CHAPTER I

INTRODUCTION

One of the goals of computational fluid dynamics (CFD) is physically accurate numerical simulation of fluid flow for a particular design. Using CFD, the design can be analyzed at less cost than using scale models and is more easily modified. Within the aerodynamic branch of CFD, a full spectrum of codes has been developed to simulate flows across airfoils, through turbomachinery, and through engines and nozzles. In water resources applications, CFD methods have been applied to open-channel flows, flows through erodible rivers and estuaries, groundwater and surface water flows, contaminant transport and salt migration, to name a few, with varying levels of complexity and accuracy. In order to use these simulation tools more effectively, they need to be modified to search the space of acceptable designs efficiently, in addition to providing flow field information. Within the field of aerodynamics, sensitivity analysis has been used to transform many high fidelity simulation codes into efficient, gradient-based design codes. Since the governing equations and solution methods within many water resources applications are similar to those used in aerodynamics, sensitivity analysis should be similarly applicable in transforming the higher fidelity simulation codes into efficient design optimization codes.

To demonstrate this transformation within the field of water resources, an existing, two-dimensional, finite-element open-channel simulation code called HIVEL2D **[1,2]** is converted into a design optimization code using discrete sensitivity analysis. Since the simulation code has been used in conjunction with scale models to assist in the analysis of potential designs, a deterministic, gradient-based design optimization code for open-channel flow is of relevance to actual design work. Coupling non-linear optimization and discrete sensitivity analysis with a finite-element simulation code that solves the shallow water equations presents several challenges due to the viscous models incorporated within the governing equations, the Petrov-Galerkin test function used to provide upwinding for the finite element method and the presence of hydraulic jumps within the domain of the objective function. Furthermore, because HIVEL2D is a higher-fidelity simulation tool, the determination of a steady-state solution is computationally expensive; hence, an efficient optimization algorithm should identify an optimal solution with as few steady-state solutions as possible.

When formulating a design optimization problem, the objective function to be optimized is chosen to be a measure of the design quality. For open-channel flow, several objective functions can be chosen, based on the particular design goals. One goal is to minimize the height and length of containment walls that are necessary to prevent flooding. When the flow depths vary greatly, the walls need to be higher for a longer stretch of the channel. The objective function used in this research is a measure of the non-uniformity of the depth of flow over the region of interest and calculates the variation of the depths from the average depth over this region. The design variables for this particular design optimization problem are similar to those variables used in current design methods. The design space derivatives, which are the derivatives of the objective function with respect to the design variables, are calculated via discrete sensitivity analysis, which is more computationally efficient than using finite differences, especially for problems where the objective function is expensive to evaluate. The complex Taylor's series expansion method is used to generate a highly accurate Jacobian matrix for use within discrete sensitivity analysis, which removes one major source of error from the derivative estimation method. Since the objective function is a least-squares function, the Gauss-Newton optimization algorithm is used to update the design variables and demonstrates rapid convergence towards an optimal solution, reducing the number of design iterations. Furthermore, by using a Levenberg-Marquardt constant, the optimization algorithm becomes quite stable, converging for each test case.

The design optimization strategy presented in this dissertation can be applied to other areas of water resources. In many time dependent problems, as well as several steady-state problems, the objective function can be naturally expressed as a nonlinear least-squares function, for which the Gauss-Newton optimization algorithm is applicable. Discrete sensitivity analysis is a mathematical tool that can be applied to almost any set of partial differential equations. For example, discrete sensitivity analysis can be applied to the St. Venant equations, the shallow water equations and the incompressible Navier-Stokes equations for use in open-channel flow, spillway flow and river and estuarine flows, to the porous media equation which governs flow in groundwater aquifers, and to the transport equations which govern contaminant transport and salinity migration. Optimization problems within these applications include parameter identification of the friction coefficient in open-channel flow, the hydraulic conductivities and storativities in groundwater modeling and the dispersion coefficient in the transport equations. Design problems include the shape of the bed and walls for open-channel and spillway flows and the shape and placement of control structures such as weirs and stilling basins. Even though the design optimization strategy presented in this research was applied to open-channel design, this procedure holds much promise for researchers in other areas of water resources to enhance their CFD codes to solve their design optimization and parameter estimation problems more efficiently and accurately.

In Chapter 2, a variety of design optimization algorithms used in recent research efforts is presented, as well as their applications within aerospace and water resources. Chapter 3 contains the components of the design optimization strategy as applied to the open-channel design code. In Chapter 4, a preliminary example is analyzed which compares the various gradient-estimation alternatives and optimization algorithms. In Chapter 5, the design optimization strategy is applied to channel contractions, expansions, bends and bridge piers, showing that the open-channel design code can be used to identify efficient designs. In Chapter 6, conclusions are drawn about the research, and suggestions for future research are made in Chapter 7. In the appendices, the equations associated with discrete sensitivity analysis are presented, as well as their implementation within the flow solver HIVEL2D, the various gradient-based optimization algorithms are reviewed, the complex Taylor's series expansion method is presented, the equation for the viscous velocity profile is derived, and the specifics of the implementation of the shallow water equations within HIVEL2D are discussed.