Estimation of diffusion and convection coefficients in an aerated hydraulic jump

K. Unami a, T. Kawachi a, M. Munir Babar b, H. Itagaki c

a Graduate School of Agricultural Science, Kyoto University, Kitashirakawa-oiwake-cho, Sakyo-ku, Kyoto 606-8502, Japan
b Institute of Irrigation and Drainage Engineering, Mehran University of Technology and Engineering, Jamshoro, Sindh, Pakistan
c Division of Biological Production System, Faculty of Agriculture, Gifu University, 1-1 Yanagido, Gifu 501-1112, Japan

Received 23 March 1999; accepted 16 October 1999

Abstract

Diffusion and convection coefficients of the aerated flow in a hydraulic jump are estimated in the framework of an optimal control problem. The specific gravity of air–water mixture is governed by a steady state convection diffusion partial differential equation. The governing equation includes the diffusion coefficient and the convection coefficient, which are taken as the control variables to minimize a domain observation type functional which evaluates the error between observed specific gravity and the solution to the governing equation. The minimum principle is deduced to characterize the optimal control variables using the adjoint partial differential equation. Solvability of the partial differential equations is discussed in terms of variational problems. An iterative numerical procedure including a finite element scheme to solve the partial differential equations is developed and demonstrated by using the observed data.

Keywords: Hydraulic jump; Aerated flow; Diffusion coefficient; Convection coefficient; Estimation; Optimal control problem

1. Introduction

In a wide horizontal rectangular channel of constant width, a hydraulic jump is formed when the state of flow changes from supercritical to subcritical one. The hydraulic jump is usually accompanied by an aerated recirculating roller on the top, where intensive turbulence results in energy dissipation and the mixing of air also takes place. The development mechanism of such a roller has been investigated using high speed video cameras [7], and it is revealed that the roller is made up of several vortices which are generated at the toe of the hydraulic jump and subsequently travel downstream growing by pairing. Thus, unsteady behaviors in the flow structure of the hydraulic jump are evident.

Despite such microscopically dynamic nature, the hydraulic jump is treated as a macroscopically steady phenomenon for engineering purposes, and temporally averaged quantities are examined. The steady state approach is rather significant for evaluating re-oxygenation effect in polluted rivers, energy dissipation effect in stilling basins of spillways, and so on. In this context, governing laws of the air-mixed water are difficult to be identified because averaged flow properties such as diffusivity and residual stress cannot be obtained from the theoretical inductions. Thus, investigations based on observations are inevitable. Especially, when measuring the concentration of contained air is relatively easy, it is interesting to clarify what is possible to know from observed air concentrations [2].

In the present work, assuming that the specific gravity, which is defined by the ratio of the density of air–water mixture to that of pure water, is governed by a steady convection diffusion equation, an inverse problem is posed to estimate its diffusion and convection coefficients from observed specific gravity data. For the sake of simplicity, considerations are restricted to vertically 2-D flow structure. Being underdetermined, the inverse problem is formulated as an optimal control problem. This type of problem, referred to as an inverse coefficient problem [4], is often studied in the area of groundwater [8,9], but the problem considered here requires particular attention to the convection term. Since the approaches to inverse coefficient problems for convection dominant equations are not very well established [5], therefore in the present work the minimum principle which characterizes the coefficients such as to give a specific gravity field closest to specified data is deduced.
The minimum principle includes the adjoint equation of the convection diffusion equation, and the solvability of these two equations are discussed in terms of variational problems. A numerical method using a finite element scheme for the resolution of the equations is proposed to iteratively estimate the diffusion and the convection coefficients. To confirm the validity of the methodology a sample computation is demonstrated by using observed data.

2. Mathematical definitions

In order to follow up the subsequent sections smoothly a brief introduction of the mathematical concepts used in these sections is delineated here. For details to these definitions, reference is made to the book of Sobolev spaces by Adams [1]. Note that the following notations are pertaining to real functions. The symbol $\Omega$ is used for a domain which is a bounded open set in 2-D Euclidean space. The inner product between two 2-D vectors $\mathbf{u}$ and $\mathbf{v}$ is denoted by $\mathbf{u} \cdot \mathbf{v}$. The absolute value of a scalar $u$ is represented by $|u|$, and the Euclidean norm of a 2-D vector $\mathbf{u}$ is also denoted by $|\mathbf{u}|$. The class of all measurable scalar valued functions $u$, defined on $\Omega$, for which $\int_{\Omega} |u|^2 \, d\Omega < \infty$ is denoted by $L^2_1$. Similarly, $L^2_2$ is defined for 2-D vector valued functions $\mathbf{u}$ for which $\int_{\Omega} |\mathbf{u}|^2 \, d\Omega < \infty$. Inner products are defined as $\langle u, v \rangle = \int_{\Omega} u \cdot v \, d\Omega$ for $u, v \in L^2_1$ and as $\langle \mathbf{u}, \mathbf{v} \rangle = \int_{\Omega} \mathbf{u} \cdot \mathbf{v} \, d\Omega$ for $\mathbf{u}, \mathbf{v} \in L^2_2$, respectively, using the same notation $\langle \cdot, \cdot \rangle$. The norms defined in $L^2_1$ and $L^2_2$ from their respective inner products are commonly denoted by $\| \cdot \|$. For a scalar function $u$, another norm $\|u\|_1$ is defined as

$$
\|u\|_1 = \sqrt{\|u\|^2 + \|\nabla u\|^2}
$$

(1)

where $\nabla$ is the 2-D del operator. Let $C^r_2$ be the class of all twice continuously differentiable functions $u$ such that $\|u\|_1 < \infty$. The completion of $C^r_2$ with respect to the norm Eq. (1) is the Sobolev space $H^1$, equipped with the norm Eq. (1). Let $C^\infty_0$ be the class of all infinite times continuously differentiable functions which have compact support in the domain $\Omega$. The closure of $C^\infty_0$ in the Sobolev space $H^1$ is another Sobolev space $H^1_0$. The Sobolev space $H^1_0$ is equipped with a norm defined by

$$
\|u\|_{H^1_0} = \|\nabla u\|
$$

(2)

for $u \in H^1_0$ and an inner product

$$
\langle u, v \rangle_{H^1_0} = \langle \nabla u, \nabla v \rangle
$$

(3)

for $u, v \in H^1_0$.

3. Problem formulation

Considering mass conservation of air and neglecting compressibility effect, the governing convection diffusion equation of the transport phenomena in steady aerated flows is written as

$$
L(a, b; \gamma) \overset{\text{def}}{=} - \nabla \cdot a \nabla \gamma + \nabla \cdot \gamma b = 0
$$

(4)

where $L$ is the differential operator of the convection diffusion equation, $a$ the diffusion coefficient, $b$ the convection coefficient, which is the vector sum of water velocity vector and air bubble rise velocity vector; and $\gamma$ is the specific gravity in the domain $\Omega$ bounded by its boundary $\Gamma$. The $x$- and $y$-coordinates are taken as the horizontal and vertical ones, respectively.

A boundary value problem of Dirichlet type is considered prescribing a boundary condition

$$
\gamma = \hat{\gamma}
$$

(5)

where $\hat{\gamma}$ is the specified boundary value on the boundary $\Gamma$. The partial differential equation system Eq. (4) with (5) is rearranged in its equivalent variational form

$$
I(a, b; u, \varphi) \overset{\text{def}}{=} \langle (a \nabla u - ab), \nabla \varphi \rangle = -I(a, b; \hat{\gamma}, \varphi)
$$

(6)

where $u$ is the state variable, $I$ the bilinear form of the convection diffusion equation, and $\hat{\gamma}$ is a particular arbitrary $H^1$ function that accords with $\hat{\gamma}$ on the boundary $\Gamma$, for all test functions $\varphi \in H^1_0$. Thus, the state variable $u$ is determined as $\gamma = \hat{\gamma}$, the residual of the specific gravity after subtracting $\hat{\gamma}$.

Generally speaking, if the coefficients $a \in L^2_1$ and $b \in L^2_2$ are predetermined, then a forward problem is solved to find $u$ which satisfies Eq. (6) in $H^1_0$. However, if the coefficients $a$ and $b$ are not given but observed data corresponding to the solution are available, then an inverse problem to reconstruct the coefficients from knowledge of the data arises. This inverse problem is underdetermined because its solution is not unique. For example, when a water velocity vector $v$ satisfies

$$
\nabla \cdot \gamma v = 0
$$

(7)

which is regarded as the governing continuity equation of air-mixed water, then both of $I(a, b; u, \varphi) = -I(a, b; \hat{\gamma}, \varphi)$ and $I(a, b + v; u, \varphi) = -I(a, b + v; \hat{\gamma}, \varphi)$ will hold. Another example is multiplication of a constant $k$ because $I(ka, kb; u, \varphi) = -I(ka, kb; \hat{\gamma}, \varphi)$ is always satisfied if $u$ is a solution to Eq. (6).

Therefore, the inverse problem is approached in the framework of an optimal control problem to minimize a prescribed functional of the coefficients $a$ and $b$, which are considered as the control variables constrained in a certain admissible set where only convexity is assumed. In the present case, a domain observation type functional $J(a, b)$ is defined by

$$
J(a, b) = \frac{1}{2} \sum_{i=1}^N \left( u(a, b) - \bar{u}_i \right)^2
$$

(8)

where $N$ is the number of observation points in the domain $\Omega$, $\bar{u}_i$ the observed value of $u$ at $i$-th observation point, and $u(a, b)$ is the solution $u$ of Eq. (6). Consid-
ering physical property of diffusion, the diffusion coefficient \( a \) is explicitly constrained under the condition of \( a > 0 \). However, since the solvability of variational problems is guaranteed only under certain conditions as discussed later, the admissible set of both coefficients \( a \) and \( b \) is implicitly determined so that the problem is meaningful.

4. Minimum principle

The optimal \( a \) and \( b \) that minimize \( J(a, b) \) are characterized by the minimum principle. Henceforth, \( J(a, b) \) is abbreviated as \( J \). Now, suppose that \( a \) and \( b \) are optimal ones and \( u = u(a, b) \). Variations in \( a \) and \( b \) are denoted by \( \delta a \) and \( \delta b \), respectively, and it is assumed that \( a' = a + \varepsilon \delta a \) and \( b' = b + \varepsilon \delta b \) are admissible for any positive \( \varepsilon \) smaller than 1. The Gâteaux differential \( \delta u \) of \( u \) is defined by

\[
\delta u = \lim_{\varepsilon \to 0} \frac{u(a', b') - u}{\varepsilon}
\]

and then the Gâteaux differential \( \delta J \) of \( J \) is deduced as

\[
\delta J = \lim_{\varepsilon \to 0} \frac{J(a', b') - J}{\varepsilon} = \sum_{i=1}^{N} (u - \tilde{u}) \delta u
\]

from Eq. (8). Since \( J(a', b') \) is not less than the minimized functional \( J \), the minimum principle is stated as the inequality \( \delta J \geq 0 \) but reduced to a convenient form using the adjoint variable \( p \in H^1_0 \) which is the solution of the adjoint equation

\[
I'(a, b; p, \varphi) = \langle a \nabla p, \nabla \varphi \rangle - \langle \nabla p, \varphi b \rangle
\]

\[
= \sum_{i=1}^{N} (u - \tilde{u}) \varphi
\]

where \( I' \) is the adjoint bilinear form of \( I \), for all test functions \( \varphi \in H^1_0 \). The bilinear forms \( I \) and \( I' \) satisfy

\[
I(a, b; \varphi, \varphi) = I'(a, b; p, \varphi)
\]

for any pair of \( p \in H^1_0 \) and \( \varphi \in H^1_0 \). Since \( \delta u \) is in \( H^1_0 \) and can be substituted into \( \varphi \) in Eq. (11), the right hand side of Eq. (10) is rewritten and transformed as

\[
\delta J = I'(a, b; p, \delta u) = I(a, b; \delta u, p)
\]

\[
= -l(\delta a, \delta b; u, p) + \langle u \nabla p, \delta b \rangle
\]

because

\[
\lim_{\varepsilon \to 0} \frac{l(a', b'; u(a', b'), p) - l(a, b; u, p)}{\varepsilon}
\]

\[
= l(a, b; \delta u, p) + l(\delta a, \delta b; u, p) = 0
\]

holds for any \( p \). Thus, the minimum principle is obtained as

\[
\delta J = \langle S_a, \delta a \rangle + \langle S_b, \delta b \rangle \geq 0
\]

where \( S_a \) and \( S_b \) are the sensitivities defined by \(-\nabla p \cdot \nabla u\) and \( u \nabla p \), respectively. This minimum principle also suggests that optimal control variables may be searched in the negative directions of the sensitivities.

5. Solvability of variational problems

The variational problems Eqs. (6) and (11) have to be solved in order to approach optimal control variables \( a \) and \( b \). Due to the constraint \( a > 0 \) imposed on the diffusion coefficient \( a \), the equivalent normalized forms of these equations are written as

\[
I\left(1, \frac{b}{a}; u, \varphi\right) = -I\left(1, \frac{b}{a}; \gamma v, \varphi\right)
\]

and

\[
I'\left(1, \frac{b}{a}; p, \varphi\right) = \sum_{i=1}^{N} \frac{1}{a} (u - \tilde{u}) \varphi
\]

for any \( \varphi \in H^1_0 \). However, it is not self-evident that solutions to Eqs. (16) and (17) uniquely exist. A sufficient condition to guarantee the solvability of Eqs. (16) and (17) is given by the Lax-Milgram’s theorem [6], in which the bilinear form is assumed to be bounded and coercive. In the present case, the bilinear forms \( I \) and \( I' \) are said to be bounded if there exists positive \( M \) such that

\[
\left| I\left(1, \frac{b}{a}; u, \varphi\right) \right| \leq M \| u \|_V \| \varphi \|_V
\]

and

\[
\left| I'\left(1, \frac{b}{a}; p, \varphi\right) \right| \leq M \| u \|_V \| \varphi \|_V
\]

for any pair of \( u \in H^1_0 \) and \( \varphi \in H^1_0 \), whereas they are said to be coercive if there exists positive \( \mu \) such that

\[
I\left(1, \frac{b}{a}; u, u\right) \geq \mu \| u \|_V^2
\]

and

\[
I'\left(1, \frac{b}{a}; u, u\right) \geq \mu \| u \|_V^2
\]

for any \( u \in H^1_0 \).

The conditions of Eqs. (18) and (19) are always satisfied when \( M \) is taken as

\[
M = 1 + \left\| \frac{b}{\lambda_1 a} \right\|
\]

where \( \lambda_1 \) is a positive finite number which is equal to \( \inf_{\| u \|_V = 1} (\| u \|_V / \| u \|) \) according to the Poincaré’s inequality, because
1. There exists a decomposition $(b/a) = r_0 + r_1$ such that $\langle r_0, \nabla \phi \rangle = 0$ for all $\phi \in H^1_0$.

2. The decomposition $(b/a) = r_0 + r_1$ is supposed to be done so as to minimize $\|r_1\|$ and $\mu$ defined by

$$\mu = 1 - \frac{\|r_1\|}{\lambda_1}$$  \hspace{1cm} (25)

is positive.

Indeed, the left hand sides of Eqs. (20) and (21) are reduced to

$$l' \left( \frac{b}{a}; u, u \right) = l' \left( \frac{b}{a}; u, u \right)$$

$$= \|u\|^2_{\Gamma} - \left( \frac{u - b}{a}, \nabla u \right)$$

$$= \|u\|^2_{\Gamma} - \left( r_0, \nabla \frac{u^2}{2} \right) - \langle u r_1, \nabla u \rangle$$

$$= \|u\|^2_{\Gamma} - \int_{\Omega} r_1 \cdot u \nabla u \, d\Omega$$

$$\geqslant \|u\|^2_{\Gamma} - \|r_1\| \|u\|_{\Gamma}$$

$$\geqslant \|u\|^2_{\Gamma} - \|r_1\|_{\lambda_1} \|u\|_{\Gamma}^2$$

$$= \mu \|u\|^2_{\Gamma}$$  \hspace{1cm} (26)

under this condition, which is satisfied if $b/a$ is nearly divergence free, so that $r_1$ is small enough. However, the positiveness of $\mu$ in Eq. (25), and thus the solvability of the variational problems, are not guaranteed in general.

6. Numerical method

6.1. Finite element solver for the partial differential equations

The finite element method is used for numerically solving the variational problems Eqs. (6) and (11). The domain $\Omega$ is discretized into a mesh comprising of finite number of triangular elements and their nodes, which are chosen in such a way that there exists a one-to-one correspondence between the set of all the observation points including ones on the boundary $\Gamma$ and the set of the nodal points in the meshing. The specified boundary value $\tilde{\gamma}$ is piecewise linearly interpolated from the observed data on the boundary $\Gamma$. The unknowns $u$ and $p$, whose nodal values are numerically resolved, are interpolated by elementwise linear functions, whereas the coefficients $a$ and $b$, which are estimated in the iterative procedure, are taken as elementwise constants.

The standard Galerkin procedure is applied for discretizing Eqs. (6) and (11). An elementwise linear function whose nodal values are equal to $\tilde{\gamma}$ on the boundary $\Gamma$ and vanish in the domain $\Omega$ is taken as $\gamma_k$. The Gauss–Jordan method is used for solving the resulting system of linear equations system because its matrix to be inverted is not diagonal dominant. If the discretized version of one of the variational problems is not regular, then the method stops.

6.2. Iterative estimation procedure

The iterative procedure remedies the control variables $a$ and $b$ to minimize the functional $J$. The estimates of the control variables at the $k$-th iteration are denoted by $a^{(k)}$ and $b^{(k)}$. The sensitivities $S_a = -\nabla p \cdot \nabla u$ and $S_b = u \nabla p$ are evaluated from the numerical solutions for $u$ and $p$ at each element, but the mean value is used for $u$ in $S_a$. Then, $a^{(k)}$ and $b^{(k)}$ are calculated as

$$a^{(k)} = a^{(k-1)} - \alpha S_a$$  \hspace{1cm} (27)

and

$$b^{(k)} = b^{(k-1)} - \beta S_b$$  \hspace{1cm} (28)

where $\alpha$ and $\beta$ are the relaxation parameters for $a$ and $b$, respectively. If $a^{(k)}$ is not greater than 0, then it is reset as $a^{(k-1)}$ to fulfill the imposition of the constraint $a > 0$.

6.3. Initial estimates

A constant value is used as an initial estimate for the diffusion coefficient $a$ in the whole domain, whereas the convection coefficient $b$ is given as the vector sum of a predetermined water velocity vector $\mathbf{v}$ and a constant air bubble rise velocity vector which has only positive vertical $y$-component. The field of the water velocity vector $\mathbf{v}$ is supposed to comprise of continuous two parts of
mainstream and roller. In the mainstream part of the field uniform velocity distribution is assumed in the vertical $y$-direction, whereas in the roller part the velocity distribution is linearly taken in the same direction. The conservation of mass with respect to the discharge entering into the domain is taken into account. In order to find such $v$ numerically, a 1-D finite difference method which assumes the hydrostatic pressure distribution is used first for determining the interface between the mainstream and the roller, and then $v$ in the mainstream is calculated. Next, a strip integral method is employed to obtain $v$ in the roller fulfilling the continuity requirement.

The field of the vector $b/a$ constructed in this way is nearly divergence free.

7. Demonstrative example

The domain $\Omega$, which models a vertical plain of flow field comprising of a hydraulic jump where the mainstream flows from the left to the right, is divided into 289 finite elements by 169 nodes as displayed in Fig. 1. The hydraulic jump has been experimentally studied by Chanson [3], and the temporally averaged void fraction has been measured at every observation point, which corresponds to one of the 169 nodes, by means of a conductivity probe system. The measured void fraction is converted into the specific gravity $\gamma$, and then it is used for the observed state variable $\bar{u}$. Fig. 2 shows vertical distributions of the specific gravity at $x = 0.00, 0.10, 0.20, 0.30, 0.45,$ and $0.65$ m. From this plot of specific gravity distribution it can be visualized that $\gamma$-value decreases in the middle layer of vertical section, however this deficiency is overcome and the distribution becomes almost uniform as the flow moves in the horizontal $x$-direction. The upstream flow depth before entering the hydraulic jump is 0.017 m, and the depth averaged velocity is 2.47 m/s, which works as another constraint imposed on the convection coefficient $b$.

Initial estimates of the coefficients $a$ and $b$ are portrayed in Fig. 3. The diffusion coefficient $a^{(0)}$ and the air bubble rise velocity are uniformly taken as 0.1 m$^2$/s and 1.0 m/s, respectively, and the corresponding specific gravity field realized by the initial estimates is depicted in Fig. 4. It can be seen from this figure that there is no significant layer of diminished specific gravity as is clearly found in the observed one.

The iterative procedure is implemented setting the values of the relaxation parameters $\alpha$ and $\beta$ as $10^{-7}$ and $10^{-6}$, respectively. Larger values are also tested, but the iterative procedure ends in failure. First order convergence of the functional value is obtained as shown in Fig. 5. After $5 \times 10^5$ iterations, the value of $J$ is reduced to $5.8 \times 10^{-4}$, and the maximum difference between the observed specific gravity and the calculated one is about 0.0104, which is considered small enough for the practical purposes. Thus, the estimated coefficients $a$ and $b$ at $5 \times 10^5$-th iteration are regarded as an approximate solution to the inverse problem and are plotted in Fig. 6.
The specific gravity field for these estimated coefficients $a$ and $b$ is shown in Fig. 7. Even though the estimated results are not unique one as mentioned in the formulation of the inverse problem, nonetheless they are considered to be close to the reality because the velocity at the upstream is constrained. The value of the diffusion coefficient $a$ ranges from $10^{-7}$ to $10^{-1}$. It is large in the layer where the specific gravity is relatively small. The convection coefficient $b$ is not much different from its initial estimates and approximately satisfies the velocity constraint at the upstream, but its vertical $y$-component in the result suddenly increases at the lower edge of the layer where the specific gravity diminishes.

8. Conclusions

The inverse problem to estimate the coefficients in the convection diffusion equation which is assumed to govern the air-mixed flow in a hydraulic jump is formulated as the optimal control problem to minimize the functional, as observed data of specific gravity are available. Solvability of the convection diffusion equation as well as its adjoint equation is guaranteed if the convection coefficient divided by the diffusion coefficient is nearly divergence free. Using the iterative procedure which includes the finite element scheme for the resolution of the two equations, the estimation is numerically implemented. In the demonstrative example, the first order convergence of the specific gravity field which the finite element scheme yields to the observed one is established without any failure in the resolution process, even though the inverse problem is underdetermined. The obtained coefficients are not unique but are considered close to the reality. It should be remarked that strong heterogeneity exists in the distribution of the diffusion coefficient and that the vertical component of the convection coefficient, which is considered as the air
bubble rise velocity, suddenly changes at the lower edge of the layer where the specific gravity decreases. The knowledge obtained from estimated results shall be used in the development of mathematical and numerical models of hydraulic jumps to analyze forward problems. For that purpose, it is still necessary to identify the absolute magnitude of the air bubble rise velocity, which depends on the bubble size and the pressure distribution. If the coefficients are far from the divergence free condition, then the procedure presented here is not effective. This may happen in other air mixed flows such as spillway chute flows, pump intakes, plunging jets, and so on. Further investigations are required for equations which have such coefficients and are not coercive.

References