ANALYSIS OF OPTIMAL BOUNDARY CONTROL FOR A THREE-DIMENSIONAL REACTION-DIFFUSION SYSTEM

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(Communicated by ?)

ABSTRACT. This paper is concerned with optimal boundary control of a three dimensional reaction-diffusion system in a more general form than what has been presented in the literature. The state equations are analyzed and the optimal control problem is investigated. Necessary and sufficient optimality conditions are derived. The model is widely applicable due to its generality. Some examples in applications are discussed.

1. Introduction. We investigate a three-dimensional semi-linear parabolic reaction-diffusion system. The model may arise in a chemical or biological process where the species involved are subject to diffusion and reaction among each other. As an example, we consider the reaction $A + B \rightarrow C$ which obeys the law of mass action. To simplify the discussion, we assume that the backward reaction $C \rightarrow A + B$ is negligible and that the forward reaction proceeds with a constant (e.g., not temperature-dependent) rate. This leads to a coupled semilinear parabolic system in three spatial
dimensions for the respective concentrations (see, e.g., [3, 8]) as the following:

\[
\begin{align*}
\frac{\partial u}{\partial t} - d_1 \Delta u + k_1 uv & = 0 \quad (x, t) \in Q, \\
\frac{\partial v}{\partial t} - d_2 \Delta v + k_2 uv & = 0 \quad (x, t) \in Q, \\
\frac{\partial w}{\partial t} - d_3 \Delta w - k_3 uv & = 0 \quad (x, t) \in Q, \\
\partial_n u & = c(t) \quad (x, t) \in \Sigma, \\
\partial_n v & = 0 \quad (x, t) \in \Sigma, \\
\partial_n w & = 0 \quad (x, t) \in \Sigma, \\
u(x, 0) & = u_0(x) \quad x \in \Omega, \\
v(x, 0) & = v_0(x) \quad x \in \Omega, \\
w(x, 0) & = w_0(x) \quad x \in \Omega.
\end{align*}
\] (1)

Here, the real constants \(d_i\), and \(k_i \geq 0, i = 1, 2, 3\), are nonnegative. The initial data \(u_0(x), v_0(x), w_0(x) \in C(\Omega)\) are given, where \(\Omega\) is a bounded open Lipschitz domain of \(\mathbb{R}^n\) with smooth boundary \(\partial \Omega\). \(T > 0\) is a fixed time, and we use the notation \(Q := \Omega \times (0, T)\) and \(\Sigma := \partial \Omega \times (0, T)\). By \(\partial_n\), we denote the outward normal derivative on \(\partial \Omega\).

The first boundary equation \(\partial_n u = c(t)\) describes the boundary flux of the first substance \(A\) by means of a given shape function \(c(t)\), while \(c(t)\) denotes the control intensity at time \(t\), which is to be determined. The remaining homogeneous Neumann boundary conditions simply correspond to a “no-outflow” condition of the substances through the boundary of the reaction vessel \(\Omega\). Our goal is to drive the above reaction-diffusion system from the given state to a desired state with minimal cost

\[
\begin{align*}
\min \quad J(u, v, w, c) &= \frac{\alpha_u}{2} \|u - u_Q\|^2_{L^2(Q)} + \frac{\alpha_v}{2} \|v - v_Q\|^2_{L^2(Q)} + \frac{\alpha_w}{2} \|w - w_Q\|^2_{L^2(Q)} \\
&+ \frac{\alpha_{uv}}{2} \|u(T) - u_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha_{uv}}{2} \|v(T) - v_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha_{uw}}{2} \|w(T) - w_\Omega\|^2_{L^2(\Omega)} \\
&+ \frac{\alpha_c}{2} \|c\|^2_{L^2(\Sigma)},
\end{align*}
\] (2)

where the real constants \(\alpha_u, \alpha_v, \alpha_w, \alpha_{uv}, \alpha_{uv}, \alpha_{uw}, \alpha_c\) are nonnegative. The given desired terminal states \(u_Q, v_Q, w_Q, u_\Omega, v_\Omega, w_\Omega\) are elements of \(L^2(Q), L^2(\Omega)\), respectively. This problem belongs to the class of optimization problems with PDF constraints [11], in particular, it is an optimal control problem with semilinear parabolic equation system, to which quite a number of publications were devoted, see e.g., [3, 12]. We note that, for instance, in [15] a nonlinear boundary condition of Stefan-Boltzmann type was considered. The papers [4, 9, 10] studied a nonlinear phase field model, and the papers [2, 14] discussed on the Pontryagin principle for parabolic control problems. Further references on the control of nonlinear parabolic equations can be found in the monographs [3, 11, 16].

The present paper studies the optimal boundary control problems governed by a system of semilinear parabolic PDEs in a very general form. Similar, but more specific optimal control problems were discussed first in the PhD thesis [6] by Griesse and later extended by Griesse and Volkwein [7, 8]. In contrast, we became interested in dealing with more general nonlinearities. Specifically, we consider the optimal
control problems (2) subject to the following class of three-dimensional reaction-diffusion systems with general right-hand terms

\[
\begin{align*}
\frac{\partial u}{\partial t} - d_1 \Delta u + k_1 u & = f_1(t, x, u, v, w), \\
\frac{\partial v}{\partial t} - d_2 \Delta v + k_2 v & = f_2(t, x, u, v, w), \quad (x, t) \in Q, \\
\frac{\partial w}{\partial t} - d_3 \Delta w + k_3 w & = f_3(t, x, u, v, w),
\end{align*}
\]

(3)
together with the Neumann boundary conditions

\[
\begin{align*}
d_1 \partial_n u + b(x, t, u) & = c(t), \\
d_2 \partial_n v + \varepsilon v & = 0, \\
\partial_n w & = 0,
\end{align*}
\]

(4)
the initial conditions

\[
\begin{align*}
u(x, 0) & = u_0(x), \\
v(x, 0) & = v_0(x), \\
w(x, 0) & = w_0(x), \\
x & \in \Omega
\end{align*}
\]

(5)
and the box constraint on control \(c\)

\[
c \in C_{ab} := \{ c \in L^\infty(\Sigma) : c_a \leq c \leq c_b \text{ on } \Sigma \}.
\]

(6)
Here, \(\varepsilon\) is a nonnegative constant. The functions \(c_a, c_b\) are given in \(L^\infty(\Sigma)\) such that \(c_a \leq c_b\) holds almost everywhere in \(\Sigma\). The control \(c(t) \in C_{ab}\) enters the right-hand side of (4), which is the first one in the inhomogeneous Neumann condition.

In [7, 8] Griesse and Volkwein studied system (3) with the following form of \(f_1, f_2, f_3\)

\[
\begin{align*}
f_1(u, v, w) & = -\gamma_1 uv, \\
f_2(u, v, w) & = -\gamma_2 uv, \\
f_3(u, v, w) & = -\gamma_3 uv
\end{align*}
\]

(7)
and added a penalized integral constraint. The cost function \(J(u, v, w, c)\) takes the following form

\[
J(u, v, w, c) = \frac{\alpha_u}{2} \| u(T) - u_0 \|_{L^2(\Omega)}^2 + \frac{\alpha_v}{2} \| v(T) - v_0 \|_{L^2(\Omega)}^2 + \frac{\alpha_w}{2} \| w(T) - w_0 \|_{L^2(\Omega)}^2 + \frac{1}{\varepsilon} \max \left( \int_0^T u(t) dt - u_c \right)^3.
\]

(8)
Under a coercivity condition on the Hessian of the Lagrange function, the optimal value of problem (8) with (7) is shown to be a directionally differentiable function of the perturbation parameters such as the reaction and diffusion constants and initial states. The derivative, termed parametric sensitivity, is characterized as the solution of an auxiliary linear-quadratic optimal control problem.

In [1], Barthel, John, and Tröltzsch considered a class of boundary control problems which are governed by a semi-linear two-dimension reaction-diffusion systems with point-wise control constraints with the following form of \(f_1, f_2\)

\[
\begin{align*}
f_1(u, v, w) & = -\gamma_1 uv, \\
f_2(u, v, w) & = -\gamma_2 uv
\end{align*}
\]

(9)
and, after discussing existence and uniqueness of the state equation with both linear and nonlinear boundary conditions, the existence of an optimal solution is shown. Necessary and sufficient optimality conditions are then derived.
Compared with [1] and [7,8], we consider more general $f_1, f_2,$ and $f_3,$ which allow wider applications of the model. We show the existence and uniqueness of a solution to the system of the state equations (3)-(6) with a general nonlinear form. The existence of a solution to the optimal control problem and necessary and sufficient optimality conditions are also derived.

The article is organized as follows. In Section 2, the state equations are analyzed and the optimal control problem is investigated. Section 3 is devoted to the necessary and sufficient optimality conditions. Some application examples are discussed in Section 4.

2. The existence of the solution for state systems and optimal control problem. In this section, we consider the systems (3)-(6) with nonlinear boundary conditions. To show an existence and uniqueness theorem for the nonlinear system, we invoke the method of ordered upper and lower solutions. This method was also used in [1, 6, 13] for the similar problem with different boundary conditions mentioned in the introduction.

We make the following blanket assumptions.

\[(H)_1:\text{ Functions } f_i(u,v,w) \in C^{1+\alpha}, i = 1, 2, 3 \text{ and satisfy}
\]

(1) the monotonicity assumption: For all $(u,v,w) \in \mathbb{R}_+^3$

$$\frac{\partial f_1}{\partial v}(u,v,w) \leq 0, \quad \frac{\partial f_1}{\partial w}(u,v,w) \leq 0,$$

$$\frac{\partial f_2}{\partial u}(u,v,w) \leq 0, \quad \frac{\partial f_2}{\partial w}(u,v,w) \leq 0,$$

$$\frac{\partial f_3}{\partial u}(u,v,w) \leq 0, \quad \frac{\partial f_3}{\partial v}(u,v,w) \leq 0.$$

(2) the derivative boundedness assumption: There exists constant $C_1 \geq 0$ such that

$$| \frac{\partial f_i}{\partial y_j}(y_1, y_2, y_3) | \leq C_1(| y_1 | + | y_2 | + | y_3 | + 1), \quad i, j = 1, 2, 3.$$

(3) for all $(u, v, w) \in \mathbb{R}_+^3$, there hold

$$f_1(0, 0, 0) = f_2(0, 0, 0) = f_3(0, 0, 0) = 0,$$

$$f_1(u, 0, 0) \leq 0, f_2(0, v, 0) \leq 0, f_3(0, 0, w) \leq 0.$$

\[(H)_2:\text{ The nonlinear function } b : \Sigma \times \mathbb{R} \to \mathbb{R} \text{ is continuous in } (x,t,u) \text{ and monotone non-decreasing with respect to } u \text{ for all } (x,t) \in \Sigma. \text{ Moreover, } b \text{ is twice continuously differentiable with respect to } u \in \mathbb{R} \text{ and } \frac{\partial^2 b(x,t,u)}{\partial u^2} \text{ is locally Lipschitz, i.e. for all } \rho > 0 \text{ there exists } L(\rho) > 0 \text{ such that}
\]

$$| \frac{\partial^2 b}{\partial u^2}(x,t,u_1) - \frac{\partial^2 b}{\partial u^2}(x,t,u_2) | \leq L(\rho)|u_1 - u_2|$$

holds for all $u_1, u_2 \in \mathbb{R}$ with $|u_i| \leq \rho, i = 1, 2$ and for all $(x,t) \in \Sigma.$

\[(H)_3:\text{ The function } b \text{ satisfies } b(x,t,0) \leq c_{\alpha}(x,t) \text{ for all } (x,t) \in \Sigma \text{ and}
\]
\[
\lim_{u \to \infty} \|b(\cdot, \cdot, u)\|_{C(\Omega)} = \infty.
\]

Let
\[
W(0, T) = \{ y \in L^2(0, T; H^1(\Omega)) \mid \partial y / \partial t \in L^2(0, T; H^1(\Omega)^*) \} \tag{10}
\]
We give the definition of a weak solution of system (3)-(5).

**Definition 2.1.** The three functions \((u, v, w) \in (W(0, T))^3\) is said to be a weak solution of systems (3)-(5), if
\[
u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad w(x, 0) = w_0(x), \tag{11}\]
and
\[
\begin{align*}
\langle \partial u / \partial t, \varphi \rangle + \int_{\partial \Omega} b(u) \varphi \, ds dt + d_1 \int_{\Omega} [\nabla u \nabla \varphi + k_1 u - f_1(u, v, w) \varphi] \, dx &= \int_{\partial \Omega} c(t) \varphi \, dx \\
\langle \partial v / \partial t, \varphi \rangle + \int_{\partial \Omega} \varepsilon v \varphi \, ds dt + d_2 \int_{\Omega} [\nabla v \nabla \varphi + k_2 v - f_2(u, v, w) \varphi] \, dx &= 0 \tag{12} \\
\langle \partial w / \partial t, \varphi \rangle + d_3 \int_{\Omega} [\nabla w \nabla \varphi + k_3 w - f_3(u, v, w) \varphi] \, dx &= 0
\end{align*}
\]
hold for all \(\varphi \in H^1(\Omega)\) and almost all \(t \in [0, T]\).

The following theorem ensures that (3)-(5) possesses a unique solution.

**Theorem 2.1.** Assume that \(u_0, v_0, w_0\) are nonnegative functions. Then, for every control \(c \in C_{ab}\), there exists a unique weak solution \((u, v, w) \in (W(0, T))^3\) satisfying (4)-(6).

**Proof.** (i) **Construction of monotone sequences:** Under Assumption \((H)_1\) and \((H)_3\), there exist constants \(M_1\) and \(M_2\), such that,
\[
M \geq \max (M_0, \|u_0\|_{C(\Omega)}, \|v_0\|_{C(\Omega)}, \|w_0\|_{C(\Omega)})
\]
and
\[
b(x, t, M) \geq \|c\|_{L^\infty(\Sigma)}.
\]
and, for all \(y_1, y_2, y_3 \in [0, M]\),
\[
| \frac{\partial f_i}{\partial y_j}(y_1, y_2, y_3) | \leq C_1 (3M + 1) =: M_1, \quad i, j = 1, 2, 3. \tag{13}
\]
holds for all \(c \in C_{ab}\). We now introduce functions \((\tilde{u}, \tilde{v}, \tilde{w})\) and \((\hat{u}, \hat{v}, \hat{w})\): \(\tilde{Q} \to \mathbb{R}\) by
\[
(\tilde{u}, \tilde{v}, \tilde{w}) = (M, M, M), \quad (\hat{u}, \hat{v}, \hat{w}) = (0, 0, 0).
\]
Then, \((\tilde{u}, \tilde{v}, \tilde{w})\) and \((\hat{u}, \hat{v}, \hat{w})\) satisfy

\[
\begin{align*}
0 &\leq \partial \tilde{u}/\partial t - d_1 \triangle \tilde{u} + (k_1 + M_1)\tilde{u} - F_1(t, x, \tilde{u}, 0, 0) \\
&\geq \partial \hat{u}/\partial t - d_1 \triangle \hat{u} + (k_1 + M_1)\hat{u} - F_1(t, x, \hat{u}, 0, 0) \\
0 &\leq \partial \tilde{v}/\partial t - d_2 \triangle \tilde{v} + (k_2 + M_1)\tilde{v} - F_2(t, x, 0, \tilde{v}, 0) \\
&\geq \partial \hat{v}/\partial t - d_2 \triangle \hat{v} + (k_2 + M_1)\hat{v} - F_2(t, x, 0, \hat{v}, 0) \\
0 &\leq \partial \tilde{w}/\partial t - d_3 \triangle \tilde{w} + (k_3 + M_1)\tilde{w} - F_3(t, x, 0, 0, \tilde{w}) \\
&\geq \partial \hat{w}/\partial t - d_3 \triangle \hat{w} + (k_3 + M_1)\hat{w} - F_3(t, x, 0, 0, \hat{w}),
\end{align*}
\]

together with the Neumann boundary conditions \(\forall (x, t) \in \Sigma\)

\[
d_1 \partial_n \tilde{u} - c(x, t) + b(x, t, \tilde{u}) \geq 0 \geq d_2 \partial_n \tilde{v} + \varepsilon \tilde{v} \geq 0 \geq d_2 \partial_n \hat{v} + \varepsilon \hat{v},
\]

\[
\partial_n \tilde{w} \geq 0 \geq \partial_n \hat{w},
\]
and the initial conditions \(\forall x \in \Omega\)

\[
\begin{align*}
\tilde{u}(x, 0) &\geq u_0(x) \geq \hat{u}(x, 0), \\
\tilde{v}(x, 0) &\geq v_0(x) \geq \hat{v}(x, 0), \\
\tilde{w}(x, 0) &\geq w_0(x) \geq \hat{w}(x, 0),
\end{align*}
\]

where \(\alpha > 0\) is taken so large that

\[-b_u(x, t, u) + \alpha \geq 0\]

and

\[F_i(y_1, y_2, y_3) = M_i y_1 + f_i(y_1, y_2, y_3), i = 1, 2, 3.\]

From (H) 1, we have that

\[
\begin{align*}
\partial F_1/\partial u(u, v, w) &\geq 0, \partial F_1/\partial v(u, v, w) \leq 0, \partial F_1/\partial w(u, v, w) \leq 0, \\
\partial F_2/\partial u(u, v, w) &\geq 0, \partial F_2/\partial u(u, v, w) \leq 0, \partial F_2/\partial w(u, v, w) \leq 0,
\end{align*}
\]

\[(17)\]

We adopt the iteration technique introduced in [13] and construct sequences \(\{(\hat{u}^k, \hat{v}^k, \hat{w}^k)\}_{k=0}^{\infty}\) and \(\{(\tilde{u}^k, \tilde{v}^k, \tilde{w}^k)\}_{k=0}^{\infty}\) as follows. We define

\[
(\tilde{u}^0, \tilde{v}^0, \tilde{w}^0) = (M, M, M), (\hat{u}^0, \hat{v}^0, \hat{w}^0) = (0, 0, 0).
\]

Initiating from \((\hat{u}^k, \hat{v}^k, \hat{w}^k)\) and \((\tilde{u}^k, \tilde{v}^k, \tilde{w}^k)\), the pair \((\hat{u}^{k+1}, \hat{v}^{k+1}, \hat{w}^{k+1})\), \((\tilde{u}^{k+1}, \tilde{v}^{k+1}, \tilde{w}^{k+1})\) is obtained by \((\hat{u}^{k+1}, \hat{v}^{k+1}, \hat{w}^{k+1}) = (u^+, v^+, w^+)\) \((\tilde{u}^{k+1}, \tilde{v}^{k+1}, \tilde{w}^{k+1}) = (u^-, v^-, w^-)\) respectively, where \((u^+, v^+, w^+)\) is the solution of the system

\[
\begin{align*}
\partial u^+/\partial t - d_1 \triangle u^+ + (k_1 + M_1)u^+ = F_1(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k), \\
\partial v^+/\partial t - d_2 \triangle v^+ + (k_2 + M_1)v^+ = F_2(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k), \\
\partial w^+/\partial t - d_3 \triangle w^+ + (k_3 + M_1)w^+ = F_3(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k),
\end{align*}
\]

\[(18)\]
together with the Neumann boundary conditions

\[
d_1 \partial_n u^+ + \alpha u^+ = G(x, t, \hat{u}^k),
\]
\[
d_2 \partial_n v^+ + \varepsilon v^+ = 0,
\]
\[
\partial_n w^+ = 0.
\]

and the initial conditions

\[
u^+(x, 0) = u_0(x), v^+(x, 0) = v_0(x), w^+(x, 0) = w_0(x).
\]

\[(u^-, v^-, w^-) \text{ is the solution of the system}
\]
\[
\partial u^- / \partial t - d_1 \triangle u^- + (k_1 + M_1)u^- = F_1(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k),
\]
\[
\partial v^- / \partial t - d_2 \triangle v^- + (k_2 + M_1)v^- = F_2(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k),
\]
\[
\partial w^- / \partial t - d_3 \triangle w^- + (k_3 + M_1)w^- = F_3(t, x, \hat{u}^k, \hat{v}^k, \hat{w}^k),
\]

\[(21)\]

together with the Neumann boundary conditions

\[
d_1 \partial_n u^- + \alpha u^- = G(x, t, \tilde{u}^k), d_2 \partial_n v^- + \varepsilon v^- = 0, \partial_n w^- = 0,
\]

and the initial conditions

\[
u^-(x, 0) = u_0(x), v^-(x, 0) = v_0(x), w^-(x, 0) = w_0(x).
\]

The two systems (18) and (21) are linear parabolic equations in a Lipschitz domain. Therefore, they have solutions in \(Y = (W(0, T) \cap C(Q))^3\). From the compare theorem for nonlinear equation in [16], we obtain as in [1] (or [13]) that the constructed sequences possess the following properties: For each \((x, t) \in Q\), the sequences \\(\{\tilde{(u)^k, \tilde{v}^k, \tilde{w}^k}\}_{k=0}^{\infty}\) are monotone non-increasing and \(\{\hat{(u)^k, \hat{v}^k, \hat{w}^k}\}_{k=0}^{\infty}\) are monotone non-decreasing, respectively. Moreover \(\{(\tilde{u}^k, \tilde{v}^k, \tilde{w}^k)\}_{k=0}^{\infty}\) is for all \(k\) an upper solution while \(\{(\hat{u}^k, \hat{v}^k, \hat{w}^k)\}_{k=0}^{\infty}\) is a lower solution. Moreover, it holds that

\[(\tilde{u}^k, \tilde{v}^k, \tilde{w}^k) \leq (\hat{u}^k, \hat{v}^k, \hat{w}^k), \forall k = 0, 1, \ldots \text{ and } (x, t) \in \bar{Q}.
\]

(ii) Convergence: The sequence \((\tilde{u}^k, \tilde{v}^k, \tilde{w}^k)\) converges uniformly to a solution of systems (3)-(5). This is seen from the following. The sequence \((\tilde{u}^k, \tilde{v}^k, \tilde{w}^k)\) is monotone non-increasing and bounded from below by \(\tilde{u} = \tilde{v} = \tilde{w} = 0\). Therefore, it has a (pointwise) limit \((\tilde{u}(x, t), \tilde{v}(x, t), \tilde{w}(x, t))\). The sequence is also bounded from above by \(M\), hence the Lebesgue dominated convergence theorem implies

\[
\lim_{k \to \infty} \int_Q |\tilde{u}^k(x, t) - \tilde{u}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\]
\[
\lim_{k \to \infty} \int_Q |\tilde{v}^k(x, t) - \tilde{v}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\]
\[
\lim_{k \to \infty} \int_Q |\tilde{w}^k(x, t) - \tilde{w}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\]

\[(24)\]
For the same reason, \( \{(\hat{u}^k, \hat{v}^k, \hat{w}^k)\}_{k=0}^{\infty} \) has a (pointwise) limit \((\hat{u}(x, t), \hat{v}(x, t), \hat{w}(x, t))\)

\[
\lim_{k \to \infty} \int_Q \int |\hat{u}^k(x, t) - \hat{u}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\]

\[
\lim_{k \to \infty} \int_Q \int |\hat{v}^k(x, t) - \hat{v}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\]

\[
\lim_{k \to \infty} \int_Q \int |\hat{w}^k(x, t) - \hat{w}(x, t)|^p \, dx \, dt = 0, \forall 1 \leq p < \infty.
\] (25)

By the same regularity argument as given in [13] the limits in (24) and (25) coincide and yield a solution of systems (3)-(5), and

\[(u(x, t), v(x, t), w(x, t)) \equiv (\hat{u}(x, t), \hat{v}(x, t), \hat{w}(x, t)) = (\hat{u}(x, t), \hat{v}(x, t), \hat{w}(x, t)).\]

(iii) Uniqueness: Let \((u_1, v_1, w_1), (u_2, v_2, w_2) \in Y^3\) be two pairs of weak solutions to systems (4)-(6). Then \((u, v, w) := (u_1 - u_2, v_1 - v_2, w_1 - w_2) \in Y^3\) satisfies \((u(0), v(0), w(0)) = (0, 0, 0)\), and

\[
\langle \partial u / \partial t, \varphi \rangle_{(H^1(\Omega))^\ast, H^1(\Omega)} + \int_{\Omega} [\nabla u \nabla \varphi + k_1 u - (f_1(u_1, v_1, w_1) - f_1(u_2, v_2, w_2)) \varphi] \, dx = 0
\]

\[
d_1 \int_{\Omega} [\nabla v \nabla \varphi + k_2 v - (f_2(u_1, v_1, w_1) - f_2(u_2, v_2, w_2)) \varphi] \, dx = 0
\]

\[
d_2 \int_{\Omega} [\nabla w \nabla \varphi + k_3 w - (f_3(u_1, v_1, w_1) - f_3(u_2, v_2, w_2)) \varphi] \, dx = 0
\]

hold for all \( \varphi \in H^1(\Omega) \) and almost all \( t \in [0, T] \). Choosing \( \varphi = u \) in (26), \( \varphi = v \) in (27), \( \varphi = w \) in (28), and adding all equations, we obtain

\[
\frac{1}{2} \frac{d}{dt} (\|u(t)\|^2_{L^2(\Omega)} + \|v(t)\|^2_{L^2(\Omega)} + \|w(t)\|^2_{L^2(\Omega)}) + d_1 \|u(t)\|^2_{H^1(\Omega)} + d_2 \|v(t)\|^2_{H^1(\Omega)} + d_3 \|w(t)\|^2_{H^1(\Omega)} +
\]

\[
\leq d_1 \|u(t)\|^2_{L^2(\Omega)} + d_2 \|v(t)\|^2_{L^2(\Omega)} + d_3 \|w(t)\|^2_{L^2(\Omega)} +
\]

\[
+ \int_{\Omega} (f_1(u_1, v_1, w_1) - f_1(u_2, v_2, w_2))(u_1 - u_2) \, dx +
\]

\[
+ \int_{\Omega} (f_2(u_1, v_1, w_1) - f_2(u_2, v_2, w_2))(v_1 - v_2) \, dx +
\]

\[
+ \int_{\Omega} (f_3(u_1, v_1, w_1) - f_3(u_2, v_2, w_2))(w_1 - w_2) \, dx +
\] (29)
for almost all $t \in [0,T]$ because $d_i \geq 0$, $i = 1, 2, 3$ and the monotonicity of $b$ with respect to $u$ implies

$$
\int_{\partial \Omega} [b(u_1) - b(u_2)](u_1 - u_2) ds dt \geq 0
$$

From $(H)_1$, we have that

$$
| f_1(u_1, v_1, w_1) - f_1(u_2, v_2, w_2) | \leq | \frac{\partial}{\partial u} f_1(\zeta, v_1, w_1)(u_1 - u_2) | + \\
+ | \frac{\partial}{\partial v} f_1(u_2, \xi, w_1)(v_1 - v_2) | + | \frac{\partial}{\partial w} f_1(u_2, \varsigma, w_1)(w_1 - w_2) | \leq C(| u_1 - u_2 | + | v_1 - v_2 | + | w_1 - w_2 |),
$$

where $(\zeta, \xi, \varsigma) \in [0,M]^3$. We have the same inequality for $f_2, f_3$:

$$
| f_2(u_1, v_1, w_1) - f_2(u_2, v_2, w_2) | \leq C_3(| u_1 - u_2 | + | v_1 - v_2 | + | w_1 - w_2 |)
$$

and

$$
| f_3(u_1, v_1, w_1) - f_3(u_2, v_2, w_2) | \leq C_4(| u_1 - u_2 | + | v_1 - v_2 | + | w_1 - w_2 |),
$$

where $C_i, i = 2, 3, 4$ are constants. Hence, (29) becomes

$$
\frac{1}{2} \frac{d}{dt} (\| u(t) \|_{L^2(\Omega)}^2 + \| v(t) \|_{L^2(\Omega)}^2 + \| w(t) \|_{L^2(\Omega)}^2) + d_1 \| u(t) \|_{H^1(\Omega)}^2 + d_2 \| v(t) \|_{H^1(\Omega)}^2 + d_3 \| w(t) \|_{H^1(\Omega)}^2 \leq C(\| u(t) \|_{L^2(\Omega)}^2 + \| v(t) \|_{L^2(\Omega)}^2 + \| w(t) \|_{L^2(\Omega)}^2)
$$

where $C$ is a constants. From the Gronwalls inequality, we have $(u, v, w) = (0, 0, 0)$. \hfill \square

We next present sufficient conditions so that the $L^2$-norm of the sum of concentrations $u, v, w$ does not increase with time.

**Proposition 2.1.** Suppose that

$$(H)_4: \quad d_1 = d_2 = d_3, f_1(u, v, w) + f_2(u, v, w) + f_3(u, v, w) \leq 0$$

(34)

Let $(u, v, w) \in (W(0,T))^3$ be the solution to systems (3)-(5). Then, we have

$$
\| u(t) + v(t) + w(t) \|_{L^2(\Omega)} \leq \| u_0 + v_0 + w_0 \|_{L^2(\Omega)}
$$

for almost all $t \in [0,T]$.

The proof is similar to the proof of theorem 2.1. We omit it. The following theorem guarantees that problem (2)-(6) has a solution.

**Theorem 2.2.** Problem (2)-(6) possesses at least one optimal control.
Proof. The claim follows by standard arguments. Let

\[ \{y^n = (u^n, v^n, w^n, c^n)\}_{n=1}^{\infty} \]

be a minimizing sequence in \( C_{ad} \) for the non-negative cost \( J \). Since \( J \) is radially unbounded, it follows from Theorem 2.1 that this sequence is bounded in \( X := (W(0, T))^3 \times L^2(0, T) \).

Therefore, there exists an element \( y^* = (u^*, v^*, w^*, c^*) \in X \), such that

\[ (u^n, v^n, w^n, c^n) \rightharpoonup (u^*, v^*, w^*, c^*) \text{ in } X, \text{ as } n \to \infty \]  

(36)

First, we consider the nonlinear terms. Using Holder’s inequality, we infer that for \( \varphi \in L^2(0, T; H^1(\Omega)) \)

\[
\begin{align*}
&\int_0^T \int_\Omega [f_1(u^n, v^n, w^n) - f_1(u^*, v^*, w^*)] \varphi \, dx \, dt \\
&\quad = \int_0^T \int_\Omega \left[ \frac{\partial f_1}{\partial u}(u^n(\zeta), v^n, w^n)(u^n - u^*) + \\
&\quad \quad + \frac{\partial f_1}{\partial v}(u^*, v^n(\xi), w^n)(v^n - v^*) + \\
&\quad \quad + \frac{\partial f_1}{\partial w}(u^*, v^*, w^n(\varsigma))(w^n - w^*) \right] \varphi \\
\end{align*}
\]

(37)

where \( \zeta, \xi, \) and \( \varsigma \) are functions between \( u^n \) and \( u^* \), \( v^n \) and \( v^* \), and \( w^n \) and \( w^* \), respectively. From \((H)_1\), we have that

\[
\begin{align*}
&\int_0^T \int_\Omega [f_1(u^n, v^n, w^n) - f_1(u^*, v^*, w^*)] \varphi \, dx \, dt \\
&\quad \leq C \left[ \|u^n - u^*\|_{L^2(0, T; L^3(\Omega))} + \|v^n - v^*\|_{L^2(0, T; L^3(\Omega))} + \|w^n - w^*\|_{L^2(0, T; L^3(\Omega))} \right] \\
&\quad + \int_0^T \int_\Omega \left[ \frac{\partial f_1}{\partial u}(u^n(\zeta), v^n, w^n) \right] \varphi \, dx \, dt \\
&\quad \leq C [\|u^n - u^*\|_{L^2(0, T; L^3(\Omega))} + \|v^n - v^*\|_{L^2(0, T; L^3(\Omega))} + \|w^n - w^*\|_{L^2(0, T; L^3(\Omega))}] \\
\end{align*}
\]

(38)

Thus, from (36) we obtain that

\[
\begin{align*}
&\lim_{n \to \infty} \int_0^T \int_\Omega [f_1(u^n, v^n, w^n) - f_1(u^*, v^*, w^*)] \varphi \, dx \, dt = 0, \\
\forall \varphi &\in L^2(0, T; H^1(\Omega))
\end{align*}
\]

(39)
Similarly, we have that
\[
\lim_{n \to \infty} \int_0^T \int_\Omega f_2(u^n, v^n, w^n) - f_2(u^*, v^*, w^*) \phi \, dx \, dt = 0, \quad \forall \phi \in L^2(0, T; H^1(\Omega))
\]
\[
(40)
\]
\[
\lim_{n \to \infty} \int_0^T \int_\Omega f_3(u^n, v^n, w^n) - f_3(u^*, v^*, w^*) \phi \, dx \, dt = 0, \quad \forall \phi \in L^2(0, T; H^1(\Omega))
\]
\[
(41)
\]
and
\[
\lim_{n \to \infty} \int_0^T \left( \int_{\partial \Omega} (b(x, t, u^n(t)) - b(x, t, u^*(t))) \varphi(t) \right) dt = 0, \quad \forall \varphi \in L^2(0, T; H^1(\Omega)).
\]
\[
(42)
\]
For all \( \varphi \in L^2(0, T; H^1(\Omega)) \), we have
\[
\lim_{n \to \infty} \int_0^T \langle \partial(u^n - u^*)/\partial t, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} = 0,
\]
\[
(43)
\]
\[
\lim_{n \to \infty} \int_0^T \langle \partial(v^n - v^*)/\partial t, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} = 0,
\]
\[
(44)
\]
\[
\lim_{n \to \infty} \int_0^T \langle \partial(w^n - w^*)/\partial t, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} = 0
\]
\[
(45)
\]
\[
\lim_{n \to \infty} \int_\Omega \int_0^T d_1 \nabla(u^n - u^*)(t) \nabla \varphi(t) \, dx \, dt = 0,
\]
\[
(46)
\]
\[
\lim_{n \to \infty} \int_\Omega \int_0^T d_2 \nabla(v^n - v^*)(t) \nabla \varphi(t) \, dx \, dt = 0,
\]
\[
(47)
\]
\[
\lim_{n \to \infty} \int_\Omega \int_0^T d_3 \nabla(w^n - w^*)(t) \nabla \varphi(t) \, dx \, dt = 0.
\]
\[
(48)
\]
Notice that
\[
\lim_{n \to \infty} \int_\Omega (u^n - u^*)(0) \varphi \, dx = 0,
\]
\[
\lim_{n \to \infty} \int_\Omega (v^n - v^*)(0) \varphi \, dx = 0,
\]
\[
\lim_{n \to \infty} \int_\Omega (w^n - w^*)(0) \varphi \, dx = 0.
\]
\[
(49)
\]
Since \( C_{ab} \) is bounded, closed, and convex, \( C_{ad} \) is also weakly closed. As \( J \) is weakly lower semi-continuous, the claim follows. \( \square \)
3. **Necessary and sufficient optimality conditions.** Let $S : c \to (u, v, w)$ be the control-to-state operator with $S : L^r(\Sigma) \to Y^3$, where we fix $r > N + 1$ throughout the following. Since the cost functional is quadratic, we obtain the next lemma by standard arguments.

**Lemma 3.1.** The cost functional $J$ is continuously Fréchet-differentiable from $Y \times Y \times L^r(\Sigma) \to \mathbb{R}$.

On the twice continuously Fréchet-differentiability of the operator $S$, we have that

**Theorem 3.1.** The control-to-state operator $S$ is twice continuously Fréchet-differentiable from $L^r(\Sigma)$ to $Y^3$.

**Proof.** First, by establishing linear and continuous solution operators

\[
S_{uQ}, S_{vQ}, S_{wQ} : L^r(Q) \to Y,
S_{u\Sigma} : L^r(\Sigma) \to Y,
S_{u0}, S_{v0}, S_{w0} : C(\bar{\Omega}) \to Y,
\]

which are associated with the following linear problem $\forall x \in Q$,

\[
\begin{align*}
\frac{\partial u}{\partial t} - d_1 \Delta u &= \psi_u, \\
\frac{\partial v}{\partial t} - d_2 \Delta v &= \psi_v, \\
\frac{\partial w}{\partial t} - d_3 \Delta w &= \psi_w,
\end{align*}
\]

with the boundary conditions, $\forall (x, t) \in \Sigma$

\[
\frac{\partial n}{\partial u} = \lambda_u, \frac{\partial n}{\partial v} = \lambda_v, \frac{\partial n}{\partial w} = \lambda_w,
\]

and the initial conditions, $\forall x \in \Omega$

\[
u(x, 0) = u_0(x), v(x, 0) = v_0(x), w(x, 0) = w_0(x),
\]

in the following sense.

\[
\begin{align*}
S_{uQ} & : \psi_u \mapsto u \text{ with } \lambda_u = 0, u_0(x) = 0; \\
S_{u\Sigma} & : \lambda_u \mapsto u \text{ with } \psi_u = 0, u_0(x) = 0; \\
S_{u0} & : u_0 \mapsto u \text{ with } \psi_u = 0, \lambda_u = 0.
\end{align*}
\]

Analogously,

\[
\begin{align*}
S_{vQ} & : \psi_v \mapsto v \text{ with } \lambda_v = 0, v_0(x) = 0; \\
S_{v\Sigma} & : \lambda_v \mapsto v \text{ with } \psi_v = 0, v_0(x) = 0; \\
S_{v0} & : v_0 \mapsto v \text{ with } \psi_v = 0, \lambda_v = 0.
\end{align*}
\]
We consider these operators with image in $C(\bar{Q})$ and reformulate the nonlinear system of (3) as

\[
0 = u - S_{uQ}(f_1(t, x, u, v, w)) - S_{u\Sigma}(c(x, t) - b(x, t, u))
\]

(56)

\[
0 = v - S_{uQ}(f_2(t, x, u, v, w)) - S_{vQ}(v_0) =: F_2(u, v, w, c);
\]

(57)

\[
0 = w - S_{uQ}(f_3(t, x, u, v, w)) - S_{wQ}(w_0) =: F_3(u, v, w, c).
\]

Since $S_{uQ}, S_{u\Sigma}, S_{wQ}, S_{vQ}, S_{v0}, S_{wQ},$ and $S_{w0}$ are linear and continuous and $f_i(t, x, u, v, w)(i = 1, 2, 3), b(x, t, u)$ are twice continuously Fréchet-differentiable, $F_i(i = 1, 2, 3)$ is a twice continuously Fréchet-differentiable mapping from $(C(\bar{Q}))^3 \times L^r(\Sigma)$ to $C(\bar{Q})$.

To use the implicit function theorem, we have to show the boundedness and continuous invertibility of the partial Fréchet derivative $F(u, v, w, c) = (F_1, F_2, F_3)^T$. To verify these properties, we first mention that the equation $F_{u,w,w}(u, v, w, c)y = z, y = (y_1, y_2, y_3), z = (z_1, z_2, z_3)$ is equivalent to the system

\[
(F_{1u}, F_{1w}, F_{1w})(y_1, y_2, y_3)^T = z_1
\]

(58)

\[
(F_{2u}, F_{2w}, F_{2w})(y_1, y_2, y_3)^T = z_2
\]

\[
(F_{3u}, F_{3w}, F_{3w})(y_1, y_2, y_3)^T = z_3
\]

i.e.,

\[
y_1 - S_{uQ}(f_1y_1 + f_1y_2 + f_1y_3) + S_{u\Sigma}b_y = z_1
\]

(59)

\[
y_2 - S_{vQ}(f_2y_1 + f_2y_2 + f_2y_3) = z_2
\]

\[
y_3 - S_{wQ}(f_3y_1 + f_3y_2 + f_3y_3) = z_3
\]

Since the mapping $z \mapsto y$ is not smooth, we substitute $r_i = z_i - y_i, i = 1, 2$, to obtain the equivalent system

\[
\partial r_1/\partial t - d_1 \triangle r_1 + f_1 r_1 + f_1 r_2 + f_1 r_3 = f_1 u y_1 + f_1 v y_2 + f_1 w y_3,
\]

(60)

\[
\partial r_2/\partial t - d_2 \triangle r_2 + f_2 r_1 + f_2 r_2 + f_2 r_3 = f_2 u y_2 + f_2 v y_2 + f_2 w y_3,
\]

\[
\partial r_3/\partial t - d_3 \triangle r_3 + f_3 r_1 + f_3 r_2 + f_3 r_3 = f_3 u y_1 + f_3 v y_2 + f_3 w y_3,
\]

together with the Neumann boundary conditions

\[
\partial_n r_1 + b_u(x, t, u)r_1 = c(t) + b_u(x, t, u)z_1, \quad \partial_n r_2 = 0, \quad \partial_n r_3 = 0.
\]
and the initial conditions

\[ r_1(x, 0) = 0, r_2(x, 0) = 0, r_3(x, 0) = 0. \]  

(62)

For every \( z \in (C(\overline{Q}))^3 \), this linear boundary value problem has a unique solution \( r \in Y^3 \) cf. e.g., Theorem 5.5 in [1]. The mapping \( z \to r \) is continuous, so is the mapping \( z \to y \). Therefore, we can invoke the implicit function theorem and obtain that the control-to-state operator \( S \) is twice continuously Fréchet differentiable. \( \square \)

**Corollary 3.1.** The derivative of the control-to-state operator \( S \) at \( \overline{c} \) in direction \( c \) is given by

\[ S'(\overline{c})c = (u, v, w) \]  

(63)

where \((u, v, w)\) is the weak solution of the linearized equation obtained by linearizing system (4) at \( S(\overline{c}) = (\overline{u}, \overline{v}, \overline{w}) \)

\[ \begin{align*}
\frac{\partial u}{\partial t} - d_1 \Delta u &= f_{1u}(\overline{u}, \overline{v}, \overline{w})u + f_{1v}(\overline{u}, \overline{v}, \overline{w})v + f_{1w}(\overline{u}, \overline{v}, \overline{w})w, \\
\frac{\partial v}{\partial t} - d_2 \Delta v &= f_{2u}(\overline{u}, \overline{v}, \overline{w})u + f_{2v}(\overline{u}, \overline{v}, \overline{w})v + f_{2w}(\overline{u}, \overline{v}, \overline{w})w, \\
\frac{\partial w}{\partial t} - d_3 \Delta w &= f_{3u}(\overline{u}, \overline{v}, \overline{w})u + f_{3v}(\overline{u}, \overline{v}, \overline{w})v + f_{3w}(\overline{u}, \overline{v}, \overline{w})w,
\end{align*} \]  

(64)

together with the Neumann boundary conditions

\[ \partial_n u + b_u(x, t, \overline{u})u = c(t), \quad \partial_n v = 0, \quad \partial_n w = 0, \]  

(65)

and the initial conditions

\[ u(x, 0) = 0, \quad v(x, 0) = 0, \quad w(x, 0) = 0. \]  

(66)

**Proof.** Let us briefly sketch the proof and omit the details. The system (4) is of the form

\[ A(S(c)) = B(S(c)) + C(S(c)) + y_0. \]  

(67)

where

\[ \begin{align*}
S(c) &= (u(c), v(c), w(c)), \\
A &= \left( \begin{array}{ccc}
\frac{\partial}{\partial t} - d_1 \Delta, & \frac{\partial}{\partial t} - d_2 \Delta, & \frac{\partial}{\partial t} - d_3 \Delta \end{array} \right)^T, \\
B(u, v, w) &= (f_1(u, v, w), f_2(u, v, w), f_3(u, v, w))^T, \\
C(u, v, w) &= (-b(u) + c, 0, 0)^T, \\
y_0 &= (u_0, v_0, w_0)^T.
\end{align*} \]  

(68)

Therefore there holds

\[ A(S'(c))c_1 = B'(S(c))S'(c)c_1 + C'(S(c))S'(c)c_1, \]  

(69)
where

\[ B'(\bar{u}, \bar{v}, \bar{w}) = (f_{1u}(\bar{u}, \bar{v}, \bar{w}) + f_{1v}(\bar{u}, \bar{v}, \bar{w}) + f_{1w}(\bar{u}, \bar{v}, \bar{w})u. \]

\[ f_{2u}(\bar{u}, \bar{v}, \bar{w}) + f_{2v}(\bar{u}, \bar{v}, \bar{w}) + f_{2w}(\bar{u}, \bar{v}, \bar{w})u, \]

\[ f_{3u}(\bar{u}, \bar{v}, \bar{w}) + f_{3v}(\bar{u}, \bar{v}, \bar{w}) + f_{3w}(\bar{u}, \bar{v}, \bar{w})u. \]

\[ C'(\bar{u}, \bar{v}, \bar{w}) = (-b_u(\bar{u}) u, 0, 0)^T, \]

\[ S'(c) c_1 = (u, v, w). \]

Similarly, we can obtain the second-order derivative of \( S \). Let

\[ f(c) := J(u(c), v(c), w(c), c) = J(S(c), c). \]

**Corollary 3.2**  The second-order derivative of \( S \) at \( \bar{c} \) in direction (\( \hat{c}, \hat{c} \)) is given by

\[ S''(c)(\hat{c}, \hat{c}) = (u, v) \] (71)

where \((u, v, w)\) is the weak solution of the system (where \((x, t) \in Q\))

\[ \frac{\partial u}{\partial t} - d_1 \Delta u = f_{1u}(\bar{u}, \bar{v}, \bar{w}) + f_{1v}(\bar{u}, \bar{v}, \bar{w}) + f_{1w}(\bar{u}, \bar{v}, \bar{w})u \]

\[ + f_{1uv}(\bar{u} + \bar{v}) + f_{1uw}(\bar{u} + \bar{w}) + f_{1vw}(\bar{v} + \bar{w}) \]

\[ \frac{\partial v}{\partial t} - d_2 \Delta v = f_{2u}(\bar{u}, \bar{v}, \bar{w}) + f_{2v}(\bar{u}, \bar{v}, \bar{w}) + f_{2w}(\bar{u}, \bar{v}, \bar{w})u \]

\[ + f_{2uv}(\bar{u} + \bar{v}) + f_{2uw}(\bar{u} + \bar{w}) + f_{2vw}(\bar{v} + \bar{w}) \]

\[ \frac{\partial w}{\partial t} - d_3 \Delta w = f_{3u}(\bar{u}, \bar{v}, \bar{w}) + f_{3v}(\bar{u}, \bar{v}, \bar{w}) + f_{3w}(\bar{u}, \bar{v}, \bar{w})u \]

\[ + f_{3uv}(\bar{u} + \bar{v}) + f_{3uw}(\bar{u} + \bar{w}) + f_{3vw}(\bar{v} + \bar{w}) \]

together with the Neumann boundary conditions (where \((x, t) \in \Sigma\))

\[ \frac{\partial u}{\partial n} + b_u(x, t, \bar{u}) u = -b_u(\bar{u}) \bar{u}, \quad \frac{\partial v}{\partial n} = 0, \quad \frac{\partial w}{\partial n} = 0. \] (73)

and the initial conditions (where \(x \in \Omega\))

\[ u(x, 0) = 0, \quad v(x, 0) = 0, \quad w(x, 0) = 0. \] (74)

**Proof.** Differentiating (74) with respect to \( c \) in direction \( c_2 \) yields

\[ A(S''(c)) [c_1, c_2] = B'(S(c)) S''(c)[c_1, c_2] + B''(S(c)) [S'(c) c_1, S'(c) c_2] \]

\[ + C'(S(c)) S''(c)[c_1, c_2] + C''(S(c)) [S'(c) c_1, S'(c) c_2], \] (75)
where

\[ c_1 = \hat{c}, \quad c_2 = \hat{c}; \]
\[ (u, v, w) = S''(c)[c_1, c_2] \]
\[ (\hat{u}, \hat{v}, \hat{w}) = S'(c)c_1 \]
\[ (\hat{\hat{u}}, \hat{\hat{v}}, \hat{\hat{w}}) = S'(c)c_2. \]

Notice that

\[ B''(u, v, w)[(\hat{u}, \hat{v}, \hat{w}), (\hat{\hat{u}}, \hat{\hat{v}}, \hat{\hat{w}})] = (B_1'', B_2'', B_3'')^T \]

where

\[ B_1'' = f_{1uu}\hat{u}\hat{u} + f_{1vv}\hat{v}\hat{v} + f_{1ww}\hat{w}\hat{w} + f_{1v}\hat{v}(\hat{u}\hat{v} + \hat{\hat{u}}\hat{\hat{v}}) + f_{1w}\hat{w}(\hat{u}\hat{w} + \hat{\hat{u}}\hat{\hat{w}}) \]
\[ B_2'' = f_{2uu}\hat{u}\hat{u} + f_{2vv}\hat{v}\hat{v} + f_{2ww}\hat{w}\hat{w} + f_{2v}\hat{v}(\hat{u}\hat{v} + \hat{\hat{u}}\hat{\hat{v}}) + f_{2w}\hat{w}(\hat{u}\hat{w} + \hat{\hat{u}}\hat{\hat{w}}) \]
\[ B_3'' = f_{3uu}\hat{u}\hat{u} + f_{3vv}\hat{v}\hat{v} + f_{3ww}\hat{w}\hat{w} + f_{3v}\hat{v}(\hat{u}\hat{v} + \hat{\hat{u}}\hat{\hat{v}}) + f_{3w}\hat{w}(\hat{u}\hat{w} + \hat{\hat{u}}\hat{\hat{w}}) \]

and

\[ C''(\hat{u}, \hat{v}, \hat{w})S''(c)[c_1, c_2] = (-b_u(u)0, 0)^T, \]
\[ C''(\hat{\hat{u}}, \hat{\hat{v}}, \hat{\hat{w}})[S'(c)c_1, S'(c)c_2] = (-b_u(u)\hat{u}\hat{u}, 0, 0)^T. \]

From (70), (72), and (78), we have that \( \forall (x, t) \in Q \)
\[ \partial u/\partial t - d_1\Delta u = f_{1u}(\hat{u}, \hat{v}, \hat{w})u + f_{1v}(\hat{u}, \hat{v}, \hat{w})v + f_{1w}(\hat{u}, \hat{v}, \hat{w})w + B''_1, \]
\[ \partial v/\partial t - d_2\Delta v = f_{2u}(\hat{u}, \hat{v}, \hat{w})u + f_{2v}(\hat{u}, \hat{v}, \hat{w})v + f_{2w}(\hat{u}, \hat{v}, \hat{w})w + B''_2, \]
\[ \partial w/\partial t - d_3\Delta w = f_{3u}(\hat{u}, \hat{v}, \hat{w})u + f_{3v}(\hat{u}, \hat{v}, \hat{w})v + f_{3w}(\hat{u}, \hat{v}, \hat{w})w + B''_3. \]

The proof is completed. \( \square \)

To formulate necessary optimality conditions, let \( \hat{c} \) be an optimal control of (2)-(6) with states \((\hat{u}, \hat{v}, \hat{w})\). Then we have \((u, v, w) = S(c)\). Let us write for short \( y = (u, v, w), \bar{y} = (\hat{u}, \hat{v}, \hat{w})\). We can obtain the following standard result.

**Lemma 3.2.** (cf. [16]). Every locally optimal control function \( \hat{c} \) of (2)-(6) satisfies the variational inequality

\[ f'(\hat{c})(c - \hat{c}) \geq 0, \forall c \in C_{ab}. \]
We determine $f'$ by the chain rule and obtain for the direction $c$

$$
f'(c)c = \int_0^T \int_\Omega (\alpha_u(\bar{u} - u_Q)u + \alpha_v(\bar{v} - v_Q)v + \alpha_w(\bar{w} - w_Q)w)dxdt + \int_\Omega (\alpha_{TV}(\bar{u}(T) - u_{QT})u(T) + \alpha_{TV}(\bar{v}(T) - v_{QT})v(T) + \alpha_{TW}(\bar{w}(T) - w_{QT})w(T))dt + \int_\Sigma \alpha_c ccdsdt.
$$

In the next, we eliminate the states $u$ and $v$ in (82) by adjoint states $(\varphi_1, \varphi_2, \varphi_3)$, defined as the solutions of the adjoint system

$$
\begin{align*}
-\partial \varphi_1/\partial t - d_1 \Delta \varphi_1 &= f_{1u} (\bar{u}, \bar{v}, \bar{w}) \varphi_1 + f_{2u} (\bar{u}, \bar{v}, \bar{w}) \varphi_2 + f_{3u} (\bar{u}, \bar{v}, \bar{w}) \varphi_3 + \alpha_u (\bar{u} - u_Q), \\
-\partial \varphi_2/\partial t - d_2 \Delta \varphi_2 &= f_{1v} (\bar{u}, \bar{v}, \bar{w}) \varphi_1 + f_{2v} (\bar{u}, \bar{v}, \bar{w}) \varphi_2 + f_{3v} (\bar{u}, \bar{v}, \bar{w}) \varphi_3 + \alpha_v (\bar{v} - v_Q), \\
-\partial \varphi_3/\partial t - d_3 \Delta \varphi_3 &= f_{1w} (\bar{u}, \bar{v}, \bar{w}) \varphi_1 + f_{2w} (\bar{u}, \bar{v}, \bar{w}) \varphi_2 + f_{3w} (\bar{u}, \bar{v}, \bar{w}) \varphi_3 + \alpha_w (\bar{w} - w_Q),
\end{align*}
$$

with the boundary conditions

$$
\partial_n \varphi_1 + b_u (x, t, \bar{u}) \varphi_1 = 0, \quad \partial_n \varphi_2 = 0, \quad \partial_n \varphi_3 = 0
$$

and the initial conditions

$$
\varphi_1 (x, T) = \alpha_{TV} (u(x, T) - u_{\Omega}(x)), \quad \varphi_2 (x, T) = \alpha_{TV} (v(x, T) - v_{\Omega}(x)), \quad \varphi_3 (x, T) = \alpha_{TW} (w(x, T) - w_{\Omega}(x)).
$$

**Lemma 3.3.** If $(u, v, w)$ is the weak solution of the linearized system (64)-(66) and $(\varphi_1, \varphi_2, \varphi_3)$ is the solution of the adjoint system (83)-(85), then it holds for all $c \in L'(\Sigma)$ that

$$
\int_\Sigma \varphi_1 (c - \bar{c}) ds dt = \int_0^T \int_\Omega (\alpha_u(\bar{u} - u_Q)u + \alpha_v(\bar{v} - v_Q)v + \alpha_w(\bar{w} - w_Q)w)dxdt + \int_\Omega (\alpha_{TV}(\bar{u}(T) - u_{QT})u(T) + \alpha_{TV}(\bar{v}(T) - v_{QT})v(T) + \alpha_{TW}(\bar{w}(T) - w_{QT})w(T))dt
$$

From this lemma and (82), we can obtain that

$$
f'(c)c = \int_\Sigma (\varphi_1 + \alpha_c \bar{c}) ds dt.
$$

It follows that
Theorem 3.2. Every locally optimal solution $\tilde{c}$ of (2)-(6) satisfies, together with the adjoint states $(\varphi_1, \varphi_2, \varphi_3)$ of the adjoint system (83)-(85), the variational inequality

$$\int \int_{\Sigma} (\varphi_1 + \alpha_c \tilde{c})(c - \tilde{c})dsdt \geq 0, \quad \forall c \in C_{ab}. \quad (88)$$

An equivalent pointwise expression of this variational inequality is

$$\min_{c_a(x,t) \leq c \leq c_b(x,t)} (\varphi_1(x,t) + \alpha_c \tilde{c}(x,t))c = (\varphi_1(x,t) + \alpha_c \tilde{c}(x,t))\tilde{c}(x,t), \quad (89)$$

which leads in a standard way to the projection formula

$$\tilde{c}(x,t) = P_{[c_a(x,t), c_b(x,t)]} \left\{ \frac{\varphi_1(x,t)}{\alpha_c} \right\} \quad (90)$$

for almost all $(x,t) \in \Sigma$, where $P_{[c_a(x,t), c_b(x,t)]: \mathbb{R} \to [c_a(x,t), c_b(x,t)]}$ denotes the projection onto $[c_a(x,t), c_b(x,t)]$.

Next, we consider the sufficient second order optimality conditions for (2)-(6) . By the chain rule, we derive for $y = (u, v, w)$ that

$$f'(c)\tilde{c} = D_y J(S(c), c)S'(c)\tilde{c} + D_c J(S(c), c)\tilde{c} \quad (91)$$

The derivative of $f'(c)\tilde{c}$ with respect to $c$ in direction $\tilde{c}$ is

$$f''(c)[\tilde{c}, \tilde{c}] = J''(S(c), c)S'(c)[(\tilde{y}, \tilde{c}), (\tilde{y}, \tilde{c})] + D_y J(S(c), c)S''(c)[\tilde{c}, \tilde{c}] \quad (92)$$

and

$$D_y J(y, c)z = \int_0^T \int_{\Omega} (\alpha_u (\dot{u} - u_Q)z_1 + \alpha_v (\dot{v} - v_Q)z_2 + \alpha_w (\dot{w} - w_Q)z_3)dxdt + \int_{\Omega} (\alpha_{uT}(\dot{u}(T) - u_{QT})z_1(T) + \alpha_{vT}(\dot{v}(T) - v_{QT})z_1(T) + \alpha_{wT}(\dot{w}(T) - w_{QT})z_3(T))dt. \quad (93)$$

Therefore, we have

$$D_y J(y, c)z = \int_0^T \int_{\Omega} [B''_1 \varphi_1 + B''_2 \varphi_2 + B''_3 \varphi_3]dxdt - \int_{\Sigma} \int_{\Omega} \varphi_1 b_{uw} \dot{u} \ddot{u} dsdt \quad (94)$$

by using the adjoint states $(\varphi_1, \varphi_2, \varphi_3)$. We then deduce

$$f''(c)[\tilde{c}, \tilde{c}] = J''(S(c), c)S'(c)[(\tilde{y}, \tilde{c}), (\tilde{y}, \tilde{c})] + \int_0^T \int_{\Omega} [B''_1 \varphi_1 + B''_2 \varphi_2 + B''_3 \varphi_3]dxdt - \int_{\Sigma} \int_{\Omega} \varphi_1 b_{uw} \ddot{u} dsdt. \quad (95)$$
To formulate our sufficient optimality conditions in a more convenient form, we introduce the Lagrange function

\[ \mathcal{L}(u, v, w, c, \varphi_1, \varphi_2, \varphi_3) = J(u, v, w, c) + \int_Q (u_t - f_1(u, v, w)) \varphi_1 \, dx \, dt + \int_Q d_1 \nabla u \nabla \varphi_1 \, dx \, dt + \int_Q (b(x, t, u) - c) \varphi_1 \, ds \, dt + \int_\Omega (u(x, 0) - u_0) \varphi_1 \, dx \]

(96)

In view of (93), we obtain

\[ \mathcal{L}''(u, v, w, c, \varphi_1, \varphi_2, \varphi_3)(u, v, w, c) = f''(c)(u, v, w, c), \quad (u, v, w) \in Y \]

(97)

To obtain the second-order sufficient conditions, \( \forall \tau > 0 \), we define

\[ A_\tau(c) := \{(x, t) \in \Sigma : |\varphi_1 + \alpha_x c| > \tau \} \]

as the set of strongly active restrictions for \( \bar{c} \). The \( \tau \)-critical cone \( C_\tau(\bar{c}) \) is made up of all \( c \in L^\infty(\Sigma) \) with

\[
c(x, t) = 0, \quad (x, t) \in A_\tau(\bar{c}),
\]

\[
c(x, t) \geq 0, \text{ for } \bar{c}(x, t) = c_a, \text{ and } (x, t) \in A_\tau(\bar{c}),
\]

\[
c(x, t) \leq 0, \text{ for } \bar{c}(x, t) = c_b, \text{ and } (x, t) \in A_\tau(\bar{c}).
\]

We have the following second-order sufficient conditions.

**Theorem 3.3.** (Second-order sufficient conditions). Suppose that the control function \( \bar{c} \) satisfies the first-order necessary optimality conditions of Theorem 3.2. If there exist positive constants \( \delta \) and \( \tau \) such that

\[ \mathcal{L}''(\bar{u}, \bar{v}, \bar{w}, \bar{c}, \varphi_1, \varphi_2, \varphi_3)(u, v, w, c)^2 \geq \delta \|c\|^2_{L^2(0, T)} \]

(98)

holds for all \( c \in C_\tau(\bar{c}) \) and all \( (u, v, w) \in Y^3 \) satisfying the linearized equation (64)-(66), then we find positive constants \( \varepsilon \) and \( \sigma \) such that the quadratic growth condition

\[ J(u, v, w, c) \geq J(\bar{u}, \bar{v}, \bar{w}, \bar{c}) + \sigma \|c - \bar{c}\|^2_{L^2(\Sigma)} \]

(99)
holds for all $c \in C_{ab}$ with $\|c - \bar{c}\|_{L^\infty(\Sigma)}$. Therefore, the control function $\bar{c}$ is locally optimal in the sense of $L^\infty(\Sigma)$.

4. Applications. In this section, we present some examples for application of the model (2)-(5).

Example 1. Consider the systems (2)-(5) with following form of $f_1, f_2, f_3, b(x, t, u)$:

\begin{align}
  f_1 &= -u(b_1 v + c_1 w), \\
  f_2 &= -v(b_2 u + c_2 w), \\
  f_3 &= -w(b_3 u + c_3 v), \\
  b(x, t, u) &= u,
\end{align}

(100)

$\forall (x, t) \in \Omega$

$$
\begin{align*}
  d_1 \partial_n u - u &= c(t), \\
  d_2 \partial_n v + \varepsilon v &= 0, \\
  \partial_n w &= 0,
\end{align*}
$$

(102)

and the initial conditions $\forall x \in \Omega$

$$
\begin{align*}
  u(x, 0) &= u_0(x), & v(x, 0) &= v_0(x), & w(x, 0) &= w_0(x).
\end{align*}
$$

(103)

Then, based on the results in Sections 2 and 3, we have the following results.

Theorem 4.1. Assume that $u_0, v_0, w_0$ and are nonnegative functions. Then, for every control $c \in C_{ab}$ , there exists a unique solution $(u, v, w) \in (W(0, T))^3$ satisfying (101)-(103).

Theorem 4.2. Problem (2) with (101)-(103) possesses at least one optimal control solution.
We introduce the adjoint system as following, \( \forall (x,t) \in Q \)

\[
-\partial \varphi_1 / \partial t - d_1 \triangle \varphi_1 + k_1 \varphi_1 = -(b_1 \bar{u} + c_1 \bar{w}) \varphi_1 - b_2 \bar{v} \varphi_2 - -b_3 \bar{w} \varphi_3,
\]

\[
-\partial \varphi_2 / \partial t - d_2 \triangle \varphi_2 + k_2 \varphi_2 = -b_1 \bar{w} \varphi_1 - (b_2 \bar{u} + c_2 \bar{w}) \varphi_2 - -c_3 \bar{w} \varphi_3,
\]

\[
-\partial \varphi_3 / \partial t - d_3 \triangle \varphi_3 + k_3 \varphi_3 = -c_1 \bar{u} \varphi_1 - c_2 \bar{v} \varphi_2 - -(b_3 \bar{u} + c_3 \bar{v}) \varphi_3,
\]

(104)

with the boundary conditions \( \forall (x,t) \in \Sigma \)

\[
\partial_n \varphi_1 + \varphi_1 = 0, \quad \partial_n \varphi_2 + \varepsilon \varphi_2 = 0, \quad \partial_n \varphi_3 = 0,
\]

(105)

and the initial conditions \( \forall x \in \Omega \)

\[
\varphi_1(x,T) = \alpha_{TU}(u(x,T) - u_\Omega(x)), \quad \varphi_2(x,T) = \alpha_{TV}(v(x,T) - v_\Omega(x)),
\]

\[
\varphi_3(x,T) = \alpha_{TW}(w(x,T) - w_\Omega(x)).
\]

(106)

**Theorem 4.3.** Every locally optimal solution \( \bar{c} \) of (101)-(103) satisfies, together with the adjoint states \((\varphi_1, \varphi_2, \varphi_3)\) of the adjoint system (104)-(106), the variational inequality

\[
\int \int_{\Sigma} (\varphi_1 + \alpha \bar{c})(c - \bar{c}) ds dt \geq 0, \forall c \in C_{ab}.
\]

(107)

**Example 2.** [8] Consider the system (4) with following form of \( f_1, f_2, f_3, b(x,t,u) \):

\[
f_1 = -b_1 u v,
\]

\[
f_2 = -b_2 u v,
\]

\[
f_3 = +b_3 u v,
\]

\[
b(x, t, u) = \varepsilon = 0,
\]

\[
b_i \geq 0, i = 1, 2, 3.
\]

(108)

Obviously, the conditions \((H)_1\) and \((H)_2\) are satisfied. The systems (4)-(6) becomes that \( \forall (x,t) \in Q \)

\[
\partial u / \partial t - d_1 \triangle u = -b_1 u v,
\]

\[
\partial v / \partial t - d_2 \triangle v = -b_2 u v,
\]

\[
\partial w / \partial t - d_3 \triangle w = b_3 u v,
\]

(109)

together with the Neumann boundary conditions \( \forall (x,t) \in \Sigma \)

\[
d_1 \partial_n u = c(t), \quad d_2 \partial_n v = 0, \quad \partial_n w = 0,
\]

(110)

and the initial conditions \( \forall x \in \Omega \)

\[
u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad w(x, 0) = w_0(x).
\]

(111)

Here, \((H)_3\) is naturally true due to \( b(x, t, 0) \equiv 0 \). It is obvious that we have the same results as following after slightly modifying the proofs of the corresponding theorems in Sections 2 and 3.
The adjoint system is as follows. \( \forall (x,t) \in Q \)

\[
-\partial \varphi_1 / \partial t - d_1 \triangle \varphi_1 = -k_1 \bar{v} \varphi_1 - k_2 \bar{v} \varphi_2 + k_3 \bar{u} \varphi_3, \\
-\partial \varphi_2 / \partial t - d_2 \triangle \varphi_2 = -k_1 \bar{u} \varphi_1 - k_2 \bar{u} \varphi_2 + k_3 \bar{u} \varphi_3, \\
-\partial \varphi_3 / \partial t - d_3 \triangle \varphi_3 = 0, 
\]

(112)

with the boundary conditions \( \forall (x,t) \in \Sigma \)

\[
\partial_n \varphi_1 = 0, \quad \partial_n \varphi_2 = 0, \quad \partial_n \varphi_3 = 0, 
\]

(113)

and the initial conditions \( \forall x \in \Omega \)

\[
\varphi_1(x,T) = \alpha_{TU}(u(x,T) - u_\Omega(x)), \quad \varphi_2(x,T) = \alpha_{TV}(v(x,T) - v_\Omega(x)), \\
\varphi_3(x,T) = \alpha_{TW}(w(x,T) - w_\Omega(x)). 
\]

(114)

Similar to Theorems 4.1-4.3, for this example, we have the following three theorems.

**Theorem 4.4.** Assume that \( u_0, v_0, w_0 \) are nonnegative functions. Then, for every control \( c \in C_{ab} \), there exists a unique solution \( (u,v,w) \in (W(0,T))^3 \) satisfying (109)-(110).

**Theorem 4.5.** The optimal control problem under (109)-(110) possesses at least one optimal control solution.

**Theorem 4.6.** Every locally optimal solution \( \bar{c} \) of (4) satisfies, together with the adjoint states \( (\varphi_1, \varphi_2, \varphi_3) \) of the adjoint system (112)-(113), the variational inequality

\[
\int \int _\Sigma (\varphi_1 + \alpha_c \bar{c})(c - \bar{c})dsdt \geq 0, \forall c \in C_{ab}. 
\]

(115)

**Example 3.** Further, we can consider the system (4) with the following general form of \( f_1, f_2, f_3 \):

\[
f_1 = a_{11}uv + a_{13}uw + a_{13}uw + b_{11}u^2 + b_{12}v^2 + b_{13}w^2, \\
f_2 = a_{21}uv + a_{22}uw + a_{23}uw + b_{21}u^2 + b_{22}v^2 + b_{23}w^2, \\
f_3 = a_{31}uv + a_{32}uw + a_{33}uw + b_{31}u^2 + b_{32}v^2 + b_{33}w^2. 
\]

(116)

Then, the conditions (H)$_1$, (H)$_2$, and (H)$_3$ are satisfied, and similar results to Theorems 4.4-4.6 can be obtained. Therefore we can extend the classical results in the literature to the general form where interactions among \( u, v, \) and \( w \) arise in the right-hand side of system (2). We omit the details.

**Acknowledgments.** The authors would like to thank the two anonymous reviewers for their constructive suggestions and comments, which help to improve the presentation of the paper.
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Received ?; 1st revision ?; final revision ?.