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CFD-BASED SHAPE OPTIMIZATION OF MICROCHANNELS USING ADJOINT VARIABLE METHOD

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Abstract. *The shape of microchannels is an important design variable to achieve the desired performance. Since most microchannels are, at present, designed by trial and error, a systematic optimal shape design method needs to be established. Computational fluid dynamics (CFD) is often used to rigorously examine the influence of the shape of microchannels on heat and mass transport phenomena in the flow field. However, the rash combination of CFD and the optimization technique based on gradients of the cost function requires enormous computation time when the number of design variables is large. Recently, the adjoint variable method has attracted the attention as an efficient sensitivity analysis method, particularly for aeronautical shape design, since it allows one to successfully obtain the shape gradient functions independently of the number of design variables. In this research, an automatic shape optimization system based on the adjoint variable method is developed using C language on a Windows platform. To validate the effectiveness of the developed system, pressure drop minimization problems of a U-shaped microchannel and a branched microchannel in incompressible flows under constant volume conditions are solved. These design examples illustrate that the pressure drops of the optimally designed microchannels are decreased by 20 ~ 40 % as compared with those of the initial shape.*

1 INTRODUCTION

In recent years, micro chemical process technology has attracted considerable industrial and academic attention in various fields ([1], [2], [3], [4], [5]). The main characteristic of micro chemical processes is the small diameter of the channels ensuring short radial diffusion time. This leads to a narrow residence time distribution, high heat and mass transfers. In addition, micro chemical processes have a high surface to volume ratio allowing efficient heat removal and high molar flux. Through the R&D activities on micro chemical processes, the necessity of developing a systematic design method of micro devices has been recognized. The design problems of micro devices are different from those of conventional devices. In a conventional design problem, the unit operations are modeled by using terms such as perfect mixing, piston flow, and overall heat transfer coefficient. In other words, each unit operation is modeled as a lumped parameter system. However, the performance of micro devices depends on the temperature distribution, the residence time distribution and/or the degree of mixing. Therefore, each micro device should be modeled as a distributed parameter system, and the shape of the device must be included in the design variables in addition to the size of the device. Namely, the design problems of micro devices are regarded as shape optimization problems, in which a cost function defined on a flow domain and/or on its boundary is minimized or maximized under several constraints.

With the advances in computational resources and algorithms, Computational Fluid Dynamics (CFD)-based optimal shape design is an interesting field for industrial applications such as aerospace, car, train, and shipbuilding ([6], [7]). In such design, the computation of the cost function gradient, i.e., the sensitivity of some performance measure, is the heart of the optimization. Recently, the adjoint variable method ([8], [9], [10]) has attracted the attention as an efficient sensitivity analysis method, since it allows successfully obtaining the shape gradient functions independently of the number of design variables. In this research, an automatic shape optimization system based on the adjoint variable method is developed using C language on a Windows platform. In addition, in order to validate the effectiveness of the developed system, the optimal shape design problems of the pressure-driven microchannels are solved in the following sections.

2 GENERAL FORMULATION OF THE ADJOINT-BASED SHAPE OPTIMIZATION

The optimization technique based on gradients of the cost function is the easiest way. For each design variable, its value is varied by a small amount, the cost function is recomputed, and the gradients with respect to it are measured. In this case, the number of CFD solutions required for N design variables is N+1. Consequently, the gradient-based method requires enormous computation time when the number of design variables is large. In this study, the adjoint variable method is adopted to obtain gradients in a more expeditious manner.

In a fluid dynamic design optimization problem, the cost function depends on design variables and the flow variables due to them. The cost function can be written as

$$I = I(\boldsymbol{W}(\boldsymbol{\beta}), \boldsymbol{\beta}) \tag{1}$$

where I is the cost function, $\boldsymbol{W}$ is the flow variable vector, and $\boldsymbol{\beta}$ is the design variable vector that represents the surface shape of channels. The cost function I is minimized or maximized subject to partial differential equation (PDE) constraints, geometric constraints, and physical constraints. Examples for the cost function I are drag or pressure drop, for PDE constraints $\boldsymbol{R}(\boldsymbol{W},\boldsymbol{\beta})=\boldsymbol{0}$ the Euler/Navier-Stokes equations, for geometric constraints $\boldsymbol{g}(\boldsymbol{\beta}) \leq \boldsymbol{0}$ the volume or cross sectional area, and for physical constraints $\boldsymbol{h}(\boldsymbol{W}) \leq \boldsymbol{0}$ a minimal pressure to prevent cavitation.

The principles of the evaluation of gradients based on adjoint variables are given here ([9], [10], [11]). A total differential in the cost function I and the PDE constraint $\boldsymbol{R}$ results in:

$$dI = \left(\frac{\partial I}{\partial \boldsymbol{W}}\right) d\boldsymbol{W} + \left(\frac{\partial I}{\partial \boldsymbol{\beta}}\right) d\boldsymbol{\beta}, \tag{2}$$

$$d\boldsymbol{R} = \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{W}}\right) d\boldsymbol{W} + \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\beta}}\right) d\boldsymbol{\beta} = \boldsymbol{0}. \tag{3}$$

Next, a Lagrange multiplier $\boldsymbol{\lambda}$ is introduced to add the flow equation to the cost function:

$$dI = \left\{ \left(\frac{\partial I}{\partial \boldsymbol{W}} \right) - \boldsymbol{\lambda}^T \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{W}} \right) \right\} d\boldsymbol{W} + \left\{ \left(\frac{\partial I}{\partial \boldsymbol{\beta}} \right) - \boldsymbol{\lambda}^T \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\beta}} \right) \right\} d\boldsymbol{\beta} \tag{4}$$

This implies that if we can solve:

$$\boldsymbol{\lambda}^T \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{W}} \right) = \left(\frac{\partial I}{\partial \boldsymbol{W}} \right), \tag{5}$$

the variation of I is given by:

$$dI = \left\{ \left(\frac{\partial I}{\partial \boldsymbol{\beta}} \right) - \boldsymbol{\lambda}^T \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\beta}} \right) \right\} d\beta = \boldsymbol{G} d\boldsymbol{\beta} \; . \tag{6}$$

Equation (6) means that the variation of I exhibits only derivatives with respect to $\boldsymbol{\beta}$, and that the shape gradient function $\boldsymbol{G}$ is independent of the number of design variables. In the case that $\boldsymbol{R}$ is PDE, the adjoint equation (5) is also PDE, and the appropriate boundary conditions must be determined. The effectiveness of the adjoint-based shape optimization is emphasized along with the increase in design variables.

3 A SHAPE OPTIMIZATION SYSTEM DEVELOPMENT

In this research, an automatic shape optimization system based on the adjoint variable method is developed using C language on a Windows platform. The procedures for building the system are shown in Fig. 1. In principle, after a new shape is obtained, a new grid is generated, and the solution is restarted. For every design cycle, the following steps are required:

1) assume an initial shape,
2) generate computational grids,
3) solve the flow equations, viz. the Navier-Stokes equations and the continuity equations, for deriving the flow velocity and the pressure,
4) solve the adjoint equations to obtain the set of Lagrange multipliers,
5) calculate the shape gradient functions,
6) obtain a new shape by moving each point on the boundary,
7) go to step 2 unless the change in the cost function is smaller than a desired convergence parameter.

Each design cycle requires a numerical solution of both the flow and the adjoint equations, whose computational time is roughly twice that required to obtain the flow solution.

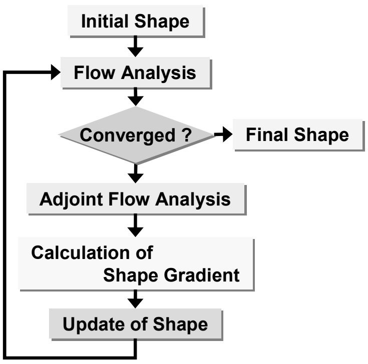

Figure 1: Flow chart of shape optimization

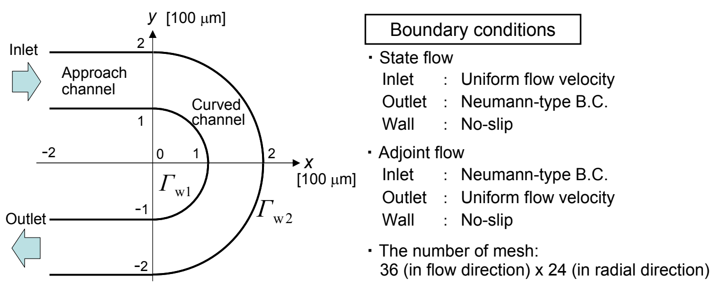

Figure 2: Analytical domain and boundary condition for a U-shaped microchannel.

4 CASE STUDY

Flow in microchannels is driven by the pressure difference or the electric potential between inlet and outlet. For pressure-driven flow, an important issue is how to reduce the pressure drop required to realize a desired flow rate in a microchannel. Curved microchannels and/or branched microchannels are often used to provide long flow passage in a compact device. Modification of the shape of curved channels and/or branched channels may decrease the pressure drop. In this study, a design example is presented to demonstrate the effectiveness of the developed system for microchannel shape optimization problems. The adjoint variable method is applied to all gradient computations. For convenience, the physical coordinates system is transformed to computational coordinates in the flow and adjoint flow analysis. The two-dimensional computations in these case studies are performed on Windows Intel® 3.0 GHz Pentium 4 processors.

The first design example is a shape optimization problem of U-shaped microchannels in incompressible flows. The goal is to minimize pressure drop for various inlet Reynolds numbers: Re = 0.1, 1, 10, and 100. The initial shape of the U-shaped microchannel and the main design conditions are shown in Fig. 2. The width of the initial shape is 100 μm. The curved channel is connected with inlet and outlet straight channels. The total number of mesh is 864. The design boundaries are assigned to Γ_{w1} and Γ_{w2}, and the design variables are associated with the grid points on both design boundaries. For pressure-driven liquid flow in a microchannel, the no-slip boundary condition is usually valid. The streamwise velocity component at the entrance is specified, and the transverse velocity component at the entrance is assumed to be zero. The prescribed pressure $p = 0$ is assumed at the exit boundary.

Design results at Re = 10 are presented here. Figure 3 shows the pressure distributions for the initial shape, the final shape under no volume constraint, and the converged shape under a constant volume constraint. Under no volume constraint, the width of the curved channel is widened, and the shape of the channel is significantly modified. The wider channel makes the flow velocity lower, and a large reduction of

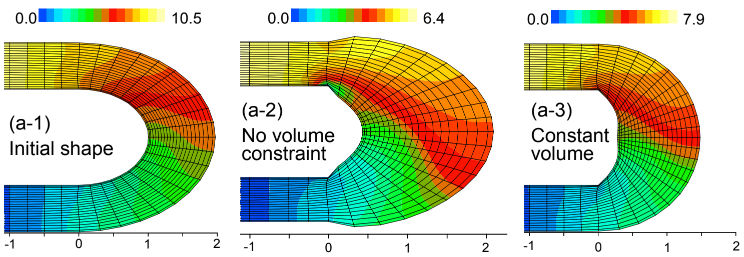

Figure 3: Pressure distributions: (a-1) initial shape, (a-2) final shape under no volume constraint, (a-3) optimal shape under a constant volume constraint. Reference frame is prepared below each shape.

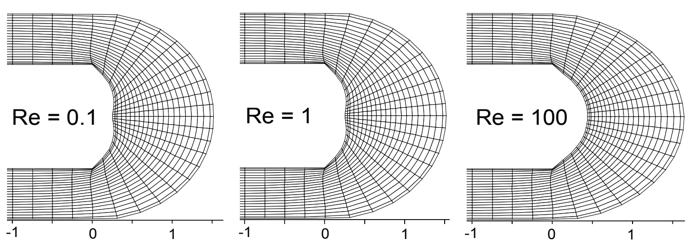

Figure 4: Optimal shape at Re = 0.1 (left), 1 (middle), and 100 (right).

pressure drop can be achieved. On the other hand, under a constant volume constraint, both the inside and outside surfaces of the curved channel are moved toward the direction of the negative *X* axis, and the flow passage is shortened.

Under a constant volume constraint, the cost function is converged in 92 design iterations and pressure drop is reduced by 27.6 %, as compared with that of the initial curved shape. Each design iteration requires approximately 10 seconds. On the other hand, without volume constraint, the design cycles are stopped in 30 design iterations due to the fluctuation of the cost function, and pressure drop is decreased by 39.3 %, as compared with that of initial curved shape.

In addition, the influence of Re on the result of shape optimization is investigated. Figure 4 shows the optimal shapes at Re = 0.1, 1, and 100 under the constant volume constraint. On the basis of these results, the corresponding reductions in pressure drop are 29.0 %, 28.9 %, and 19.6 %, respectively, as compared with that of initial curved shape. The optimal shapes at Re = 0.1 and 1 are almost the same as that at Re = 10. The optimal shape at Re =100 is different from the others, and its curvature is small due to large flow inertia.

5 CONCLUSIONS

In this work, an automatic shape optimization system based on the adjoint variable method is developed by using C language on a Windows platform. Since the pressure drop in microchannels is an important characteristic related to the energy demand for process optimization, the developed system is applied to the pressure drop minimization problems of microchannels. The last section demonstrates by representative examples that the adjoint variable method can be used to formulate computationally feasible procedures for the shape design of pressure-driven microchannels. The computational time of each design cycle is of the same order as two flow solutions, since the adjoint equation is of comparable complexity to the flow equation. The developed system is quite general and is not limited to particular choice of cost function. Our future work will focus on the extension of the developed system to shape optimization problems of thermo-fluidic microdevices.

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