MIXING ENHANCEMENT BY OPTIMAL FLOW ADVECTION[*]

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Abstract. We consider the problem of optimal mixing control. Our objective is to best enhance mixing by flow advection while the flow is optimized in the sense that it is almost steady and is of the least magnitude and the least rotation. For this we define a mixing efficiency functional by penalizing the average of variance of a diffusive scalar, the average of the flow, and the average of its acceleration and strain tensor. By variational principles, we prove the existence of an optimal flow and derive optimality conditions that consist of a system of nonlinear advection-diffusion equations, wave equations, and Laplace's equation.

1. Introduction. A fluid mixture consists of diffusive physical quantities and a fluid in which the physical quantities are immersed. Typical examples of such a mixture include fuel and air in a combustor and chemical pollutants and water in the environment. These physical quantities can be mathematically regarded as scalars. If a scalar such as the fuel does not significantly influence the fluid motion, it is called a passive scalar. If chemical reactions can be neglected, then the scalar usually undergoes two processes: molecular diffusion and flow advection. These two processes can be mathematically modeled by the advection-diffusion equation

$$(1) \qquad \frac{\partial c}{\partial t} + (\mathbf{v} \cdot \nabla)c = \kappa \nabla^2 c, \quad c(\mathbf{x}, 0) = c^0(\mathbf{x}) \quad \text{in } \Omega, \quad \text{and} \quad \frac{\partial c}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega$$

in the absence of a source or sink. In the above equation, $c = c(\mathbf{x}, t)$ denotes the concentration of the scalar, $c^0(\mathbf{x})$ is an initial concentration, $\kappa > 0$ denotes the molecular diffusivity of the scalar, Ω is a bounded domain in $\mathbb{R}^n$, $\frac{\partial}{\partial \mathbf{n}}$ denotes the normal derivative along the boundary $\partial\Omega$, $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$ denotes an incompressible velocity field ($\nabla \cdot \mathbf{v} = 0$), $\nabla = (\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n})$, and $\nabla^2 = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}$. We assume that $\mathbf{v}$ satisfies no-penetration boundary conditions on the boundary $\partial\Omega$ ($\mathbf{n} \cdot \mathbf{v} = 0$ with $\mathbf{n}$ denoting the unit normal on the boundary).

Often a certain level of homogeneity of a mixture is desired. For instance, before fuel is burned in a combustor, it is required to be well mixed so that the combustor can achieve its best efficiency. Hence, it is important to design efficient and practical mixing enhancement techniques.

Because a turbulent flow can greatly enhance mixing [4, 10, 11, 12, 13, 15, 22, 26], a useful mixing enhancement technique is to destabilize a flow so that it becomes as turbulent or chaotic as possible. In the design of a stainless cylindrical microcombustor,

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a critical component for micropower systems using hydrogen and hydrocarbon fuels as an energy source, Yang et al. [28] used the backward facing step to provide a simple yet effective solution to enhance the mixing of the fuel mixture, prolong the residence time, control the position of the flame, and widen the operational range of the flow rate and H_2/air ratio. Charyulu et al. [7] studied mixing enhancement with two-dimensional (2D) lobed nozzles in a dual stream supersonic flow facility, and their results indicated an enormous enhancement in mixing when a 2D lobed nozzle was employed in comparison with a conventional plain 2D nozzle. The enhanced mixing performance could be attributed to the large-scale axial vortices observed in the flow field. In addition to the use of these passive control devices, a flow can be destabilized by open-loop active excitations through flaps, wall-jets, or other devices [14] so that the flow is separated and large-scale coherent structures are developed in the flow. Active feedback controllers were developed by Aamo, Krstic, and Bewley [1] for destabilization of 2D channel flows; by Balogh, Aamo, and Krstic [5] for destabilization of three-dimensional (3D) pipe flows; by Yuan, Krstic, and Bewley [29] for destabilization of jet nozzle flows; and by Wang et al. [27] for generation of flow separation in bluff body shear flows.

In these control designs, the optimization of control efforts is ignored. While we try to enhance mixing by destabilizing a flow, it is desirable to minimize this destabilization effort. For instance, after mixing has been enhanced, the destabilization should be stopped to save the control efforts. The goal of this paper is to characterize a flow that best enhances mixing and is optimized in some sense.

Mixing will be best enhanced if the scalar variance $\|c(t; \mathbf{v}) - \langle c(t; \mathbf{v}) \rangle\|$ is made as small as possible [19], where $c(\mathbf{x}, t; \mathbf{v})$ is the solution of (1) corresponding to the velocity $\mathbf{v}$ and $\langle c(t; \mathbf{v}) \rangle$ denotes the mean concentration. As for the control efforts, we could say that the flow velocity $\mathbf{v}$ is optimal if the flow is almost steady and irrotational. This implies that the flow, its acceleration, and its strain tensor need to be minimized. Therefore we define a mixing efficiency functional by penalizing the average of variance of the scalar, the average of the flow velocity, the average of the strain tensor, and the average of the acceleration. We show that the functional is weakly lower semicontinuous and then it attains its minimum. The minimizer of the functional is called an optimal flow. By variational principles, we then derive optimality conditions that consist of a system of nonlinear partial differential equations.

There are different measures for mixing efficiency such as Lagrangian and Eulerian time averages of a flow [3], the mixing variance coefficient [6], and the Mix-Norm defined by Mathew, Mezić, and Petzold [20]. For the convenience of treatment of our optimal control problem, we use the L_2 norm of a scalar variance as the mixing efficiency measurement.

The optimal mixing problem has been studied in the literature. Using the entropy of automorphisms of dynamical systems as the measure of mixing efficiency, D'Alessandro, Dahleh, and Mezic [2] formulated an optimal mixing problem by maximizing the entropy among all permissible periodic sequences composed of two shear flows orthogonal to each other. They derived the form of the protocol which maximizes the entropy by developing appropriate ergodic-theoretic tools. Another optimal mixing problem was defined by Noack et al. [21], who used the flux across a recirculation region as the measure of mixing efficiency and then maximized the flux among all permissible controlled vortex motions. These optimal mixing problems are different from the one discussed here. First, in our case, the advection-diffusion equation is used to describe the fluid mixing, while a system of ordinary differential equations was used in their studies. Second, the measures of mixing efficiency are different. Third,

the optimal objectives are different. While mixing and flow are both optimized in our case, the optimization of flow was not considered in their cases. Finally, because of these differences, the characterizations of the optimal flow are different. In our case, the optimal flow is characterized by a system of nonlinear partial differential equations, while, in their cases, the optimal sequence of flow is given by the sequence of period 2 of two matrices in [2], and the optimal vortex motion was identified in [21] by finding the optimal flat output trajectory which maximizes the flux.

The paper is organized as follows. We define a mixing efficiency functional in section 2 and prove the existence of an optimal flow in section 3. Optimality conditions are presented in section 4 and are proved in sections 5 and 6.

2. Mixing efficiency functionals. Throughout this paper, $H^s(\Omega)$ denotes the usual Sobolev space [9] for any $s \in \mathbb{R}$. For $s \geq 0$, $H_0^s(\Omega)$ denotes the completion of $C_0^\infty(\Omega)$ in $H^s(\Omega)$, where $C_0^\infty(\Omega)$ denotes the space of all infinitely differentiable functions on Ω with a compact support in Ω.

We will need the following vector function spaces:

$$\mathbf{L}^2(\Omega) = \{L^2(\Omega)\}^n,$$

$$\mathbf{H}^1(\Omega) = \{H^1(\Omega)\}^n,$$

$$\mathbf{H}^2(\Omega) = \{H^2(\Omega)\}^n,$$

$$\mathbf{H}_{div}^1(\Omega) = \{\mathbf{v} \in \mathbf{H}^1(\Omega) \ : \ \text{div}(\mathbf{v}) = 0 \text{ in } \Omega\},$$

$$\mathbf{L}_{div}^2(\Omega) = \text{ the closure of } \mathbf{H}_{div}^1(\Omega) \text{ in } \mathbf{L}^2(\Omega).$$

The $\mathbf{L}^2$ norm of a function $\mathbf{f}(\mathbf{x}) \in \mathbf{L}^2(\Omega)$ is denoted by

$$\|\mathbf{f}\| = \left(\int_\Omega |\mathbf{f}(\mathbf{x})|^2 dV\right)^{1/2}.$$

We will also need spaces involving time. Let X denote a Banach space with a norm $\|\cdot\|$ and $0 < T$. The space $L^2(0, T; X)$ consists of all measurable functions $\mathbf{v} : [0, T] \to X$ with

$$\|\mathbf{v}\|_{L^2(0,T;X)} = \left(\int_0^T \|\mathbf{v}(t)\|^2 dt\right)^{1/2} < \infty.$$

The Sobolev space $H^1(0, T; X)$ consists of all functions $\mathbf{v} \in L^2(0, T; X)$ such that $\mathbf{v}'$ exists in the weak sense and belongs to $L^2(0, T; X)$. The norm is defined by

$$\|\mathbf{v}\|_{H^1(0,T;X)} = \left(\int_0^T (\|\mathbf{v}(t)\|^2 + \|\mathbf{v}'(t)\|^2) dt\right)^{1/2}.$$

We denote

$$H_0^1(0, T; X) = \{\mathbf{v} \in H^1(0, T; X) \mid \mathbf{v}(0) = \mathbf{v}(T) = 0\}.$$

The space $C([0, T]; X)$ consists of all continuous functions $\mathbf{v} : [0, T] \to X$ with

$$\|\mathbf{v}\|_{C([0,T];X)} = \max_{0 \leq t \leq T} \|\mathbf{v}(t)\| < \infty.$$

The strain tensor of the velocity $\mathbf{v} = (v_1, v_2, v_3)$ is denoted by

$$\nabla\mathbf{v} = \begin{pmatrix} \dfrac{\partial v_1}{\partial x_1} & \dfrac{\partial v_1}{\partial x_2} & \dfrac{\partial v_1}{\partial x_3} \\[2mm] \dfrac{\partial v_2}{\partial x_1} & \dfrac{\partial v_2}{\partial x_2} & \dfrac{\partial v_2}{\partial x_3} \\[2mm] \dfrac{\partial v_3}{\partial x_1} & \dfrac{\partial v_3}{\partial x_2} & \dfrac{\partial v_3}{\partial x_3} \end{pmatrix}.$$

The mean concentration of $c(\mathbf{x}, t; \mathbf{v})$ is defined by

$$\langle c(t; \mathbf{v}) \rangle = \frac{1}{\text{mes}(\Omega)} \int_\Omega c(\mathbf{x}, t; \mathbf{v}) dV.$$

Mixing will be best enhanced if the scalar variance $\|c(t; \mathbf{v}) - \langle c(t; \mathbf{v})\rangle\|$ is made as small as possible. While mixing is best enhanced, the velocity $\mathbf{v}$ is desired to be optimized in the sense that it is almost steady and is of the least magnitude $\|\mathbf{v}\|$ and the least rotation. The least magnitude ensures that the cost of generating the flow will be lowest, and the least rotation guarantees that the flow is not too turbulent and chaotic. A development of rotation in a flow requires shear stress to be present on a fluid particle surface. The shear stress depends on the strain tensor $\nabla\mathbf{v}$ of the velocity $\mathbf{v}$ [23]. Thus, to have the least rotation, the magnitude $\|\nabla\mathbf{v}\|$ needs to be minimized. To make the flow almost steady, the acceleration magnitude $\|\frac{\partial \mathbf{v}(t)}{\partial t}\|$ needs to be minimized. This motivates us to define the following mixing efficiency functional:

$$J(\mathbf{v}) = \int_0^T \left(\|c(t; \mathbf{v}) - \langle c(t; \mathbf{v})\rangle\|^2 + \alpha\|\mathbf{v}(t)\|^2 + \beta\|\nabla\mathbf{v}(t)\|^2 + \gamma \left\|\frac{\partial \mathbf{v}(t)}{\partial t}\right\|^2 \right) dt$$

$$(2) \qquad + \mu\|c(T; \mathbf{v}) - \langle c(T; \mathbf{v})\rangle\|^2,$$

where $T > 0$ is some desired time, and $\alpha > 0, \beta, \gamma, \mu \geq 0$ are weight constants. In optimal control theory, the first two terms $\|c(t; \mathbf{v}) - \langle c(t; \mathbf{v})\rangle\|^2, \alpha\|\mathbf{v}(t)\|^2$, which penalize the averages of the scalar variance and the controlling cost, are standard [8, 16]. The variance $\|c(T; \mathbf{v}) - \langle c(T; \mathbf{v})\rangle\|^2$ at the final time is optional but included in this functional to ensure that the highest level of homogenization of the scalar will be achieved. Another standard functional in optimal control theory is the one over an infinite time interval for a regulator problem. For the problem of mixing enhancement, this functional is not appropriate since mixing needs to be enhanced in a desired finite time.

The weight constants in (2) play an important role in determining the control strength. For small values of α, β, γ, the functional will result in an optimal solution with a small variance of the scalar but with big magnitudes of the velocity $\mathbf{v}$, of the strain tensor $\nabla\mathbf{v}$, and of the acceleration $\frac{\partial \mathbf{v}}{\partial t}$. This implies that the smaller the weights, the more turbulent the optimal flow, and then the better the mixing enhancement.

We note that the mean is conserved. In fact, integrating (1) over Ω gives

$$\frac{d}{dt} \langle c \rangle = \frac{\kappa}{\text{mes}(\Omega)} \int_\Omega \nabla^2 c \, dV = 0,$$

where we have used the boundary conditions on $\mathbf{v}$ and c. Therefore we can assume zero mean without loss of generality. With the zero-mean assumption, the cost functional reduces to

$$J(\mathbf{v}) = \int_0^T \left(\|c(t; \mathbf{v})\|^2 + \alpha\|\mathbf{v}(t)\|^2 + \beta\|\nabla\mathbf{v}(t)\|^2 + \gamma \left\| \frac{\partial \mathbf{v}(t)}{\partial t} \right\|^2 \right) dt$$

(3) $+ \mu\|c(T; \mathbf{v})\|^2.$

Then the optimal control problem is to minimize J in an admissible velocity space $\mathcal{V} = H_0^1(0, T; \mathbf{H}_{div}^1(\Omega))$:

(4) $$J(\mathbf{v}^*) = \min_{\mathbf{v} \in \mathcal{V}} J(\mathbf{v}).$$

The minimizer $\mathbf{v}^*$ is called an *optimal flow*.

In deriving optimality conditions for the optimal flow below, control flows are required to satisfy the condition $\mathbf{v}(0) = \mathbf{v}(T) = 0$. This mathematical condition, in fact, is quite realistic because the control flows should start from the rest and return back to the rest at the final time when the mixing has been enhanced. For instance, before coffee is stirred, the flow is at rest.

In this theoretical study, we assume that an arbitrary unsteady flow can be generated. This may not be realistic. In a future work, we will consider specific velocity fields such as $\mathbf{v} = \sum_{i=1}^N \mathbf{v}_i(\mathbf{x})u_i(t)$, where $\mathbf{v}_i(\mathbf{x})$ $(i = 1, \ldots, N)$ are given steady flows which prescribe how the control action is distributed in the flow field.

3. Existence of optimal flows. For convenience, we state a well-known estimate about the solution of (1) as follows.

LEMMA 3.1. *Let $\mathbf{v} \in L^2(0, T; \mathbf{L}_{div}^2(\Omega))$. Then the solution c of (1) satisfies the following estimate:*

(5) $$\|c(t)\|^2 + 2\kappa \int_0^t \|\nabla c(s)\|^2 \, ds = \left\|c^0\right\|^2.$$

Proof. Multiplying (1) by c and using the boundary conditions, we obtain the equation

(6) $$\frac{1}{2}\frac{d}{dt}\|c\|^2 = -\kappa \|\nabla c\|^2.$$

Integrating over $[t_0, t]$ gives (5).   □

To prove the existence of an optimal flow, we need the following weakly lower semicontinuity of the function J.

LEMMA 3.2. *The functional J defined by (3) is weakly lower semicontinuous. That is, if $\mathbf{v}_n$ converges weakly to $\mathbf{v}_0$ in $H^1(0, T; \mathbf{H}_{div}^1(\Omega))$, then*

$$J(\mathbf{v}_0) \leq \liminf_{n \to \infty} J(\mathbf{v}_n).$$

Proof. Let $\mathbf{v}_n$ converge weakly to $\mathbf{v}_0$ in $H^1(0, T; \mathbf{H}_{div}^1(\Omega))$ and let $c_n(\mathbf{x}, t; \mathbf{v}_n)$ be the solution of

(7) $\dfrac{\partial c_n}{\partial t} + (\mathbf{v}_n \cdot \nabla)c_n = \kappa\nabla^2 c_n, \quad c_n(\mathbf{x}, 0) = c^0(\mathbf{x}) \quad \text{in } \Omega, \quad \text{and} \quad \dfrac{\partial c_n}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega.$

Then $\mathbf{v}_n$ converges strongly to $\mathbf{v}_0$ in $L^2(0,T;\mathbf{L}^2_{div}(\Omega))$. Moreover, it follows from (5) that there exists a subsequence of $c_n(\mathbf{x},t;\mathbf{v}_n)$, still denoted by itself for convenience, that converges weakly to c_0^* in $L^2(0,T;H^1(\Omega))$. Therefore we can pass to the limit in (7) and obtain

$$\frac{\partial c_0^*}{\partial t} + (\mathbf{v}_0 \cdot \nabla)c_0^* = \kappa\nabla^2 c_0^*, \quad c_0^*(\mathbf{x},0) = c^0(\mathbf{x}) \quad \text{in } \Omega, \quad \text{and} \quad \frac{\partial c_0^*}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega.$$

Since any norm of a Banach space is weakly lower semicontinuous [17], it therefore follows that

$$\liminf_{n\to\infty} J(\mathbf{v}_n) \geq \liminf_{n\to\infty} \int_0^T \left(\|c_n(t;\mathbf{v}_n)\|^2 + \alpha\|\mathbf{v}_n(t)\|^2 \right.$$

$$\left. + \beta\|\nabla\mathbf{v}_n(t)\|^2 + \gamma\left\|\frac{\partial\mathbf{v}_n(t)}{\partial t}\right\|^2 \right) dt$$

$$+ \mu\liminf_{n\to\infty} \|c_n(T;\mathbf{v}_n)\|^2$$

$$\geq \int_0^T \left(\|c_0^*(t;\mathbf{v}_0)\|^2 + \alpha\|\mathbf{v}_0(t)\|^2 + \beta\|\nabla\mathbf{v}_0(t)\|^2 + \gamma\left\|\frac{\partial\mathbf{v}_0(t)}{\partial t}\right\|^2 \right) dt$$

$$+ \mu\|c_0^*(T;\mathbf{v}_0)\|^2$$

$$= J(\mathbf{v}_0).$$

So the functional J is weakly lower semicontinuous. $\quad\square$

From this lemma, we can readily prove the following existence theorem.

THEOREM 3.1. *If $\beta,\gamma > 0$, then there exists an optimal flow $\mathbf{v}^* \in \mathcal{V} = H^1(0,T;\mathbf{H}^1_{div}(\Omega))$ such that*

$$(8) \qquad\qquad\qquad J(\mathbf{v}^*) = \min_{\mathbf{v}\in\mathcal{V}} J(\mathbf{v}).$$

Proof. Let $\mathbf{v}_n$ be the minimizing sequence in $H^1(0,T;\mathbf{H}^1_{div}(\Omega))$. That is,

$$\lim_{n\to\infty} J(\mathbf{v}_n) = \min_{\mathbf{v}\in\mathcal{V}} J(\mathbf{v}).$$

Then $\mathbf{v}_n$ is bounded in $H^1(0,T;\mathbf{H}^1_{div}(\Omega))$. This implies that there exists a subsequence, still denoted by $\mathbf{v}_n$, that converges weakly to $\mathbf{v}^*$ in $H^1(0,T;\mathbf{H}^1_{div}(\Omega))$. It therefore follows from Lemma 3.2 that

$$J(\mathbf{v}^*) \leq \lim_{n\to\infty} J(\mathbf{v}_n) = \min_{\mathbf{v}\in\mathcal{V}} J(\mathbf{v}),$$

which implies (8). $\quad\square$

If $\beta = \gamma = 0$, the existence is open. In this case, the minimizing sequence $\mathbf{v}_n$ is bounded only in $L^2(0,T;\mathbf{L}^2_{div}(\Omega))$ and then may not converge strongly to $\mathbf{v}_0$ in $L^2(0,T;\mathbf{L}^2_{div}(\Omega))$. Thus passing to the limit in (7) cannot be guaranteed. Also the uniqueness of the optimal flow is open because we could not prove that the functional J is convex.

4. Optimality conditions.

THEOREM 4.1. *If $\mathbf{v}^*$ is an optimal flow under the cost functional J defined by (3), then it satisfies the following equations:*

$$
(9) \qquad\qquad \frac{\partial c}{\partial t} + (\mathbf{v}^* \cdot \nabla)c = \kappa \nabla^2 c,
$$

$$
(10) \qquad\qquad \frac{\partial g}{\partial t} + (\mathbf{v}^* \cdot \nabla)g = -\kappa \nabla^2 g + c(\mathbf{v}^*),
$$

$$
(11) \qquad\qquad \nabla^2 p(\mathbf{x}, t) = \nabla g(\mathbf{x}, t; \mathbf{v}^*) \cdot \nabla c(\mathbf{x}, t; \mathbf{v}^*) + g(\mathbf{x}, t; \mathbf{v}^*) \nabla^2 c(\mathbf{x}, t; \mathbf{v}^*),
$$

$$
(12) \quad -\alpha \mathbf{v}^* + \beta \nabla^2 \mathbf{v}^* + \gamma \frac{\partial^2 \mathbf{v}^*}{\partial t^2} = g(\mathbf{x}, t; \mathbf{v}^*) \nabla c(\mathbf{x}, t; \mathbf{v}^*) - \nabla p,
$$

$$
(13) \qquad\qquad \frac{\partial c}{\partial \mathbf{n}} = \frac{\partial g}{\partial \mathbf{n}} = \frac{\partial p}{\partial \mathbf{n}} = 0,\ \mathbf{v}^* = 0 \quad on\ \partial\Omega,
$$

$$
(14) \qquad\qquad \mathbf{v}^*(\mathbf{x}, 0) = \mathbf{v}^*(\mathbf{x}, T) = 0 \quad in\ \Omega,
$$

$$
(15) \qquad\qquad c(\mathbf{x}, 0) = c^0(\mathbf{x}), \quad g(\mathbf{x}, T) = -\mu c(\mathbf{x}, T; \mathbf{v}^*) \quad in\ \Omega.
$$

We will prove this theorem in the next two sections.

If $\beta = 0$, we can solve (12) to obtain

$$
\begin{aligned}
\mathbf{v}^* = {} & \frac{1}{2}\sqrt{\frac{1}{\alpha\gamma}} \int_0^t \left(\nabla p(\mathbf{x}, s) - g(\mathbf{x}, s)\nabla c(\mathbf{x}, s)\right) \left(e^{\sqrt{\alpha/\gamma}(s-t)} - e^{\sqrt{\alpha/\gamma}(t-s)}\right) ds \\
& + \frac{1}{2}\sqrt{\frac{1}{\alpha\gamma}} \frac{e^{-t\sqrt{\alpha/\gamma}} - e^{t\sqrt{\alpha/\gamma}}}{e^{-T\sqrt{\alpha/\gamma}} - e^{T\sqrt{\alpha/\gamma}}} \\
& \times \int_0^T \left(\nabla p(\mathbf{x}, s) - g(\mathbf{x}, s)\nabla c(\mathbf{x}, s)\right) \left(e^{\sqrt{\alpha/\gamma}(T-s)} - e^{\sqrt{\alpha/\gamma}(s-T)}\right) ds.
\end{aligned}
$$

This control law shows that the optimal control flow depends on all the concentration gradients during the whole time period from 0 to T.

Solving the system (9)–(15) numerically or analytically is a challenging problem since it is highly nonlinear. As an initial attempt, we give a preliminary numerical result.

One potential method for solving (9)–(15) could be the iteration method. We first solve the advection-diffusion (9) with a given velocity $\mathbf{v}_1$. Then with this solution $c(\mathbf{v}_1)$, we solve (10) and then (11). Through (12), we obtain a new velocity $\mathbf{v}_2$. With this $\mathbf{v}_2$, we repeat the above procedure, and so on.

To test whether or not this iteration method works, we consider a simplified case where $\beta = \gamma = \mu = 0$ and the system is considered in a 2D domain. Under this simplification, this testing could be purely numerical, as real mixing may take place only in the 3D space. Since $\beta = \gamma = 0$, the boundary condition (14) is not needed, and then $\mathbf{v}^*(\mathbf{x}, 0)$ may not be equal to zero in this case.

In our computations, the domain $\Omega = (0, 1) \times (0, 1)$, the initial condition $c^0(x, y) = \sin(2\pi x)\sin(2\pi y)$, the diffusivity $\kappa = 0.01$, the starting velocity $\mathbf{v}_1 = \mathbf{0}$, $T = 2$, $\alpha = 0.5$, and $\beta = \gamma = \mu = 0$. All equations are solved by the finite element method developed in [25] (with some modifications for this particular problem).
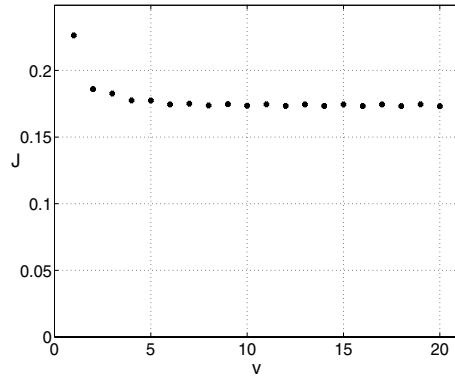
FIG. 1. *Starting with the velocity* $\mathbf{v}_1 = 0$, *the functional J reaches its minimum after a number of iterations and then stays there.*

Figure 1 shows that the functional J reaches its minimum after a number of iterations and then stays there. The approximate optimal flow $\mathbf{v}^*$ obtained via 20 iterations in this numerical experiment is shown in Figure 2. From this figure it can be seen that the flow is decreasing to zero. This could imply that after the scalar is well advected, no further advection is needed to save the control efforts.

To see how this optimal flow enhances mixing, we compare the variance decay in the case of $\mathbf{v}_1 = 0$ with the variance decay in the case of the optimal flow, where the variance is defined by

$$V(t) = \|c(t; \mathbf{v}) - \langle c(t; \mathbf{v}) \rangle \|^2.$$

Figure 3 shows that the variance of the scalar advected by the optimal flow decays much faster than the one without advection.

To further test whether or not the functional $J(\mathbf{v})$ really attains the minimum at the optimal flow obtained above, we consider a couple of other model flows. One of them is the following time-periodic velocity [18], denoted by $\mathbf{v}_{p_1}$:

$$v_1(x, y, t) = \begin{cases} \sin(\pi x)\cos(\pi y) & \text{if } n \le t < n + 0.5; \\ -\sin(2\pi x)\cos(\pi y) & \text{if } n + 0.5 \le t < n + 1; \end{cases}$$

(16)
$$v_2(x, y, t) = \begin{cases} -\cos(\pi x)\sin(\pi y) & \text{if } n \le t < n + 0.5; \\ 2\cos(2\pi x)\sin(\pi y) & \text{if } n + 0.5 \le t < n + 1. \end{cases}$$

As above, we can compute the value of the functional $J(\mathbf{v}_{p_1})$ at this flow and obtain

$$J(\mathbf{v}_{p_1}) = 1.0429,$$

which is greater than the value of the functional at the above optimal flow:

$$J(\mathbf{v}^*) = 0.1731.$$

Another flow is the simplified model flow, denoted by $\mathbf{v}_{p_2}$, of time-aperiodic Rayleigh–Bénard convection. The velocity field of the flow is derived from the stream function

(17)
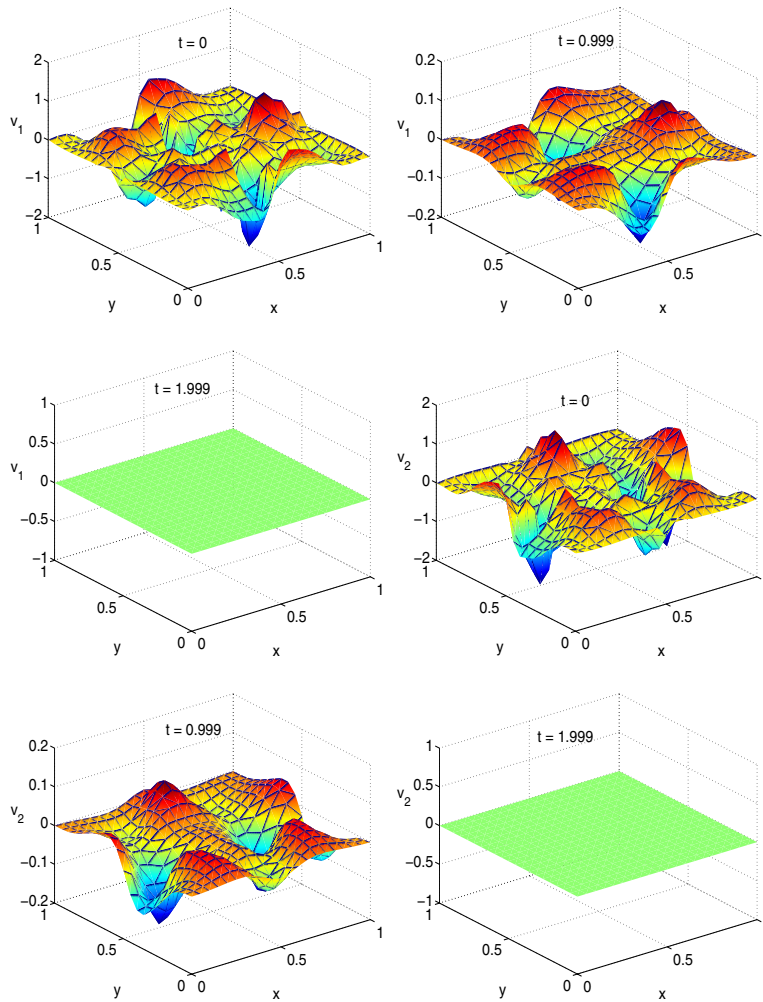$$\Psi = \frac{A}{n}\sin(2\pi x)\sin\{n[x + B\sin(\omega t)]\}W(y),$$

FIG. 2. *The x-component v_1 (top row and middle row (left)) and y-component v_2 (middle row (right) and bottom row) of the optimal flow $\mathbf{v}^*$ at $t = 0, 0.999, 1.999$, obtained via 20 iterations starting with the velocity $\mathbf{v}_1 = 0$.*

where A is a positive constant, n is the wave number $2\pi/\lambda$ with a constant λ, and $W(y)$ is a function that satisfies the rigid boundary conditions at the top and bottom surfaces. Here we use the following function $W(y)$:

$$W(y) = (1 - y)y.$$

This stream function is obtained by adding the factor $\sin(2\pi x)$ to a stream function used in [24] to make it satisfy the no-penetration boundary condition. In this computation, $A = 1.8, B = 0.06, \omega = 2\pi$, and $\lambda = 2$. The value of the functional at this flow is

$$J(\mathbf{v}_{p_2}) = 0.2801.$$

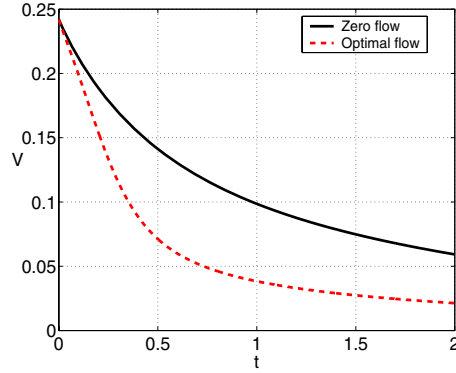As before, it is also greater than $J(\mathbf{v}^*) = 0.1731$.

FIG. 3. *The variance of a scalar advected by the optimal flow decays much faster than the one without advection.*

The above is a very preliminary attempt. The complete resolution of the problem could require an extensive regularity analysis of solutions and applications of fixed point theorems.

The asymptotic behavior of solutions of the system (9)–(15) in the zero limit of the diffusivity κ is a singular perturbation problem. This problem is interesting but difficult. The resolution of the problem will require extensive asymptotic analysis such as the decomposition of inner and outer solutions and boundary layer analysis. This is beyond the reach of the paper.

5. Gâteaux differentials. The space $C(\Omega)$ consists of all continuous functions f on Ω with

$$\|f\|_\infty = \max_{\mathbf{x} \in \Omega} |f(\mathbf{x})| < \infty.$$

The function vector space $\mathbf{C}(\Omega) = \{C(\Omega)\}^n$.

THEOREM 5.1. *Let the functional J be defined by (3). If $\mathbf{v} = (v_1, v_2, v_3) \in H^1(0, T; \mathbf{H}^1_{div}(\Omega))$ and $\mathbf{u} = (u_1, u_2, u_3) \in H^1(0, T; \mathbf{H}^1_{div}(\Omega) \cap \mathbf{C}(\Omega))$, then the Gâteaux differential of J is given by*

$$\langle J'(\mathbf{v}), \mathbf{u} \rangle = \lim_{\varepsilon \to 0} \frac{J(\mathbf{v} + \varepsilon \mathbf{u}) - J(\mathbf{v})}{\varepsilon}$$

$$= 2 \int_0^T \int_\Omega c(\mathbf{v}) h(\mathbf{v}, \mathbf{u}) dV\, dt + 2\mu \int_\Omega c(T; \mathbf{v}) h(T; \mathbf{v}, \mathbf{u}) dV$$

(18)
$$+ 2 \int_0^T \int_\Omega \left(\alpha \mathbf{v} \cdot \mathbf{u} + \beta \nabla \mathbf{v} \cdot \nabla \mathbf{u} + \gamma \frac{\partial \mathbf{v}}{\partial t} \cdot \frac{\partial \mathbf{u}}{\partial t} \right) dV\, dt,$$

where $\nabla \mathbf{v} \cdot \nabla \mathbf{u} = \sum_{i,j=1}^3 \frac{\partial v_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}$ and h is the solution of

(19)
$$\frac{\partial h}{\partial t} + (\mathbf{v} \cdot \nabla) h = \kappa \nabla^2 h - (\mathbf{u} \cdot \nabla) c(\mathbf{v}) \quad in\ \Omega,$$

$$h(\mathbf{x}, 0) = 0 \quad in\ \Omega, \quad and\quad \frac{\partial h}{\partial \mathbf{n}} = 0 \quad on\ \partial \Omega.$$

To prove this theorem, we need the following lemma. For a positive constant ε and $\mathbf{v}, \mathbf{u} \in L^2(0, T; \mathbf{L}^2_{div}(\Omega))$, we denote by $c(\mathbf{v})$ and $c_\varepsilon(\mathbf{v}, \mathbf{u})$ the solutions of (1) corresponding the velocities $\mathbf{v}$ and $\mathbf{v} + \varepsilon \mathbf{u}$, respectively.

LEMMA 5.1. *Let $\mathbf{u} \in L^2(0, T, \mathbf{L}^2_{div}(\Omega) \cap \mathbf{C}(\Omega))$ and denote $h_\varepsilon(\mathbf{v}, \mathbf{u}) = c_\varepsilon(\mathbf{v}, \mathbf{u}) - c(\mathbf{v})$. Then the h_ε satisfies the following estimates:*

$$(20) \qquad \max_{0 \le s \le t} \|h_\varepsilon(s)\|^2 \le \frac{2\varepsilon^2}{\kappa} \|c^0\|^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds,$$

$$(21) \qquad \frac{1}{2} \|h_\varepsilon(t)\|^2 + \kappa \int_0^t \|\nabla h_\varepsilon(s)\|^2 ds \le \frac{\varepsilon^2}{\kappa} \|c^0\|^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds,$$

$$(22) \qquad \max_{0 \le s \le t} \left\| \frac{h_\varepsilon(s)}{\varepsilon} - h(s) \right\|^2 \le \frac{4\varepsilon^2}{\kappa^2} \|c^0\|^2 \left(\int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \right)^2.$$

Proof. A direct calculation shows that h_ε satisfies

$$(23) \qquad \frac{\partial h_\varepsilon}{\partial t} + (\mathbf{v} \cdot \nabla) h_\varepsilon = \kappa \nabla^2 h_\varepsilon - \varepsilon (\mathbf{u} \cdot \nabla) c_\varepsilon(\mathbf{v}, \mathbf{u}) \quad \text{in } \Omega,$$

$$h_\varepsilon(\mathbf{x}, 0) = 0 \quad \text{in } \Omega, \quad \text{and} \quad \frac{\partial h_\varepsilon}{\partial \mathbf{n}} = 0 \quad \text{on } \partial \Omega.$$

Multiplying (23) by h_ε and using the boundary conditions, we obtain the equation

$$\frac{1}{2} \frac{d}{dt} \|h_\varepsilon(t)\|^2 = -\kappa \|\nabla h_\varepsilon\|^2 - \varepsilon \int_\Omega h_\varepsilon (\mathbf{u} \cdot \nabla) c_\varepsilon dV$$

$$(24) \qquad \qquad \le \varepsilon \|\mathbf{u}(t)\|_\infty \|h_\varepsilon(t)\| \|\nabla c_\varepsilon(t)\|.$$

Integrating over $[t_0, t]$ gives

$$\|h_\varepsilon(t)\|^2 \le 2\varepsilon \max_{0 \le s \le t} \|h_\varepsilon(s)\| \int_0^t \|\mathbf{u}(s)\|_\infty \|\nabla c_\varepsilon(s)\| ds$$

$$\le 2\varepsilon \max_{0 \le s \le t} \|h_\varepsilon(s)\| \left(\int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \right)^{1/2} \left(\int_0^t \|\nabla c_\varepsilon(s)\|^2 ds \right)^{1/2},$$

which implies that

$$\max_{0 \le s \le t} \|h_\varepsilon(s)\|^2 \le 2\varepsilon \max_{0 \le s \le t} \|h_\varepsilon(s)\| \left(\int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \right)^{1/2} \left(\int_0^t \|\nabla c_\varepsilon(s)\|^2 ds \right)^{1/2}$$

$$\le \frac{1}{2} \left(\max_{0 \le s \le t} \|h_\varepsilon(s)\| \right)^2 + 2\varepsilon^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \int_0^t \|\nabla c_\varepsilon(s)\|^2 ds.$$

It then follows from (5) that

$$\max_{0 \le s \le t} \|h_\varepsilon(s)\|^2 \le 4\varepsilon^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \int_0^t \|\nabla c_\varepsilon(s)\|^2 ds$$

$$(25) \qquad \qquad \le \frac{2\varepsilon^2}{\kappa} \|c^0\|^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds.$$

This proves (20).

To prove (21), we use (24) again and derive that

$$\frac{1}{2}\|h_\varepsilon(t)\|^2 + \kappa \int_0^t \|\nabla h_\varepsilon(s)\|^2 \, ds$$

$$\leq \varepsilon \max_{0 \leq s \leq t} \|h_\varepsilon(s)\| \int_0^t \|\mathbf{u}(s)\|_\infty \|\nabla c_\varepsilon(s)\| ds$$

$$\leq \varepsilon \max_{0 \leq s \leq t} \|h_\varepsilon(s)\| \left(\int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \right)^{1/2} \left(\int_0^t \|\nabla c_\varepsilon(s)\|^2 ds \right)^{1/2}.$$

It then follows from (5) and (20) that

$$\frac{1}{2}\|h_\varepsilon(t)\|^2 + \kappa \int_0^t \|\nabla h_\varepsilon(s)\|^2 \, ds \leq \varepsilon^2 \frac{\sqrt{2}}{\sqrt{\kappa}} \|c^0\| \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \frac{\|c^0\|}{\sqrt{2\kappa}}$$

(26)
$$\leq \frac{\varepsilon^2}{\kappa} \|c^0\|^2 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds.$$

To prove (22), we denote $f_\varepsilon = \frac{h_\varepsilon}{\varepsilon} - h$. A direction calculation shows that

(27)
$$\frac{\partial f_\varepsilon}{\partial t} + (\mathbf{v} \cdot \nabla) f_\varepsilon = \kappa \nabla^2 f_\varepsilon - (\mathbf{u} \cdot \nabla) h_\varepsilon \quad \text{in } \Omega,$$

$$f_\varepsilon(\mathbf{x}, 0) = 0 \quad \text{in } \Omega, \quad \text{and} \quad \frac{\partial f_\varepsilon}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega.$$

In the same way as above, we can derive that

$$\max_{0 \leq s \leq t} \|f_\varepsilon(s)\|^2 \leq 4 \int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \int_0^t \|\nabla h_\varepsilon(s)\|^2 ds$$

$$\leq \frac{4\varepsilon^2}{\kappa^2} \|c^0\|^2 \left(\int_0^t \|\mathbf{u}(s)\|_\infty^2 ds \right)^2. \qquad \Box$$

We are now ready to prove Theorem 5.1. Using the estimates (20) and (22), we derive that

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^T \int_\Omega [|c(\mathbf{v} + \varepsilon \mathbf{u})|^2 - |c(\mathbf{v})|^2] dV dt$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^T \int_\Omega [|c(\mathbf{v}) + h_\varepsilon(\mathbf{v}, \mathbf{u})|^2 - |c(\mathbf{v})|^2] dV dt$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^T \int_\Omega [2c(\mathbf{v}) h_\varepsilon(\mathbf{v}, \mathbf{u}) + (h_\varepsilon(\mathbf{v}))^2] dV dt$$

(28)
$$= 2 \int_0^T \int_\Omega c(\mathbf{v}) h(\mathbf{v}, \mathbf{u}) dV dt.$$

In the same way, we can show that

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{\Omega} [|c(T; \mathbf{v} + \varepsilon\mathbf{u})|^2 - |c(T; \mathbf{v})|^2] dV$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{\Omega} [|c(T; \mathbf{v}) + h_\varepsilon(T; \mathbf{v}, \mathbf{u})|^2 - |c(\mathbf{v})|^2] dV$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{\Omega} [2c(T; \mathbf{v})h_\varepsilon(T; \mathbf{v}, \mathbf{u}) + (h_\varepsilon(T; \mathbf{v}, \mathbf{u}))^2] dV$$

$$= 2 \int_{\Omega} c(T; \mathbf{v})h(T; \mathbf{v}, \mathbf{u}) dV.$$

Using these limits, we then readily prove Theorem 5.1.

6. Proof of Theorem 4.1. If the flow $\mathbf{v}^*$ is an optimal flow under the functional J defined by (3), then it satisfies

$$\langle J'(\mathbf{v}), \mathbf{u} \rangle = 0$$

for all $\mathbf{u} \in H_0^1(0, T; \mathbf{H}_{div}^1(\Omega))$. It then follows from (18) that

$$(29) \quad \int_0^T \int_{\Omega} c(\mathbf{x}, t; \mathbf{v}^*)h(\mathbf{x}, t; \mathbf{u}, \mathbf{v}^*) dV dt + \mu \int_{\Omega} c(\mathbf{x}, T; \mathbf{v}^*)h(\mathbf{x}, T; \mathbf{u}, \mathbf{v}^*) dV$$

$$+ \int_0^T \int_{\Omega} \left(\alpha\mathbf{v}^* \cdot \mathbf{u} + \beta\nabla\mathbf{v}^* \cdot \nabla\mathbf{u} + \gamma\frac{\partial\mathbf{v}^*}{\partial t} \cdot \frac{\partial\mathbf{u}}{\partial t} \right) dV dt = 0$$

for all $\mathbf{u} \in H_0^1(0, T; \mathbf{H}_{div}^1(\Omega) \cap \mathbf{C}(\Omega))$. Consider the adjoint equation

$$(30) \quad \frac{\partial g}{\partial t} + (\mathbf{v}^* \cdot \nabla)g = -\kappa\nabla^2 g + c(\mathbf{v}^*) \quad \text{in } \Omega,$$

$$g(\mathbf{x}, T) = -\mu c(\mathbf{x}, T; \mathbf{v}^*) \quad \text{in } \Omega, \quad \text{and} \quad \frac{\partial g}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega.$$

Multiplying (30) by h and (19) by g and integrating over $\Omega \times [0, T]$, we obtain

$$(31) \quad \int_0^T \int_{\Omega} c(\mathbf{x}, t; \mathbf{v}^*)h(\mathbf{x}, t; \mathbf{u}, \mathbf{v}^*) dV dt + \mu \int_{\Omega} c(\mathbf{x}, T; \mathbf{v}^*)h(\mathbf{x}, T; \mathbf{u}, \mathbf{v}^*) dV$$

$$= \int_0^T \int_{\Omega} (\mathbf{u} \cdot \nabla c(\mathbf{x}, t; \mathbf{v}^*)) g(\mathbf{x}, t; \mathbf{v}^*) dV dt.$$

After integration by parts with respect to t, we deduce from (29) and (31) that

$$(32) \quad \int_0^T \int_{\Omega} \mathbf{u} \cdot \left(\alpha\mathbf{v}^* - \beta\nabla^2\mathbf{v}^* - \gamma\frac{\partial^2\mathbf{v}^*}{\partial t^2} + g(\mathbf{x}, t; \mathbf{v}^*)\nabla c(\mathbf{x}, t; \mathbf{v}^*) \right) dV dt = 0,$$

which implies that there exists a potential function p such that

$$(33) \quad \alpha\mathbf{v}^* - \beta\nabla^2\mathbf{v}^* - \gamma\frac{\partial^2\mathbf{v}^*}{\partial t^2} + g(\mathbf{x}, t; \mathbf{v}^*)\nabla c(\mathbf{x}, t; \mathbf{v}^*) = \nabla p.$$

To determine p, we apply the divergence operation to the above equation and then obtain

$$(34) \quad \nabla^2 p = \nabla g(\mathbf{x}, t; \mathbf{v}^*) \cdot \nabla c(\mathbf{x}, t; \mathbf{v}^*) + g(\mathbf{x}, t; \mathbf{v}^*)\nabla^2 c(\mathbf{x}, t; \mathbf{v}^*).$$

Thus we have proved Theorem 4.1.

7. Conclusions. We have studied the problem of optimal mixing control whose objective is to best enhance mixing by flow advection while the flow is optimized in the sense that it is almost steady and is of the least magnitude and the least rotation. In solving this problem, we defined a mixing efficiency functional by penalizing the average of variance of the scalar, the average of the flow, and the average of the strain tensor and acceleration of the flow. We showed that the functional is weakly lower semicontinuous and then it attains its minimum. By variational principles, we then derived optimality conditions that consist of a system of nonlinear partial differential equations.

A number of issues are left open. Solving the optimality partial differential equations numerically or analytically is challenging since nonlinearity is presented in the advection term, which, like in the study of Navier–Stokes equations, is difficult to estimate. The resolution of the problem could require the regularity analysis of solutions and applications of fixed point theorems. The uniqueness of the optimal flow is open because we could not prove that the efficiency functional J is convex. Another interesting problem is the singular perturbation problem for the optimality partial differential equations in the zero limit of diffusivity. The resolution of the problem will require an extensive asymptotic analysis such as the decomposition of inner and outer solutions and boundary layer analysis.

Results presented in this paper could have potential applications in aerospace engineering and mixing-related industry. Often a certain level of homogeneity of a fluid mixture is desired. For instance, before fuel is burned in a combustor, it is required to be well mixed so that the combustor has its best efficiency. Hence, optimality conditions derived in this paper could serve as guidelines in implementing an efficient and practical control technique for mixing enhancement.

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