) and accumulate to a certain critical concentration level, at which the rebar begins to corrode. Since the density of corrosion product is lower than that of steel, the corrosion product occupies larger volume than the volume of steel consumed in the corrosion process. This volumetric mismatch will generate very high tensile stress in the concrete cover that may lead to concrete cracking and/or spalling.

The other necessary conditions for the rebar corrosion to take place are low pH value, and sufficient oxygen and moisture present in the rebar-concrete interface. For non-saturated concrete (e.g. the concrete not submerged in water), oxygen supply is usually not an issue. For old concrete structures, pH value of the concrete is usually much lower than new concrete (pH is about 12.5 to 13). Therefore the diffusion of moisture in the concrete is just as important as the diffusion of chloride ions in terms of the corrosion process of rebars. Although moisture is the carrier of chloride ions, the moisture and the chloride ions can diffuse in the same or opposite

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directions depending on the boundary (environmental) and initial conditions of a structure. When the moisture and chloride diffusions are considered as two fully coupled diffusion processes, the computational program is very complicated.

Chloride-induced rebar corrosion has been one of the major causes of deterioration in reinforced concrete structures. In some states of the U.S., chloride-induced deterioration may govern the service life of reinforced concrete structures. With the increasing acceptance of durability-based design for reinforced concrete structures, it is very important to develop both material models and computational tools that are able to accurately simulate the processes of chloride ion penetration and moisture diffusion in concrete. This study is aimed to address both aspects: development of theoretical models and computational techniques for coupled chloride and moisture diffusion in concrete.

The material models and governing partial differential equations for chloride ions penetration and moisture diffusion are time dependent and complex. Thus, various numerical approaches have been developed as effective tools to solve the problem. In this study, a finite element method is employed to solve the coupled chloride penetration and moisture diffusion equations. The space discretization is carried out based on a Galerkin procedure and time discretization based on mid-point time integration method.

The diffusion processes of moisture and chloride take place only in a thin layer of concrete structures (5 to 10 cm), and therefore, very small finite elements must be used in the diffusion analysis to deal with drastic variation of the moisture profiles and chloride concentration profiles. For large scale structures with different environmental conditions on their surfaces, the number of elements required for a durability analysis is enormous. If we want to further combine the diffusion analysis with stress analysis for the damage development due to the steel corrosion, the computational time will be escalated even at a higher rate, resulting in a computationally intensive program. With increased availability of parallel computing facilities, it becomes natural to implement parallel finite element method for the diffusion analysis. In this study, a parallel finite element program is implemented on a cluster of PCs using the Linux operating system, and the parallel architecture is classified as a distributed memory system.

The development of parallel finite element program used to be a time consuming and complicated process. Now, with the help of higher level libraries for parallel implementation such as PETSc (Portable, Extensible Toolkit for Scientific Computation), parallel finite element program can be developed in a relatively simple manner. PETSc provides a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. PETSc employs the MPI (Message Passing Interface) standard for all message-passing communication.

2. Governing differential equations and material parameters

2.1. Governing equations. We derive the governing partial differential equations for chloride penetration and moisture diffusion in concrete based on Fick's law and the mass balance equations for chloride and moisture in concrete. The two resulting equations are coupled and must be solved simultaneously. First of all, the flux of chloride ions (J_{Cl}) through a unit area of porous media depends on the gradient of chloride ions as well as the gradient of moisture, i.e.:

$$J_{Cl} = -\left(D_{Cl}\nabla C_f + \varepsilon D_H \nabla H\right), \tag{1}$$