

INVERSE PROBLEMS FOR COMPRESSIBLE FLOW OF NEWTONIAN FLUID

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ABSTRACT. We consider the problem of identification of fundamental parameters for a compressible viscous flow of a Newtonian fluid. The flow is governed by time dependent Navier-Stokes equation subject to given boundary conditions. The objective of this study is to find an optimal set of parameters of the compressible viscous fluid so that the corresponding model solution matches with the observed data. This method of identification can be applied to blood flow through an artificial heart chamber and the dynamic modeling of aquifers as special cases.

Key Words: Inverse Problem, Fundamental Parameters, Viscous Flow, Compressible Newtonian Fluid

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1. INTRODUCTION

Fluids which obey a linear relationship between stress and rate of deformation are known as Newtonian fluids. The viscosity of these fluids are normally assumed to be constant although it may also be a function of space and time. In a compressible flow the density of the fluid changes in most of the fluid flow systems. This change in density is mainly caused by the variation of pressure in various locations of the fluid medium. Microscopic analysis shows that the motion of the fluid molecules is highly influenced by the propagation of pressure pulses in the fluid medium whereas in a macroscopic sense these pressure pulses cause small disturbances in the thermodynamic properties of the fluid.

In practice many flows can be modeled by assuming them to be isentropic. An isentropic flow is a flow in which viscous losses are not significant. There are many flows in which the major part of the flow can be considered to be isentropic. For instance, in internal flows the effects of viscosity are restricted to thin layers near the walls and the rest of the flow can be treated by assuming it to be isentropic. Similarly in external flows the effects of viscosity are restricted to the wakes, shock waves and the boundary layers whereas the flow is considered to be isentropic far away from the boundary. Thus this approach has been adopted in our analysis of the flow.

Weak solutions present the most suitable formulation for the mathematical framework of the laws of conservation arising in continuum fluid dynamics. The theory of weak solutions has emerged as an integral part of modern analysis of physical and engineering applications. This theory has been adopted by Temam [1], Lions [2], Caffarelli et al. [3], and many others. These investigators studied incompressible fluids where the weak solutions were expected to be regular based on the function spaces of Sobolev type. The theory of compressible fluids significantly depend on the notion of weak solutions involving various types of discontinuities and other irregularities (see e.g., [4–7]). A more rigorous theory of compressible flows with large data was studied by Lions [8]. Hoff [9] discussed a fundamental idea of weak continuity property of the so-called effective viscous pressure in order to deal with possible density fluctuations. Some authors [10–12] have developed the theory of measure solutions to describe oscillations that may develop in a finite time. One can find some useful results in this direction in the monographs [13, 14].

The objective of this study is to identify the fundamental parameters of the compressible flow of a viscous fluid. This is an inverse problem. The layout of the paper is portrayed as follows. In Section 2, the formulation for the identification problem of the flow is developed along with the system equations. The objective functional and the variational equations are presented in Section 3. Existence of optimal parameters and necessary conditions of optimality applied to identification problems are discussed in Section 4. In Section 5, we develop the computational scheme giving two algorithms for identification of the model parameters.

2. SYSTEM DYNAMICS AND PROBLEM FORMULATION

We consider a compressible viscous Newtonian fluid surrounded by an open bounded domain Ω in a time interval $I \equiv (0, T)$. The flow is governed by the continuity equation (conservation of mass) and the time dependent Navier-Stokes equation (conservation of linear momenta) together with the initial-boundary conditions given by

$$(2.1) \quad \frac{\partial \rho}{\partial t} = -\operatorname{div}(\rho \mathbf{u}),$$

$$(2.2) \quad \frac{\partial}{\partial t}(\rho \mathbf{u}) = -\operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \operatorname{div} \mathbb{T} + \rho \mathbf{f},$$

$$(2.3) \quad \mathbf{u}(0, \cdot) = \mathbf{u}_0, \quad \rho(0, \cdot) = \rho_0,$$

$$\mathbf{u}(t, \cdot)|_{\partial\Omega} = 0, \quad \rho(t, \cdot)|_{\partial\Omega} = 0,$$

where Ω , an open bounded connected subset of \mathbb{R}^3 , is the domain of the flow regime and $\partial\Omega$ is its boundary which is assumed to be sufficiently smooth. In the above expressions ρ is the mass density of the fluid, \mathbf{u} the velocity field, \mathbf{f} the volume force, \mathbb{T} the Cauchy stress tensor and \mathbb{I} the identity tensor.

The constitutive relation for a compressible Newtonian fluid is given by

$$\mathbb{T} = \mathbb{S} - p\mathbb{I},$$

where

$$(2.4) \quad \mathbb{S} = \left[\mu \{ \nabla \mathbf{u} + (\nabla \mathbf{u})' \} + \left(\eta - \frac{2}{3} \mu \right) (\operatorname{div} \mathbf{u}) \mathbb{I} \right],$$

with μ and η being the shear and bulk viscosity coefficients respectively. In the above expression \mathbb{S} is the viscous stress tensor, p denotes the pressure and the prime over the velocity gradient represents its transpose. We consider the flow to be an isentropic one. Therefore we use the relation $p = \Gamma(\rho)$ in the subsequent expressions where Γ is a C^1 function representing the constitutive law. Here it should be noted that the second law of thermodynamics requires that $\mu, \eta \geq 0$. These are the two fundamental parameters that we wish to identify on the basis of observed data.

Theorem 1 (Existence theorem). *Consider the following assumptions on the data*

$$\begin{aligned} \rho_0 \in L^1(\Omega) \cap L^\gamma(\Omega), \quad \rho_0 \geq 0, \quad \mathbf{f} \in L^1(0, T; L^{2\gamma/(\gamma-1)}(\Omega, \mathbb{R}^3)), \quad \forall T > 0, \\ \rho \mathbf{u}_0 = \mathbf{m}_0 \in L^{2\gamma/(\gamma+1)}(\Omega, \mathbb{R}^3), \quad \frac{|\mathbf{m}_0|^2}{\rho_0} \in L^1(\Omega), \quad \rho_0 \neq 0, \quad \mathbf{m}_0 = 0 \text{ a.e on } \{\rho_0 = 0\}. \end{aligned}$$

Then, the system (2.1)–(2.3) has a weak solution $(\rho, \mathbf{u}) \in L_{loc}^\infty(0, \infty; L^\gamma(\Omega)) \times L_{loc}^2(0, \infty; H_0^1(\Omega, \mathbb{R}^3))$ satisfying

$$\begin{aligned} \rho \in C([0, \infty); L^p(\Omega)) \quad \text{if } 1 \leq p < \gamma, \\ \rho |\mathbf{u}|^2 \in L_{loc}^\infty(0, \infty; L^1(\Omega)), \quad \rho \mathbf{u} \in C([0, \infty); L_\omega^{2\gamma/(\gamma+1)}(\Omega, \mathbb{R}^3)), \\ \rho \in L_{loc}^r([0, \infty) \times \Omega), \quad \text{for } r = \gamma - 1 + 2\gamma/3, \end{aligned}$$

where we denote by $C([0, \infty); L_\omega^{2\gamma/(\gamma+1)}(\Omega, \mathbb{R}^3))$ the space of continuous functions with values in the Lebesgue space $L^{2\gamma/(\gamma+1)}(\Omega, \mathbb{R}^3)$ which is endowed with the weak topology.

Proof. The proof of this theorem can be found in Lions [8]. He proved the existence theorem and presented sufficient conditions for existence of global solution to the aforementioned system with large initial data. One can also refer to the work of Desjardins [16] on the weak solutions of compressible Navier-Stokes equations. \square

2.1. Problem Formulation. Given the parameters (μ, η) and the boundary data including the volume force, one considers the question of existence of solutions $\{p, \rho, \mathbf{u}\}$ (often in the weak sense) and finally the computation thereof. This is the direct problem. On the other hand, the inverse problem is to find the parameters (μ, η) given some functional of the observed response or true solutions $\{p, \rho, \mathbf{u}\}$. Here we are interested in the inverse problem. Clearly, the solution $\{p, \rho, \mathbf{u}\}$ is dependent on the parameters (μ, η) . Thus there are two maps involved. One is the direct map

$(\mu, \eta) \longrightarrow \{p, \rho, \mathbf{u}\}$ and the other is the inverse map $\{p, \rho, \mathbf{u}\} \longrightarrow (\mu, \eta)$. Even if the direct map is single valued (unique), the inverse map may be multi valued. However this multi valued character may not be physically important to real world users. Such users are perfectly satisfied if the mathematical model produces results close to the naturally observed data. Usually scientific experiments are designed to determine these fundamental parameters often assuming that they are constant. However it is quite conceivable that they may also depend on time and space in a dynamic environment of the fluid flow. Let (μ^0, η^0) denote the true underlying parameters unknown to the observer and $\{p^0, \rho^0, \mathbf{u}^0\}$ the corresponding (weak) solution satisfying the following system of equations:

$$(2.5) \quad \frac{\partial \rho^0}{\partial t} = -\operatorname{div}(\rho^0 \mathbf{u}^0),$$

$$(2.6) \quad \begin{aligned} \frac{\partial}{\partial t}(\rho^0 \mathbf{u}^0) &= -\operatorname{div} [\rho^0 \mathbf{u}^0 \otimes \mathbf{u}^0 + p^0 \mathbb{I}] \\ &\quad + \operatorname{div} [\mu^0 \{\nabla \mathbf{u}^0 + (\nabla \mathbf{u}^0)'\}] \\ &\quad + \operatorname{div} \left[\left(\eta^0 - \frac{2}{3} \mu^0 \right) (\operatorname{div} \mathbf{u}^0) \mathbb{I} \right] + \rho^0 \mathbf{f}, \end{aligned}$$

$$(2.7) \quad \begin{aligned} \mathbf{u}^0(0, \cdot) &= \mathbf{u}_0^0, \quad \rho^0(0, \cdot) = \rho_0^0, \\ \mathbf{u}^0(t, \cdot)|_{\partial\Omega} &= 0, \quad \rho^0(t, \cdot)|_{\partial\Omega} = 0. \end{aligned}$$

Thus in order to determine these parameters one introduces a functional, often called cost functional, which is a measure of discrepancy between the observables and the true solutions of the dynamic system corresponding to the assumed (trial) parameters (μ, η) . Let $\{p, \rho, \mathbf{u}\}$ denote the solution of the model system corresponding to (μ, η) and $\{p^0, \rho^0, \mathbf{u}^0\}$ the solution corresponding to the true parameters (μ^0, η^0) which is unknown to the observer. If the true solution $\{p^0, \rho^0, \mathbf{u}^0\}$ is observable, the natural objective functional is given by the following expression,

$$(2.8) \quad \begin{aligned} J(\mu, \eta) &\equiv \int_{I \times \Omega} |(p - p^0)^2 + (\rho - \rho^0)^2 + |\mathbf{u} - \mathbf{u}^0|^2| d\mathbf{x} dt \\ &\quad + \int_{\Omega} |(p(T, \mathbf{x}) - p^0(T, \mathbf{x}))^2 + (\rho(T, \mathbf{x}) - \rho^0(T, \mathbf{x}))^2 + |\mathbf{u}(T, \mathbf{x}) - \mathbf{u}^0(T, \mathbf{x})|^2| d\mathbf{x}. \end{aligned}$$

From a practical point of view it is not possible to measure this functional as all the physical quantities under consideration are continuously distributed in the domain $I \times \Omega$. However, in order to have a reasonable error estimation we can select some accessible regions of the domain and evaluate the cost functional based on the available data. This is given in its general form in the following section.

3. PERFORMANCE MEASURE AND VARIATIONAL EQUATION

Since the flow is assumed to be isentropic p is given by a function of ρ only as indicated by the expression $p = \Gamma(\rho)$. Therefore, it suffices to consider the pair (ρ, \mathbf{u})

as the state variable. In general we consider the following cost functional

$$(3.1) \quad J(\mu, \eta) = \int_{I \times \Omega} \ell(t, \mathbf{x}, \rho, \mathbf{u}) \, d\mathbf{x} \, dt + \int_{\Omega} L(\mathbf{x}, \rho(T, \mathbf{x}), \mathbf{u}(T, \mathbf{x})) \, d\mathbf{x},$$

where $\ell : I \times \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$ and $L : \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$ are suitable functions which represent the mismatch between the observed data and the data produced by the model corresponding to the parameter (μ, η) with $\{\rho, \mathbf{u}\}$ being the corresponding solutions (response) of the model system (2.1)–(2.3). Let \mathcal{C} be a closed convex bounded set in \mathbb{R}^2 defined as

$$\mathcal{C} \equiv \{(\mu, \eta) \in \mathbb{R}^2 : 0 \leq \mu_1 \leq \mu \leq \mu_2, \quad 0 \leq \eta_1 \leq \eta \leq \eta_2\}.$$

In general, the parameters (μ, η) are measurable functions defined on $I \times \Omega$ with values in the set \mathcal{C} . This class of functions is denoted by $\mathcal{P} = \mathcal{B}_{\infty}(I \times \Omega, \mathcal{C}) \subset B_{\infty}(I \times \Omega, \mathbb{R}^2)$ where $\mathcal{B}_{\infty}(I \times \Omega, \mathbb{R}^2) \subset L_{\infty}(I \times \Omega, \mathbb{R}^2)$ is the space of bounded measurable functions defined on $I \times \Omega$. Furnished with the supnorm topology, this is a closed subspace of the Banach space $L_{\infty}(I \times \Omega, \mathbb{R}^2)$ and hence a Banach space. Our objective is to find $(\mu^0, \eta^0) \in \mathcal{P}$ such that

$$J(\mu^0, \eta^0) \leq J(\mu, \eta) \quad \forall (\mu, \eta) \in \mathcal{P}.$$

We define $\mu^{\epsilon} = \mu^0 + \epsilon(\mu - \mu^0)$ and $\eta^{\epsilon} = \eta^0 + \epsilon(\eta - \eta^0)$ for any $\epsilon \in [0, 1]$. Since \mathcal{C} is a closed convex set, \mathcal{P} is also a closed convex subset of $B_{\infty}(I \times \Omega, \mathbb{R}^2)$ and so we have $(\mu^{\epsilon}, \eta^{\epsilon}) \in \mathcal{P}$. Thus

$$(3.2) \quad J(\mu^0, \eta^0) \leq J(\mu^{\epsilon}, \eta^{\epsilon}) \quad \forall \epsilon \in [0, 1] \quad \text{and} \quad \forall (\mu, \eta) \in \mathcal{P},$$

where

$$(3.3) \quad J(\mu^{\epsilon}, \eta^{\epsilon}) = \int_{I \times \Omega} \ell(t, \mathbf{x}, \rho^{\epsilon}, \mathbf{u}^{\epsilon}) \, d\mathbf{x} \, dt + \int_{\Omega} L(\mathbf{x}, \rho^{\epsilon}(T, \mathbf{x}), \mathbf{u}^{\epsilon}(T, \mathbf{x})) \, d\mathbf{x}$$

with $(\rho^{\epsilon}, \mathbf{u}^{\epsilon})$ being the solution of (2.1)–(2.3) corresponding to the parameter $(\mu^{\epsilon}, \eta^{\epsilon})$ and

$$(3.4) \quad J(\mu^0, \eta^0) = \int_{I \times \Omega} \ell(t, \mathbf{x}, \rho^0, \mathbf{u}^0) \, d\mathbf{x} \, dt + \int_{\Omega} L(\mathbf{x}, \rho^0(T, \mathbf{x}), \mathbf{u}^0(T, \mathbf{x})) \, d\mathbf{x},$$

corresponding to the parameter (μ^0, η^0) . Let us denote the Gâteaux differential of J at (μ^0, η^0) in the direction $(\mu - \mu^0, \eta - \eta^0)$ by $dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0)$. Then using the inequality (3.2) to compute the differential quotient and letting $\epsilon \downarrow 0$ one can easily verify that

$$(3.5) \quad dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) \geq 0 \quad \forall (\mu, \eta) \in \mathcal{P}.$$

Using the differentiability assumptions on ℓ and L , and the expressions (3.3) and (3.4), one can easily verify that the directional derivative dJ is given by

$$(3.6) \quad dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) = \int_{I \times \Omega} \langle \ell_{\rho}(t, \mathbf{x}^0, \rho^0, \mathbf{u}^0), q \rangle \, d\mathbf{x} \, dt$$

$$\begin{aligned}
& + \int_{I \times \Omega} \langle \ell_{\mathbf{u}}(t, \mathbf{x}, \rho^0, \mathbf{u}^0), \mathbf{w} \rangle d\mathbf{x} dt \\
& + \int_{\Omega} \langle L_{\rho}(\mathbf{x}, \rho^0(T, \mathbf{x}), \mathbf{u}^0(T, \mathbf{x})), q(T, \mathbf{x}) \rangle d\mathbf{x} \\
& + \int_{\Omega} \langle L_{\mathbf{u}}(\mathbf{x}, \rho^0(T, \mathbf{x}), \mathbf{u}^0(T, \mathbf{x})), \mathbf{w}(T, \mathbf{x}) \rangle d\mathbf{x}
\end{aligned}$$

where (ℓ_{ρ}, L_{ρ}) and $(\ell_{\mathbf{u}}, L_{\mathbf{u}})$ are the partial derivatives of ℓ and L with respect to ρ and \mathbf{u} respectively. The mass density field q and velocity vector \mathbf{w} in the last expression are given by the limits:

$$q = \lim_{\epsilon \rightarrow 0} \frac{(\rho^{\epsilon} - \rho^0)}{\epsilon}, \quad \mathbf{w} = \lim_{\epsilon \rightarrow 0} \frac{(\mathbf{u}^{\epsilon} - \mathbf{u}^0)}{\epsilon}.$$

By straightforward variational argument it is easy to verify that the pair (q, \mathbf{w}) satisfies the following set of partial differential equations together with the initial-boundary conditions:

$$(3.7) \quad K_1(q, \mathbf{w}) = G_1^0(\mu - \mu^0, \eta - \eta^0),$$

$$(3.8) \quad \mathbf{K}_2(q, \mathbf{w}) = \mathbf{G}_2^0(\mu - \mu^0, \eta - \eta^0),$$

$$q(0, \cdot) = 0, \quad \mathbf{w}(0, \cdot) = 0,$$

$$(3.9) \quad q(t, \cdot)|_{\partial\Omega} = 0, \quad \mathbf{w}(t, \cdot)|_{\partial\Omega} = 0,$$

in which the differential operators K_1 and \mathbf{K}_2 are given by

$$(3.10) \quad K_1(q, \mathbf{w}) = \frac{\partial q}{\partial t} + \operatorname{div}(q\mathbf{u}^0 + \rho^0\mathbf{w}),$$

$$\begin{aligned}
(3.11) \quad \mathbf{K}_2(q, \mathbf{w}) &= \frac{\partial}{\partial t}(q\mathbf{u}^0 + \rho^0\mathbf{w}) \\
&+ \operatorname{div} \{q(\mathbf{u}^0 \otimes \mathbf{u}^0) + \rho^0(\mathbf{w} \otimes \mathbf{u}^0 + \mathbf{u}^0 \otimes \mathbf{w}) + q d\Gamma(\rho^0)\} \\
&- \operatorname{div} \left[\mu^0 \{(\nabla \mathbf{w}) + (\nabla \mathbf{w})'\} + (\eta^0 - \frac{2}{3}\mu^0)(\operatorname{div} \mathbf{w}) \mathbb{I} \right] - q\mathbf{f},
\end{aligned}$$

$$(3.12) \quad G_1^0(\mu - \mu^0, \eta - \eta^0) = 0 \text{ and}$$

$$\begin{aligned}
\mathbf{G}_2^0(\mu - \mu^0, \eta - \eta^0) &= \operatorname{div} [(\mu - \mu^0) \{(\nabla \mathbf{u}^0) + (\nabla \mathbf{u}^0)'\}] \\
&+ \operatorname{div} \left[\left\{ (\eta - \eta^0) - \frac{2}{3}(\mu - \mu^0) \right\} (\operatorname{div} \mathbf{u}^0) \mathbb{I} \right].
\end{aligned}$$

In view of the above analysis we have the following result.

Lemma 2 (Variational equations (3.7)–(3.8)). *Let $(\rho, \mathbf{u})(\mu, \eta)$ denote the weak solution of the system (2.1)–(2.3) corresponding to $(\mu, \eta) \in \mathcal{P}$. Then at each point $(\mu^0, \eta^0) \in \mathcal{P}$, the function $(\mu, \eta) \rightarrow (\rho, \mathbf{u})(\mu, \eta)$ has weak Gâteaux differential in the direction $(\mu - \mu^0, \eta - \eta^0)$, denoted $(\widehat{\rho}, \widehat{\mathbf{u}})(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0)$ and it is the weak solution (q, \mathbf{w}) of the system of variational equations (3.7)–(3.8) satisfying $(\widehat{\rho}, \widehat{\mathbf{u}}) \in L_{loc}^{\infty}(0, \infty; L^{\gamma}(\Omega)) \times L_{loc}^2(0, \infty; H_0^1(\Omega, \mathbb{R}^3))$, where $(\rho, \mathbf{u})(\mu^0, \eta^0)$ is the solution of the system (2.1)–(2.3) corresponding to the pair $(\mu, \eta) = (\mu^0, \eta^0)$.*

Proof. We omit the proof since the basic arguments leading to the proof is identical to that of Lemma 2.1 in [15]. \square

4. NECESSARY CONDITIONS FOR IDENTIFICATION

As stated before, our objective is to find optimal parameters $(\mu^0, \eta^0) \in \mathcal{P}$ which minimizes the cost functional (3.1) subject to the given initial boundary value problem (2.1)–(2.3). For this we need some basic assumptions on differentiability of $\{\ell, L\}$ as stated below:

(A1): ℓ is continuously differentiable with respect to the third and fourth argument satisfying $\ell_{\mathbf{u}}(\cdot, \cdot, \rho(\cdot, \cdot), \mathbf{u}(\cdot, \cdot)) \in L^2(I, H^{-1}(\Omega, \mathbb{R}^3))$ and $\ell_{\rho}(\cdot, \cdot, \rho(\cdot, \cdot), \mathbf{u}(\cdot, \cdot)) \in L^1(I, L^r(\Omega))$ for any feasible solution (ρ, \mathbf{u}) .

(A2): L is continuously differentiable with respect to the second and the third argument satisfying $L_{\mathbf{u}}(\cdot, \rho(T, \cdot), \mathbf{u}(T, \cdot)) \in H^{-1}(\Omega, \mathbb{R}^3)$ and $L_{\rho}(\cdot, \rho(T, \cdot), \mathbf{u}(T, \cdot)) \in L^r(\Omega)$ for any feasible solution (ρ, \mathbf{u}) .

Using the above assumptions we can develop the necessary conditions of optimality. This is presented as Theorem 3 at the end of this section. The reader may also be referred to Theorem 2.1 in reference [15]. Let $\{(\rho^\epsilon, \mathbf{u}^\epsilon), (\rho^0, \mathbf{u}^0)\}$ denote the solutions of the system (2.1)–(2.3) corresponding to the pairs $(\mu^\epsilon, \eta^\epsilon)$ and (μ^0, η^0) respectively. For the pair $(\mu^0, \eta^0) \in \mathcal{P}$ to be optimal it is necessary that $J(\mu^\epsilon, \eta^\epsilon) - J(\mu^0, \eta^0) \geq 0$ for all $\epsilon \in [0, 1]$ and for all $(\mu, \eta) \in \mathcal{P}$. From this inequality it is easy to verify that the differential dJ at (μ^0, η^0) in the direction $(\mu - \mu^0, \eta - \eta^0)$ must satisfy the inequality $dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) \geq 0$ for all $(\mu, \eta) \in \mathcal{P}$. Using the expressions on the right-hand side of (3.6) giving the directional derivative, and the assumptions (A1)–(A2), we observe that the map

$$(q, \mathbf{w}) \longrightarrow dJ$$

is a continuous linear functional on the Banach space $L^\infty(I, L^r(\Omega)) \times L^2(I, H_0^1(\Omega, \mathbb{R}^3))$. Also it is noted that

$$(G_1^0, \mathbf{G}_2^0) \longrightarrow (q, \mathbf{w})$$

is a continuous linear map from the Hilbert space $L^2(I, H_0^1) \times L^2(I, H^{-1}(\Omega, \mathbb{R}^3))$ to the Banach space $L^\infty(I, L^r(\Omega)) \times L^2(I, H_0^1(\Omega, \mathbb{R}^3))$. Then the composition map

$$(G_1^0, \mathbf{G}_2^0) \longrightarrow (q, \mathbf{w}) \longrightarrow dJ$$

is a continuous linear functional on $L^2(I, H_0^1) \times L^2(I, H^{-1}(\Omega, \mathbb{R}^3))$. Hence there exists a pair $(\Phi, \Psi) \in L^2(I, H^{-1}) \times L^2(I, H_0^1(\Omega, \mathbb{R}^3))$ such that

$$(4.1) \quad dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) = \int_{I \times \Omega} (\langle G_1^0, \Phi \rangle + \langle \mathbf{G}_2^0, \Psi \rangle) \, dx \, dt.$$

Thus it follows from equation (3.5) that

$$(4.2) \quad \int_{I \times \Omega} (\langle G_1^0, \Phi \rangle + \langle G_2^0, \Psi \rangle) dx dt \geq 0, \quad \forall (\mu, \eta) \in \mathcal{P}.$$

Using the equations (3.7) and (3.8) the expression on the right of equation (4.1) can be written as

$$(4.3) \quad \int_{I \times \Omega} (\langle G_1^0, \Phi \rangle + \langle G_2^0, \Psi \rangle) dx dt = \int_{I \times \Omega} (\langle K_1, \Phi \rangle + \langle K_2, \Psi \rangle) dx dt.$$

Now integrating by parts, the expression on right of equation (4.3) gives

$$(4.4) \quad \int_{I \times \Omega} (\langle G_1^0, \Phi \rangle + \langle G_2^0, \Psi \rangle) dx dt = \int_{I \times \Omega} (\langle q, K_1^*(\Phi, \Psi) \rangle + \langle \mathbf{w}, \mathbf{K}_2^*(\Phi, \Psi) \rangle) dx dt \\ + \int_{\Omega} q(T, \mathbf{x}) \langle \mathbf{u}^0(T, \mathbf{x}), \Psi(T, \mathbf{x}) \rangle dx + \int_{\Omega} \rho^0(T, \mathbf{x}) \langle \mathbf{w}(T, \mathbf{x}), \Psi(T, \mathbf{x}) \rangle dx \\ + \int_{\Omega} q(T, \mathbf{x}) \Phi(T, \mathbf{x}) dx.$$

where $K_1^*(\Phi, \Psi)$ and $\mathbf{K}_2^*(\Phi, \Psi)$ are the adjoint differential operators given by

$$(4.5) \quad K_1^*(\Phi, \Psi) = -\frac{\partial \Phi}{\partial t} - \left\langle \mathbf{u}^0, \frac{\partial \Psi}{\partial t} \right\rangle - tr \{(\mathbf{u}^0 \otimes \mathbf{u}^0)(\nabla \Psi)'\} \\ - tr(\mathbf{u}^0(\nabla \Phi)') - \langle \mathbf{f}, \Psi \rangle - d\Gamma(\rho^0)tr((div \Psi) \mathbb{I})$$

$$(4.6) \quad \mathbf{K}_2^*(\Phi, \Psi) = -\rho^0 \frac{\partial \Psi}{\partial t} - div\{\rho^0(\nabla \Psi + (\nabla \Psi)') \mathbf{u}^0\} + div\{\mu^0(\nabla \Psi + (\nabla \Psi)')\} \\ + div\left\{\left(\eta^0 - \frac{2}{3}\mu^0\right)((div \Psi) \mathbb{I})\right\} - \rho^0(\nabla \Phi)'.$$

On comparison of the integrals in expressions (3.6) and (4.4), we get the following adjoint differential equations together with the corresponding terminal and boundary conditions:

$$(4.7) \quad \frac{\partial \Phi}{\partial t} + \left\langle \mathbf{u}^0, \frac{\partial \Psi}{\partial t} \right\rangle = -tr \{(\mathbf{u}^0 \otimes \mathbf{u}^0)(\nabla \Psi)'\} \\ - tr(\mathbf{u}^0(\nabla \Phi)') - \langle \mathbf{f}, \Psi \rangle - d\Gamma(\rho^0)tr((div \Psi) \mathbb{I}) \\ - \ell_{\rho}(t, \mathbf{x}, \rho^0(t, \mathbf{x}), \mathbf{u}^0(t, \mathbf{x})),$$

$$(4.8) \quad \rho^0 \frac{\partial \Psi}{\partial t} = -div\{\rho^0(\nabla \Psi + (\nabla \Psi)') \mathbf{u}^0\} + div\{\mu^0(\nabla \Psi + (\nabla \Psi)')\} \\ + div\left\{\left(\eta^0 - \frac{2}{3}\mu^0\right)tr((div \Psi) \mathbb{I})\right\} - \rho^0(\nabla \Phi)' - \ell_{\mathbf{u}}(t, \mathbf{x}, \rho^0(t, \mathbf{x}), \mathbf{u}^0(t, \mathbf{x})),$$

$$(4.9) \quad \Phi(T, \mathbf{x}) + \langle \mathbf{u}^0(T, \mathbf{x}), \Psi(T, \mathbf{x}) \rangle = L_{\rho}(\mathbf{x}, \rho^0(T, \mathbf{x}), \mathbf{u}^0(T, \mathbf{x})), \\ \rho^0(T, \mathbf{x}) \Psi(T, \mathbf{x}) = L_{\mathbf{u}}(\mathbf{x}, \rho^0(T, \mathbf{x}), \mathbf{u}^0(T, \mathbf{x})), \\ \Phi(T, \cdot)|_{\partial \Omega} = 0, \quad \Psi(T, \cdot)|_{\partial \Omega} = 0.$$

The above system of equations can also be expressed in the following matrix form:

$$(4.10) \quad \mathbf{S} \frac{\partial \mathbf{Z}}{\partial t} = \mathbf{E}(\mathbf{Z}) + \mathbf{F},$$

where

$$\mathbf{S} = \begin{pmatrix} 1 & u_1^0 & u_2^0 & u_3^0 \\ 0 & \rho^0 & 0 & 0 \\ 0 & 0 & \rho^0 & 0 \\ 0 & 0 & 0 & \rho^0 \end{pmatrix}, \quad \mathbf{Z} = \begin{pmatrix} \Phi \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}, \quad \mathbf{E}(\mathbf{Z}) = \begin{pmatrix} K_1^*(\Phi, \Psi) \\ \mathbf{K}_2^*(\Phi, \Psi) \end{pmatrix} \quad \text{and} \quad \mathbf{F} = \begin{pmatrix} -\ell_{\mathbf{u}} \\ -\ell_{\rho} \end{pmatrix}.$$

In summary we have proved the following theorem.

Theorem 3 (Necessary conditions of optimality). *Consider the system (2.1)–(2.3) with the performance functional given by (3.1) and suppose the assumptions (A1) and (A2) hold. Then, for the $(\mu^0, \eta^0) \in \mathcal{P}$ to be optimal it is necessary that the system of equations (2.5)–(2.7) and the adjoint equations (4.7)–(4.9), and the inequality (4.2) hold.*

5. A COMPUTATIONAL SCHEME

Here we present an algorithm for identification of the fundamental parameters determining the dynamics of the system. In order to carry out this it is convenient to express the necessary inequality $dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) \geq 0$ given by (4.1) and (4.2) in the following form

$$\begin{aligned} (5.1) \quad dJ(\mu^0, \eta^0; \mu - \mu^0, \eta - \eta^0) &= \int_{I \times \Omega} (\mu - \mu^0) \text{tr} \{ (\nabla \mathbf{u}^0 + (\nabla \mathbf{u}^0)') (\nabla \Psi^0)' \} \, d\mathbf{x}dt \\ &\quad + \int_{I \times \Omega} \left\{ (\eta - \eta^0) - \frac{2}{3}(\mu - \mu^0) \right\} \text{tr} \{ ((\text{div} \mathbf{u}^0) \mathbb{I}) (\nabla \Psi^0)' \} \, d\mathbf{x}dt \\ &= \int_{I \times \Omega} (\mu - \mu^0) \text{tr} \left\{ (\nabla \mathbf{u}^0 + (\nabla \mathbf{u}^0)') \nabla \Psi^0 - \frac{2}{3} ((\text{div} \mathbf{u}^0) \mathbb{I}) (\nabla \Psi^0)' \right\} \, d\mathbf{x}dt \\ &\quad + \int_{I \times \Omega} (\eta - \eta^0) \text{tr} \{ ((\text{div} \mathbf{u}^0) \mathbb{I}) (\nabla \Psi^0)' \} \, d\mathbf{x}dt \geq 0 \quad \forall (\mu, \eta) \in \mathcal{P}. \end{aligned}$$

We use this inequality to construct the algorithm.

Step 1: Let $(\mu^n, \eta^n) \in \mathcal{P}$ denote the value of the parameter pair at n th stage of iteration and let (ρ^n, \mathbf{u}^n) denote the corresponding (weak) solution of the system equations (2.1)–(2.3).

Step 2: Use $\{\mu^n, \eta^n\}$ and $\{\rho^n, \mathbf{u}^n\}$ in the adjoint equations (4.7)–(4.9) and solve for $\{\Phi^n, \Psi^n\}$.

Step 3: Use this set $\{\mu^n, \eta^n, \rho^n, \mathbf{u}^n, \Phi^n, \Psi^n\}$ to determine if the following inequality is satisfied.

$$\begin{aligned} (5.2) \quad dJ(\mu^n, \eta^n; \mu - \mu^n, \eta - \eta^n) &= \\ &\int_{I \times \Omega} (\mu - \mu^n) \text{tr} \left\{ (\nabla \mathbf{u}^n + (\nabla \mathbf{u}^n)') (\nabla \Psi^n)' - \frac{2}{3} ((\text{div} \mathbf{u}^n) \mathbb{I}) (\nabla \Psi^n)' \right\} \, d\mathbf{x}dt \\ &\quad + \int_{I \times \Omega} (\eta - \eta^n) \text{tr} \{ ((\text{div} \mathbf{u}^n) \mathbb{I}) (\nabla \Psi^n)' \} \, d\mathbf{x}dt \geq 0, \quad \forall (\mu, \eta) \in \mathcal{P}. \end{aligned}$$

If the inequality (5.2) is satisfied then (μ^n, η^n) is the optimal pair and this ends the algorithm. Otherwise take

$$(5.3) \quad \begin{aligned} \mu^{n+1} &= \mu^n - \epsilon \operatorname{tr} \left\{ (\nabla \mathbf{u}^n + (\nabla \mathbf{u}^n)') (\nabla \Psi^n)' - \frac{2}{3} ((\operatorname{div} \mathbf{u}^0) \mathbb{I}) (\nabla \Psi^n)' \right\} \\ &\equiv \mu^n - \epsilon \operatorname{tr}(\mathbf{A}_n) \end{aligned}$$

$$(5.4) \quad \begin{aligned} \eta^{n+1} &= \eta^n - \epsilon \operatorname{tr} \left\{ ((\operatorname{div} \mathbf{u}^0) \mathbb{I}) (\nabla \Psi^n)' \right\} \\ &\equiv \eta^n - \epsilon \operatorname{tr}(\mathbf{B}_n) \end{aligned}$$

so that for sufficiently small $\epsilon > 0$, $(\mu^{n+1}, \eta^{n+1}) \in \mathcal{P}$. For this choice of (μ, η) in (5.2) one can easily verify that at $(n+1)$ -th iteration we have

$$(5.5) \quad \begin{aligned} J(\mu^{n+1}, \eta^{n+1}) &= J(\mu^n, \eta^n) + dJ(\mu^n, \eta^n; \mu^{n+1} - \mu^n, \eta^{n+1} - \eta^n) + o(\epsilon) \\ &= J(\mu^n, \eta^n) - \epsilon \int_{I \times \Omega} \left\{ (\operatorname{tr} \mathbf{A}_n)^2 + (\operatorname{tr} \mathbf{B}_n)^2 \right\} d\mathbf{x}dt + o(\epsilon). \end{aligned}$$

For ϵ sufficiently small, it follows from the above expression that

$$J(\mu^{n+1}, \eta^{n+1}) < J(\mu^n, \eta^n).$$

Thus it is evident that this process will generate a monotone convergent sequence $\{J(\mu^n, \eta^n), n \in N\}$.

Step 4: Using the pair (μ^{n+1}, η^{n+1}) , go to **Step 1** and continue till a desired level of accuracy is achieved. For example, for sufficiently small $\delta > 0$, we may require that

$$|J(\mu^{n+1}, \eta^{n+1}) - J(\mu^n, \eta^n)| \leq \delta.$$

This may be chosen as the stopping criterion.

5.1. An Algorithm for Constant Parameters. In the previous algorithm we have assumed that the parameters are functions of time and space belonging to the set \mathcal{P} . In case one wishes to find the best constant parameter from the set \mathcal{C} one can easily modify the previous algorithm as follows. Replace the equation (5.2) by the following equation

$$(5.6) \quad \begin{aligned} dJ(\mu^n, \eta^n; \mu - \mu^n, \eta - \eta^n) &= \\ &(\mu - \mu^n) \int_{I \times \Omega} \operatorname{tr} \left\{ (\nabla \mathbf{u}^n + (\nabla \mathbf{u}^n)') (\nabla \Psi^n)' - \frac{2}{3} (\operatorname{div}(\mathbf{u}^0 \mathbb{I})) (\nabla \Psi^n)' \right\} d\mathbf{x}dt \\ &+ (\eta - \eta^n) \int_{I \times \Omega} \operatorname{tr} \left\{ (\operatorname{div}(\mathbf{u}^0 \mathbb{I})) (\nabla \Psi^n)' \right\} d\mathbf{x}dt \geq 0, \quad \forall (\mu, \eta) \in \mathcal{C}. \end{aligned}$$

In this case equations (5.3) and (5.4) take the form

$$(5.7) \quad \begin{aligned} \mu^{n+1} &= \mu^n - \epsilon \int_{I \times \Omega} \operatorname{tr} \left\{ (\nabla \mathbf{u}^n + (\nabla \mathbf{u}^n)') (\nabla \Psi^n)' - \frac{2}{3} (\operatorname{div}(\mathbf{u}^0 \mathbb{I})) (\nabla \Psi^n)' \right\} d\mathbf{x}dt \\ &\equiv \mu^n - \epsilon \int_{I \times \Omega} \operatorname{tr}(\mathbf{A}_n) d\mathbf{x}dt \end{aligned}$$

$$\begin{aligned}
(5.8) \quad \eta^{n+1} &= \eta^n - \epsilon \int_{I \times \Omega} \text{tr} \{ (\text{div}(\mathbf{u}^0 \mathbb{I})) (\nabla \Psi^n)' \} \, d\mathbf{x} dt \\
&\equiv \eta^n - \epsilon \int_{I \times \Omega} \text{tr}(\mathbf{B}_n) \, d\mathbf{x} dt.
\end{aligned}$$

Thus choosing $(\mu, \eta) = (\mu^{n+1}, \eta^{n+1})$ as given above we have

$$\begin{aligned}
(5.9) \quad J(\mu^{n+1}, \eta^{n+1}) &= J(\mu^n, \eta^n) + dJ(\mu^n, \eta^n; \mu^{n+1} - \mu^n, \eta^{n+1} - \eta^n) + o(\epsilon) \\
&= J(\mu^n, \eta^n) - \epsilon \left\{ \left(\int_{I \times \Omega} \text{tr}(A_n) d\mathbf{x} dt \right)^2 + \left(\int_{I \times \Omega} \text{tr}(B_n) d\mathbf{x} dt \right)^2 \right\} + o(\epsilon).
\end{aligned}$$

Again, for $\epsilon > 0$ sufficiently small, we have

$$J(\mu^{n+1}, \eta^{n+1}) < J(\mu^n, \eta^n).$$

Thus by appropriate choice of the sequence $\{(\mu^n, \eta^n), n \in N\}$ as shown above we can construct a monotone sequence of the cost functionals $\{J(\mu^n, \eta^n), n \in N\}$ decreasing to a local minimum.

Remark 4. With reference to the first algorithm, note that the set \mathcal{P} is a weak star compact subset of $L_\infty(I \times \Omega, \mathbb{R}^2)$. Hence every sequence from \mathcal{P} has a weak star convergent subsequence. Thus, there exists an element $(\mu^0, \eta^0) \in \mathcal{P}$ such that the sequence generated by the first algorithm will converge in the weak star sense to (μ^0, η^0) and the local minimum is given by $J(\mu^0, \eta^0)$.

With reference to the second algorithm, where the parameters are required to be constant taking values from the compact set $\mathcal{C} \subset \mathbb{R}^2$, similar conclusions hold.

If one wishes to determine whether or not the algorithm gives a global minimum, one must choose and start the algorithm with different initial values for (μ, η) and examine if $J(\mu^n, \eta^n)$ converges to the same minimum. There are some adhoc algorithms such as RRS (recursive random search) that can do the job.

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