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Analysis of the local well-posedness of optimization-constrained differential equations by local optimality conditions

Xiao Zhao[1] | Tobias Ploch[2] | Stephan Noack[1] | Wolfgang Wiechert[1,3] | Alexander Mitsos[2,3,4] | Eric von Lieres[1,3]

[1]IBG-1: Biotechnology, Forschungszentrum Jülich, Germany

[2]Process Systems Engineering (AVT.SVT), RWTH Aachen University, Germany

[3]Center for Simulation and Data Science, JARA, Germany

[4]Institute of Energy and Climate Research, Energy Systems Engineering (IEK-10), Forschungszentrum Jülich, Germany

Correspondence
Eric von Lieres, IBG-1, Biotechnology, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany.
Email: e.von.lieres@fz-juelich.de

Alexander Mitsos, Process Systems Engineering (AVT.SVT), RWTH Aachen University, 52074 Aachen, Germany.
Email: alexander.mitsos@avt.rwth-aachen.de

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Abstract

Optimization-constrained differential equations (OCDE) are a class of mathematical problems where differential equations are constrained by an embedded algebraic optimization problem. We analyze the well-posedness of the local solutions of OCDE based on local optimality. By assuming linear independence constraint qualification and applying the Karush-Kuhn-Tucker optimality conditions, an OCDE is transformed into a complementarity system (CS). Under second-order sufficient condition we show that (a) if strict complementary condition (SCC) holds, the local solution of OCDE is well-posed, which corresponds to a mode of the derived CS; (b) at points where SCC is violated, a local solution of OCDE exists by sequentially connecting the local solutions of two selected modes of the derived CS. We propose an event-based algorithm to numerically solve OCDE. We illustrate the approach and algorithm for microbial cultivation, single flash unit and contrived numerical examples.

KEYWORDS

complementarity system, KKT conditions, optimization-constrained differential equations, parametric optimization

1 | INTRODUCTION

Hybrid systems refer to dynamic systems whose states have continuous as well as discrete components.[1,2] Changes occur both in response to discrete, instantaneous events and in response to dynamics as described by differential or difference equations in time.[2] There exist different types of hybrid systems, including differential inclusions, switched systems and complementarity systems (CS).[3,4]

CS are a class of hybrid systems,[5-10] which contain complementarity variables for all time points. Two scalar variables are said to be complementary, if they are both non-negative and at least one of these two scalar variables equals zero. This gives rise to systems that can experience discrete events, the so-called mode switches. A mode of CS refers to a derived differential-algebraic equations (DAE) system, which is embedded in CS. Between two switches, CS behave as continuous differential systems within a mode, and the neighboring two modes are two different continuous differential systems. Well-posedness of CS, that is, the existence and uniqueness of the solutions of CS, has been studied.[5,7,10-12] Commonalities and differences between CS and other types of hybrid systems were studied.[9,13]

Herein, we analyze so-called optimization-constrained differential equation systems (OCDE),[14] that is, differential equations constrained by

an embedded algebraic optimization problem. The right-hand side of the differential equations depends on an optimal solution of the embedded optimization problem, while the embedded algebraic optimization problem is parameterized by the state variables of the differential equations. Solutions of OCDE are the trajectories of the state and the optimization variables, which satisfy both the differential equations and the algebraic optimization problem. OCDE has been applied to simulate dynamic phase transition for a single atmospheric aerosol particle that exchanges mass with surrounding gas.[14-16] They have also been applied to model the cell metabolism under changes in the environment by using metabolic networks.[17] Models resulting from dynamic flux analysis are a special type of OCDE.[18-21]

More specifically, we study local well-posedness of OCDE. Well-posedness of a dynamic system in general means that its solution exists and is unique. Local well-posedness of OCDE means that a local solution of OCDE exists and is locally unique given the same initial conditions. We will introduce this concept more formally later. Sufficient conditions are given to analyze the local existence and uniqueness of local solutions of OCDE. In particular, an OCDE is first reformulated into a CS by applying Karush-Kuhn-Tucker (KKT) conditions.[14,20,21] We show that (1) under local optimality conditions, namely linear independence constraint qualification (LICQ), strict complementarity condition (SCC) and second-order sufficient condition (SOSC), the local solution of OCDE is well-posed, which corresponds to a single mode of the derived CS, (2) under LICQ, SOSC and transversality conditions, a local solution of the original OCDE can be obtained by activating or deactivating an inequality constraint. Due to activation or deactivation of inequality constraints, OCDE belong to hybrid systems.

Although a CS can be derived by applying KKT conditions to OCDE, the latter is fundamentally different from CS, because (1) KKT conditions are local optimality conditions, while OCDE require the embedded optimization problem to be solved to global optimality, (2) KKT conditions are necessary, not sufficient for local optimality. One cannot guarantee that local optimality is obtained. Therefore, well-posedness of the derived CS does not necessarily guarantee well-posedness of the original OCDE. We consider only local optimality of the embedded algebraic optimization. Ensuring global optimality along the solution trajectory of OCDE is important, but beyond the scope of this article. We note also that this manuscript deals with the simulation task of OCDE. Optimization of the entire OCDE is beyond the scope of this manuscript.

In comparison to the work of Landary et al.[14] and our previous work,[20,21] we do not target a specific engineering problem but rather aim to mathematically analyze the general form of OCDE. A CS-based reformulation is presented along with rigorous formulations to construct local solutions of the original OCDE through the derived CS. Contrasting with our previous work,[20] we give here a set of rigorous conditions, including LICQ, SCC, SOSC and transversality condition, to analyze the local well-posedness of OCDE. The proposed conditions (cf. Theorem 3.4) are more general than condition (3.3) in the work.[20] Contrasting with the work,[21] we consider here OCDE with nonlinear optimization problems and the focus is on mathematical analysis and algorithm development.

This work is largely influenced by the literature of parametric optimization, in particular the developments by Jongen, Fiacco and their coauthors,[22-27] and can be viewed as an application of the results therein to OCDE. Other important works in parametric optimization also include the treatment of linear/nonlinear parametric optimization with and without integer variables.[28-32] Herein, the variational analysis of local minima for each mode is a special type of nondegenerate critical points (points of type 1^{22}). Fiacco[24] discusses sufficient conditions in parametric optimization that guarantee smooth parametric solution (cf. Theorem 3.3). Switching points, where switching of modes happens (cf. Section 3.3), are a special type of critical points (points of type 2^{22}). There exist also other types of degenerate critical points,[22] which are not treated here. These types of critical points have typically stronger conditions, but in our examined engineering problems and based on own experiences they seem less likely to happen. Extending the current results to these types of critical points is not straightforward. Note that for parametric quadratic programming,[33,34] it could be shown that the solution can be described by continuous piecewise affine functions, and analytical expressions were derived. For parametric nonlinear programming, Sakizlis et al. applied KKT conditions to the optimal control problem and derived a dynamic system, which was constrained by inequality constraints.[35] Switching of the active set was discussed under the assumption that a solution exists.

The article is organized as follows. In Section 2, we present a problem formulation and a CS-based reformulation by applying KKT conditions. In Section 3, we discuss the local solution of OCDE with the help of CS. In Section 4, we present an event-based numerical algorithm to solve OCDE. We demonstrate theory and algorithm using examples from systems biotechnology and chemical engineering in Section 5. Contrived numerical examples are also presented in the Supplemental Material.

2 | PROBLEM DEFINITION AND REFORMULATION

2.1 | OCDE definition

An OCDE takes the following form

$$\dot{x}(t) = f(x(t), z(t)), x(t_0) = x_0 \tag{1a}$$

$$z(t) \in \underset{\hat{z} \in \mathbb{R}^n}{\arg\min}\, g(x(t), \hat{z}) \tag{1b}$$

$$s.t.\ h_i(x(t), \hat{z}) = 0, i = 1, \ldots, I, \tag{1c}$$

$$l_j(x(t), \hat{z}) \le 0, j = 1, \ldots, J, \tag{1d}$$

where $x(t) \in \mathbb{R}^m$ are the differential states, $z(t) \in \mathbb{R}^n$ are the algebraic variables. $f : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}^m$, g, h_i, $l_j : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ are assumed to be twice continuously differentiable, that is, $\mathcal{C}^2$. I, $J \in \mathbb{N}$ are fixed, and $\mathcal{I} := \{1, \ldots, I\}$, $\mathcal{J} := \{1, \ldots, J\}$. Equation (1a) refers to the (upper-level) differential part, while Equations (1b)–(1d) refer to the (lower-level) algebraic optimization part. $g(x(t), \hat{z})$ is the objective function, while Equations (1c) and (1d) are equality and inequality constraints, respectively. We use "algebraic optimization" to distinguish from optimization with dynamic systems, that is, we point out that both objective

function and constraints in algebraic optimization are algebraic functions. $t_0 \in \mathbb{R}$ denotes the start time.

At any fixed time $t = t^*$ and states $x(t^*)$, the optimization problem (1b)–(1d) searches for a minimizer, denoted by $\hat{z}^*$. Recall that in this article, we do not consider global optimality of the lower-level optimization problem and we restrict the discussion to local optimality. This minimizer $\hat{z}^*$ is then fed back to the differential part (1a) through setting $z(t^*) = \hat{z}^*$. $x(t^*)$ and $z(t^*)$ in turn determine the right-hand side of Equation (1a), namely $\dot{x}(t^*)$. In this way, the lower-level optimization and the upper-level differential parts are coupled with each other. In the following, we use $P(x(t))$ to denote the lower-level optimization problem (1b)–(1d), in which $P(\cdot)$ is parameterized by $x(t)$. Note that $P(x(t))$ indicates that t is the ultimate parameter for parameterization of the lower-level optimization, following the sequence t, $x(t)$, $P(x(t))$, however, for better understanding and later discussion we suggest to consider $x(t)$ as a whole to parameterize the lower-level optimization problem, since $x(t)$ is not a known function.

Denote $I_T = (t_0 - \epsilon, t_0 + \epsilon)$, $\epsilon > 0$, as an open time interval. Continuous functions $x(t) : I_T \to \mathbb{R}^m$ and $z(t) : I_T \to \mathbb{R}^n$ are called a local solution of OCDE (1) for the time interval I_T, if $\forall t \in I_T$, (i)

$$x(t) = x_0 + \int_{t_0}^{t} f(x(\tau), z(\tau))d\tau,$$

(ii) $z(t)$ is a local minimizer of $P(x(t))$. If one can find such functions $x(t)$ and $z(t)$ for $t \in I_T$, we say that a solution of OCDE (1) locally exists. In particular, if we can find continuous functions $x(t)$ and $z(t)$ fulfilling the above condition (i) and (ii) for half-open intervals $I_T = [t_0, t_0 + \epsilon)$ or $I_T = (t_0 - \epsilon, t_0]$, we say that a solution of OCDE exists for the half-open interval I_T. If ϵ can be increased to infinity, we say that a solution globally exists. Note that this article considers only local existence.

For $t \in I_T$, denote $(x(t)^\top, z(t)^\top)^\top$ as a local solution of OCDE (1), fulfilling initial condition $x(t_0) = x_0$, $z(t_0) = z_0$. This local solution is called locally unique, if for $t \in I_T$ there do not exist other solutions, denoted as $\left(\tilde{x}(t)^\top, \tilde{z}(t)^\top\right)^\top$, satisfying $\tilde{x}(t_0) = x_0$, $\tilde{z}(t_0) = z_0$. So local uniqueness requires that there exists only one solution starting from $\left(x_0^\top, z_0^\top\right)^\top$. OCDE is called locally well-posed with reference to an initial point $\left(x_0^\top, z_0^\top\right)^\top$, if a local solution exists and it is locally unique.

Remarks: (1) According to the above definition, both $x(t)$ and $z(t)$ are confined to be continuous functions in I_T. Although there may exist discontinuous local solutions of OCDE (1), in which $x(t)$ or $z(t)$ is discontinuous, we have excluded this case from our discussion. (2) As a special type of hybrid systems, OCDE may have different definitions of their solutions and the corresponding well-posedness. We will stick to the above definition.

Denote $V \in \mathbb{R}^m$ as a neighborhood of x_0. Assume that $\forall x(t) \in V$, the lower-level parametric optimization problem $P(x(t))$ has a local solution $z^{opt}(x(t))$, where $z^{opt}(\cdot) : \mathbb{R}^m \to \mathbb{R}^n$. In this case, OCDE (1) can be transformed into

$$\dot{x}(t) = f\left(x(t), z^{opt}(x(t))\right), x(t_0) = x_0, \tag{2}$$

To numerically solve OCDE (1), one can apply the time-step methods[4,36] to Equation (2), which has a non-smooth right-hand side. These types of methods evaluate $z^{opt}(x(t))$ by calling an internal local optimizer/solver repeatedly and use the evaluated value of $z^{opt}(x(t))$ to integrate forwards. Thus, one does not need to provide an event function for locating the non-smoothness of the right-hand side of Equation (2). The local optimizer behaves like a black box for integration and it is not relevant to take care what happens inside the optimizer. However, switching points may be hard to locate for the optimizer and jumps of the solution trajectory may be missed. Moreover, because a theoretical expression of the exact local minimum function $z^{opt}(\cdot)$ is typically difficult to obtain, iterative numerical optimization algorithms have to be applied to approximate $z^{opt}(\cdot)$. The cost of optimization calls may be high.

2.2 | CS-based reformulation

This section presents a CS-based reformulation of OCDE (1), derived by applying KKT conditions to the lower-level optimization problem $P(x(t))$. In the following sections, we will discuss the solution of the derived CS and its relationship to the solution of the original OCDE. For any function $f : \mathbb{R}^m \to \mathbb{R}$, we denote the gradient ∇f as a row vector of first-order partial derivatives.

It is well-known that under constraint qualifications (e.g., LICQ, cf. Definition 2.1) every local minimizer $z(t)$ of $P(x(t))$ fulfills the so-called KKT conditions (cf. e.g., the book of Nocedal and Wright[37])

$$0 = \nabla_z L(x(t), z(t), \lambda(t), \mu(t)), \tag{3a}$$

$$0 = h_i(x(t), z(t)),\ i \in \mathcal{I}, \tag{3b}$$

$$0 \le \mu_j(t) \perp -l_j(x(t), z(t)) \ge 0,\ j \in \mathcal{J}, \tag{3c}$$

where

$$L(x(t), z(t), \lambda(t), \mu(t)) := g(x(t), z(t)) + \sum_{i \in \mathcal{I}} \lambda_i(t) h_i(x(t), z(t)) + \sum_{j \in \mathcal{J}} \mu_j(t) l_j(x(t), z(t))$$

denotes the Lagrangian function. $\lambda(t) = (\lambda_1(t), \ldots, \lambda_I(t))^\top \in \mathbb{R}^I$ and $\mu(t) = (\mu_1(t), \ldots, \mu_J(t))^\top \in \mathbb{R}^J$ denote the Lagrangian multipliers for equality and inequality constraints, respectively. The complementarity constraints (3c) require $\forall j \in \mathcal{J}$,

$$0 \le \mu_j(t),\ \ 0 \le -l_j(x(t), z(t)), \tag{4a}$$

$$0 = \mu_j(t) l_j(x(t), z(t)). \tag{4b}$$

For notational simplicity, denote $y(t) := (x(t)^\top, z(t)^\top, \lambda(t)^\top, \mu(t)^\top)^\top$ and define

$$\mathcal{A}(x(t), z(t)) := \{\, j \in \mathcal{J} \mid l_j(x(t), z(t)) = 0 \,\} \tag{5}$$

as the active set of inequality constraints evaluated at $(x(t)^\top, z(t)^\top)^\top$. A point $y(t)$ is called a KKT point, if it satisfies KKT conditions (3). For time point $t = t^*$, we also denote $x^* = x(t^*)$, $z^* = z(t^*)$, $\lambda^* = \lambda(t^*)$, $\mu^* = \mu(t^*)$, $y^* = y(t^*)$ and similarly $\mathcal{A}^* = \mathcal{A}(x(t^*), z(t^*))$ to simplify the notation.

Replacing the lower-level optimization problem $P(x(t))$ by KKT system (3) in Equation (1), we obtain a nonlinear complementarity system (CS)

$$\dot{x}(t) = f(x(t), z(t)), x(t_0) = x_0, \tag{6a}$$

$$0 = \nabla_z L(x(t), z(t), \lambda(t), \mu(t)), \tag{6b}$$

$$0 = h_i(x(t), z(t)), i \in \mathcal{I}, \tag{6c}$$

$$0 \le \mu_j(t) \perp -l_j(x(t), z(t)) \ge 0, j \in \mathcal{J}. \tag{6d}$$

We will discuss the local solution of OCDE (1) with the help of several concepts, developed for the derived CS (6). In particular, we are interested in: How does the solution of OCDE locally look like? Under which conditions does the OCDE locally have a solution? Is the solution of OCDE locally unique?

Remarks: (1) Since KKT conditions are only necessary optimality conditions, one cannot in general conclude that the solutions of CS (6) correspond to the local minima of $P(x(t))$. Hence, a solution of CS may not be a solution of OCDE. As we will see later, SOSC will be used to ensure this. (2) Comparing CS (6) with a typical DAE system, CS (6) requires in addition that inequality constraints (4a) to be fulfilled along the solution trajectory. As we will see later, this leads to a typical feature of hybrid system, that is, the solution trajectories are continuous, but have discontinuous derivatives at certain points.

2.3 | Modes of derived CS

Denote $\mathcal{S}$ as any subset of $\mathcal{J}$, i.e., $\mathcal{S} \subseteq \mathcal{J}$ ($\mathcal{S}$ can be the empty set). For $t = t^*$, the following DAE system is called "mode $\mathcal{S}$" of CS (6)[5]:

$$\dot{x}(t) = f(x(t), z(t)), x(t^*) = x^*, \tag{7a}$$

$$0 = \nabla_z L(x(t), z(t), \lambda(t), \mu(t)), \tag{7b}$$

$$0 = h_i(x(t), z(t)), i \in \mathcal{I}, \tag{7c}$$

$$0 = l_j(x(t), z(t)),\ j \in \mathcal{S}, \tag{7d}$$

$$0 = \mu_j(t),\ j \in \mathcal{J}/\mathcal{S}. \tag{7e}$$

CS (6) has in total 2^J different modes. Each mode $M(\mathcal{S})$ has as many equations as variables, that is, no degrees of freedom. The initial time of mode $M(\mathcal{S})$ is t^* and its initial states are x^*. Denote $V^{\mathcal{S}}$ as the set of consistent initial points of $M(\mathcal{S})$. If $x(t^*) \in V^{\mathcal{S}}$, we denote the solution of $M(\mathcal{S})$ by $y^{\mathcal{S}}(t) = \left(x^{\mathcal{S}}(t)^\top, z^{\mathcal{S}}(t)^\top, \lambda^{\mathcal{S}}(t)^\top, \mu^{\mathcal{S}}(t)^\top\right)^\top$. Note that if $t^* = t_0$ and $x^* = x_0$ are taken as a special case, mode $M(\mathcal{S})$ is initialized by the initial condition of CS (6).

Remark: Compared to system (6), system (7) does not have inequality constraints embedded in Equation (4a). So in general, solutions of system (7) may not satisfy all inequality constraints in Equation (4a).

We now summarize the conditions and notations, which will be used later in this manuscript to analyze local well-posedness of OCDE.

Definition 2.1 (LICQ[37]). *Linear independence constraint qualification (LICQ) is said to hold at point $(x^{*\top}, z^{*\top})^\top$, if vectors $\nabla_z h_i(x^*, z^*)$, $i \in \mathcal{I}$, $\nabla_z l_j(x^*, z^*)$, $j \in \mathcal{A}(x^*, z^*)$ are linearly independent.*

Definition 2.2 (SCC[37]). *For any fixed $\mathcal{S} \subseteq \mathcal{J}$, strict complementarity condition (SCC) is said to hold at y^*, if*

$$\begin{cases} \mu_j^* > 0,\ l_j(x^*, z^*) = 0,\ \forall j \in \mathcal{S}, \\ \mu_j^* = 0,\ l_j(x^*, z^*) < 0,\ \forall j \in \mathcal{J} \setminus \mathcal{S}. \end{cases} \tag{8}$$

Note that $\mathcal{S}$ is allowed to be an empty set.

For any point $y^* = (x^{*\top}, z^{*\top}, \lambda^{*\top}, \mu^{*\top})^\top$, define

$$\Gamma^* := \Gamma(x^*, z^*, \lambda^*, \mu^*) = \left\{ j \in \mathcal{J} \mid l_j(x^*, z^*) = 0, \mu_j^* = 0 \right\}.$$

If $\Gamma^* \neq \emptyset$, SCC is violated $\forall \mathcal{S}$.

Definition 2.3 (SOSC, cf. Theorem 2.1[24]). *Second-order sufficient condition (SOSC) is said to hold at a KKT point y^*, if*

$$s^\top \nabla_z^2 L(x^*, z^*, \lambda^*, \mu^*) s > 0, \tag{9}$$

for all $s \neq 0$ such that

$$\begin{aligned} &\nabla_z l_j(x^*, z^*, \lambda^*, \mu^*) s \le 0,\ \text{for all } j \in \mathcal{J}, \text{where } l_j(x^*, z^*) = 0, \\ &\nabla_z l_j(x^*, z^*, \lambda^*, \mu^*) s = 0,\ \text{for all } j \in \mathcal{J}, \text{where } \mu_j^* > 0, \\ &\nabla_z h_i(x^*, z^*, \lambda^*, \mu^*) s = 0,\ i \in \mathcal{I}. \end{aligned} \tag{10}$$

Definition 2.4 (TC). *Denote y^* as a KKT point and assume Γ^* to contain a single element, that is, $\Gamma^* = \{j^*\}$. Transversality condition (TC) is said to hold at $y^* = y(t^*)$ for $t = t^*$, if*

$$\dot{\mu}_{j^*}^{\mathcal{A}^* \setminus \Gamma^*}(t^*) \cdot \dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) > 0. \tag{11}$$

TC will be later assumed for point y^*, for which SCC is violated. By imposing TC we intend to ensure that SCC is violated only at $t = t^*$ so that by activating or deactivating the j^*-th inequality constraint a

local solution can be obtained. The idea of formulating the above TC is learned from Equation (1.6)[38] and Equation (5).[39]

We summarize also the used assumptions in this manuscript as follows:

Assumption 1 *Functions f, g, h_i, $\forall i \in \mathcal{I}$, l_j, $\forall j \in \mathcal{J}$, are twice continuously differentiable.*

Assumption 2 *At $t = t^*$, LICQ holds at point $(x(t^*)^\top, z(t^*)^\top)^\top$.*

Assumption 3 *At $t = t^*$, SOSC holds at KKT point $y(t^*)$.*

Assumption 4 *At KKT point $y(t^*)$, either SCC holds, that is, $\Gamma^* = \emptyset$, or only one inequality constraint violates SCC, that is, $\Gamma^* = \{j^*\}$.*

Assumption 5 *If SCC is violated for the j^*-th constraint at $t = t^*$, TC holds.*

3 | LOCAL SOLUTION OF OCDE

We now analyze the local well-posedness of OCDE in this section by applying the conditions introduced above. In Section 3.1, we show that under the proposed conditions, modes of derived CS are index-1 DAE systems. In Section 3.2, SOSC is applied to points satisfying SCC, which guarantees that the local solution of each mode is identical to the local solution of OCDE, which is also locally unique. In Section 3.3, we discuss the situation when SCC fails and we show that mode switching of derived CS can generate a local solution of the original OCDE.

3.1 | Regularity conditions for modes

This section shows that under certain conditions originated from parametric optimization, the derived modes are index-1 DAE systems. And therefore, these DAE systems have well-posed local solutions. The results can be applied both to the cases when SCC is satisfied or not.

For any matrix $B \in \mathbb{R}^{n\times k}$, $k \le n$, $Ker\, B^\top := \{s \in \mathbb{R}^n |\ B^\top s = 0\}$ denotes the kernel of $B^\top$. Denote $H \in \mathbb{R}^{n\times n}$ as a symmetric real matrix and let $T \subseteq \mathbb{R}^n$ be a linear subspace of $\mathbb{R}^n$. $H|_T$ is said to be non-singular (positive definite), if and only if, $\forall a \in T\backslash\{0\}$, $a^\top H a \neq 0$ ($a^\top H a > 0$).

Lemma 3.1 (Lemma 2.4.3[23]). *Let A be a symmetric $n \times n$ real matrix, B be a $n \times k$ real matrix and C be a $k \times k$ real matrix. Matrix*

$$\begin{pmatrix} A & B \\ CB^\top & 0 \end{pmatrix}$$

is non-singular, if and only if, C is non-singular, $rank(B) = k$ and $A|_{KerB^\top}$ is non-singular.

For any mode $M(\mathcal{S})$, denote

$$F^{\mathcal{S}}(x(t),z(t),\lambda(t),\mu(t)) = \begin{pmatrix} \nabla_z L^\top(x(t),z(t),\lambda(t),\mu(t)) \\ h_{\mathcal{F}}(x(t),z(t)) \\ l_{\mathcal{S}}(x(t),z(t)) \\ \mu_{\mathcal{J}\mathcal{S}}(t) \end{pmatrix} \tag{12}$$

as the right-hand side of Equations (7b)–(7e). $h_{\mathcal{F}}(x(t), z(t)) := (..., h_i(x(t), z(t)), ...)^\top$, $i \in \mathcal{F}$, $l_{\mathcal{S}}(x(t),z(t)) := (..., l_j(x(t),z(t)),...)^\top$, $j \in \mathcal{S}$ and $\mu_{\mathcal{J}\backslash\mathcal{S}}(t) := (..., \mu_j(t), ...)^\top$, $j \in \mathcal{J}\backslash\mathcal{S}$. Denote matrix

$$E^{\mathcal{S}} = \left(\underbrace{..., \nabla_z h_i^\top, ...}_{i\in\mathcal{F}}, \underbrace{..., \nabla_z l_j^\top, ...}_{j\in\mathcal{S}} \right) \in \mathbb{R}^{n\times(l+|\mathcal{S}|)}$$

as the matrix containing the gradients (column vectors) of all equality constraints $\nabla_z h_i^\top$, $i \in \mathcal{F}$, and the inequality constraints $\nabla_z l_j^\top$, $j \in \mathcal{S}$.

Theorem 3.1 (Non-singularity of $\nabla_{(z^\top,\lambda^\top,\mu^\top)^\top} F^{\mathcal{S}}$) *$\nabla_{(z^\top,\lambda^\top,\mu^\top)^\top} F^{\mathcal{S}}$ is non-singular, if and only if*

$$(\mathrm{i})\ E^{\mathcal{S}} \text{ has full column rank,} \tag{13a}$$

$$(\mathrm{ii})\ \nabla_z^2 L|_{Ker(E^{\mathcal{S}})^\top} \text{ is non-singular.} \tag{13b}$$

Proof. Apply Lemma 3.1 to

$$\nabla_{(z^\top,\lambda^\top,\mu^\top)^\top} F^{\mathcal{S}} = \begin{pmatrix} \nabla_z^2 L & \nabla_z h_{\mathcal{F}}^\top & \nabla_z l_{\mathcal{S}}^\top & \nabla_z l_{\mathcal{J}\backslash\mathcal{S}}^\top \\ \nabla_z h_{\mathcal{F}} & 0 & 0 & 0 \\ \nabla_z l_{\mathcal{S}} & 0 & 0 & 0 \\ 0 & 0 & 0 & diag(1,...,1)^\top \end{pmatrix}$$

by choosing matrix C in Lemma 3.1 as

$$C = diag\left(\underbrace{1,...,1}_{l}, \underbrace{1,...,1}_{|\mathcal{S}|} \right).$$

By applying the Implicit Function Theorem (IFT, cf. Theorem 2.4.1[25]), Equations (7b)–(7e) uniquely determine $z(t)$, $\lambda(t)$ and $\mu(t)$ in a neighborhood of $x(t)$. Hence, Theorem 3.1 results in an important consequence that mode $M(\mathcal{S})$, defined in Equation (7), is an index-1 DAE. And hence, the well-posedness of Equation (7) can be deduced from the existing results of index-1 DAE system.

In the following of this subsection we show that conditions in Theorem 3.1 can be actually deduced, if the optimization problem $P(x)$ fulfills certain moderate conditions.

Lemma 3.2 (Lemma 2.1[24]). *If SOSC holds at a KKT point y^*, then z^* is a locally isolated (locally unique) minimizer of $P(x^*)$.*

Note that Lemma 3.2 does not require SCC.

Define

$$\Omega^-\left(\mathcal{A}^*,\Gamma^*\right):=\left\{s\in\mathbb{R}^m \mid \begin{array}{c}\nabla_z l_j s\le 0, j\in\Gamma^*\\ \nabla_z l_j s=0, j\in\mathcal{A}^*\setminus\Gamma^*\\ \nabla_z h_i s=0, i\in\mathcal{I}\end{array}\right\}, \tag{14}$$

$$\Omega^+\left(\mathcal{A}^*,\Gamma^*\right):=\left\{s\in\mathbb{R}^m \mid \begin{array}{c}\nabla_z l_j s\ge 0, j\in\Gamma^*\\ \nabla_z l_j s=0, j\in\mathcal{A}^*\setminus\Gamma^*\\ \nabla_z h_i s=0, i\in\mathcal{I}\end{array}\right\}=\{s\in\mathbb{R}^m \mid -s\in\Omega^-\}. \tag{15}$$

Lemma 3.3 *If SOSC is fulfilled at a KKT point y^*, i.e., $s^\top\nabla_z^2 L(x^*,z^*,\lambda^*,\mu^*)s>0$, $\forall s\in\Omega^-\setminus\{0\}$, and if Γ^* contains a single element, that is, $\Gamma^*=\{j^*\}$, then:*

(1) $\nabla_z^2 L(x^*,z^*,\lambda^*,\mu^*)\big|_{Ker\left(E^{\mathcal{A}^*}\right)^\top}$ is positive definite,
(2) $\nabla_z^2 L(x^*,z^*,\lambda^*,\mu^*)\big|_{Ker\left(E^{\mathcal{A}^*\setminus\Gamma^*}\right)^\top}$ is positive definite.

Proof. $\forall s\in\Omega^+\setminus\{0\}$, $-s\in\Omega^-\setminus\{0\}$ and $s^\top\nabla_z^2 L s=(-s)^\top\nabla_z^2 L(-s)>0$. Because Γ^* contains a single element,

$$\Omega^+\cup\Omega^-=Ker\left(E^{\mathcal{A}^*\setminus\Gamma^*}\right)^\top.$$

Hence, when $\forall s\in Ker\left(E^{\mathcal{A}^*\setminus\Gamma^*}\right)^\top\setminus\{0\}$, $s^\top\nabla_z^2 L s>0$, namely item (2) holds. Item (1) is a direct consequence of item (1), because

$$Ker\left(E^{\mathcal{A}^*}\right)^\top\subseteq Ker\left(E^{\mathcal{A}^*\setminus\Gamma^*}\right)^\top.$$

Now we summarize the first important result of this work as follows.

Theorem 3.2 *If LICQ and SOSC hold at a KKT point y^*, Γ^* contains at most a single element, then*

$$|\nabla_z F^{\mathcal{A}^*\setminus\Gamma^*}|\neq 0,\quad |\nabla_z F^{\mathcal{A}^*}|\neq 0. \tag{16}$$

Proof. From Theorem 3.1, we prove that Condition (13) is fulfilled for $\mathcal{S}=\mathcal{A}^*\setminus\Gamma^*$ and $\mathcal{S}=\mathcal{A}^*$. Condition (13a) follows directly from LICQ condition, while Condition (13b) follows from Lemma 3.3.

The consequences of Theorem 3.2 are that: (1) Modes $M(\mathcal{A}^*)$ and $M(\mathcal{A}^*\setminus\Gamma^*)$ are index-1 DAE systems, whose local solutions are well-posed. (2) When SCC is fulfilled, among all modes there exists only one mode $M(\mathcal{A}^*)$, whose solution passes through KKT point y^*. (3) When SCC is violated for a single inequality constraint, that is, $\Gamma^*=\{j^*\}$, there exist in total two modes, $M(\mathcal{A}^*)$ and $M(\mathcal{A}^*\setminus\Gamma^*)$, whose solutions pass through KKT point y^*, refer to Section 3.3.

3.2 | Local solutions when SCC holds

From Theorem 3.2, when SCC holds at a KKT point y^*, mode $M(\mathcal{A}^*)$ is an index-1 DAE system and there exists $\epsilon>0$ such that inequality constraints (4a) are fulfilled, $\forall t\in(t^*-\epsilon,t^*+\epsilon)$. So the solution $y^{\mathcal{A}^*}(t)$ of mode $M(\mathcal{A}^*)$ is a solution of CS (6), taking $t^*=t_0$ and $x^*=x_0$ as initial condition. To guarantee that $y^{\mathcal{A}^*}(t)$ is also a solution of the original OCDE, one needs in addition to ensure that $z^{\mathcal{A}^*}(t)$ are the local minima of $P\left(x^{\mathcal{A}^*}(t)\right)$. In this section, we show that this can be actually deduced if SOSC at the single KKT point y^* is fulfilled.

Theorem 3.3 (Local minima of $P(x(t))$, Theorem 2.1[24]). *If (i) the SOSC for a local minimizer of $P(x^*)$ holds at $(x^{*\top},z^{*\top})^\top$ with associated Lagrange multipliers λ^* and μ^*, (ii) LICQ condition of $P(x^*)$ holds at $(x^{*\top},z^{*\top})^\top$, (iii) SCC of $P(x^*)$ holds at $(x^{*\top},z^{*\top},\lambda^{*\top},\mu^{*\top})^\top$, then:*

(1) *z^* is a local isolated minimizer of $P(x^*)$ and the associated Lagrange multipliers λ^* and μ^* are unique.*

(2) *For any $x'\in\mathbb{R}^m$ in a neighborhood of x^*, there exists a unique once-continuously differentiable function $(z^f(x')^\top,\lambda^f(x')^\top,\mu^f(x')^\top)^\top$, implicitly defined by $0=F^{\mathcal{A}^*}(x,z,\lambda,\mu)$, satisfying the SOSC for a local minimum of problem $P(x')$ such that $z^f(x^*)=z^*$, $\lambda^f(x^*)=\lambda^*$, $\mu^f(x^*)=\mu^*$, and hence, $z^f(x')$ is a locally unique local minimizer of $P(x')$ with associated unique Lagrange multipliers $\lambda^f(x')$ and $\mu^f(x')$.*

(3) *SCC and LICQ hold at $z^f(x')$ for x' near x^*.*

In other words, under LICQ, SOSC and SCC at a KKT point, the points on solution trajectory $z^{\mathcal{A}^*}(t)$ of mode $M(\mathcal{A}^*)$ are not only KKT points, but also local minima of $P(x(t))$. Therefore, the local solution $y^{\mathcal{A}^*}(t)$ of mode $M(\mathcal{A}^*)$ is locally a solution of the original OCDE, that is, the local existence of the solution of OCDE is deduced.

Local uniqueness of the solution of OCDE can be deduced from Theorem 3.3 and local well-posedness of index-1 DAE systems as follows.

Corollary 3.1 *If conditions in Theorem 3.3 are fulfilled, $\left(x^{\mathcal{A}^*}(t)^\top,z^{\mathcal{A}^*}(t)^\top\right)^\top$ is a local solution of OCDE (1), which is locally unique.*

Proof. Because local solution is considered, the initial condition of OCDE (1) can be shifted to $t_0=t^*$, $x_0=x^*$. Assume that $\left(\tilde{x}(t)^\top,\tilde{z}(t)^\top\right)^\top$, $t\in I_T(\epsilon)$, is another local solution of OCDE with $\tilde{x}(t^*)=x^*$, $\tilde{z}(t^*)=z^*$. Because $\tilde{x}(t)$ and $\tilde{z}(t)$ are continuous, for $t\in I_T(\epsilon)$, $\left(\tilde{x}(t)^\top,\tilde{z}(t)^\top\right)^\top$ are in a close neighborhood of $(x^{*\top},z^{*\top})^\top$. From point (3) of Theorem 3.3, we have $z^f(\tilde{x}(t))=\tilde{z}(t)$. From point (3) of Theorem 3.3, LICQ and SCC hold for $\left(\tilde{x}(t)^\top,\tilde{z}(t)^\top\right)^\top$. So there exist unique $\tilde{\lambda}(t)$ and $\tilde{\mu}(t)$, such that $F^{\mathcal{A}^*}\left(\tilde{x}(t),\tilde{z}(t),\tilde{\lambda}(t),\tilde{\mu}(t)\right)=0$ and $\dot{\tilde{x}}(t)=f(\tilde{x}(t),\tilde{z}(t))$. In other words, $\tilde{y}(t):=\left(\tilde{x}(t)^\top,\tilde{z}(t)^\top,\tilde{\lambda}(t)^\top,\tilde{\mu}(t)\right)^\top$ is another solution of mode $M(\mathcal{A}^*)$ except from $y^{\mathcal{A}^*}(t)$, starting from $x(t^*)=x^*$, $z(t^*)=z^*$, $\lambda(t^*)=\lambda^*$ and $\mu(t^*)=\mu^*$. This is a contradiction, because mode $M(\mathcal{A}^*)$ is an index-1 DAE system and local solution of index-1 DAE system is unique.

3.3 | Local solutions when SCC fails

When SCC holds, Theorem 3.2 and 3.3 imply that the OCDE is well-posed. This section discusses a special type of degenerated situations, in which SCC fails for the j^*-th inequality constraint at a KKT point $(x^{*\top},z^{*\top},\lambda^{*\top},\mu^{*\top})^\top$ at $t=t^*$, i.e.

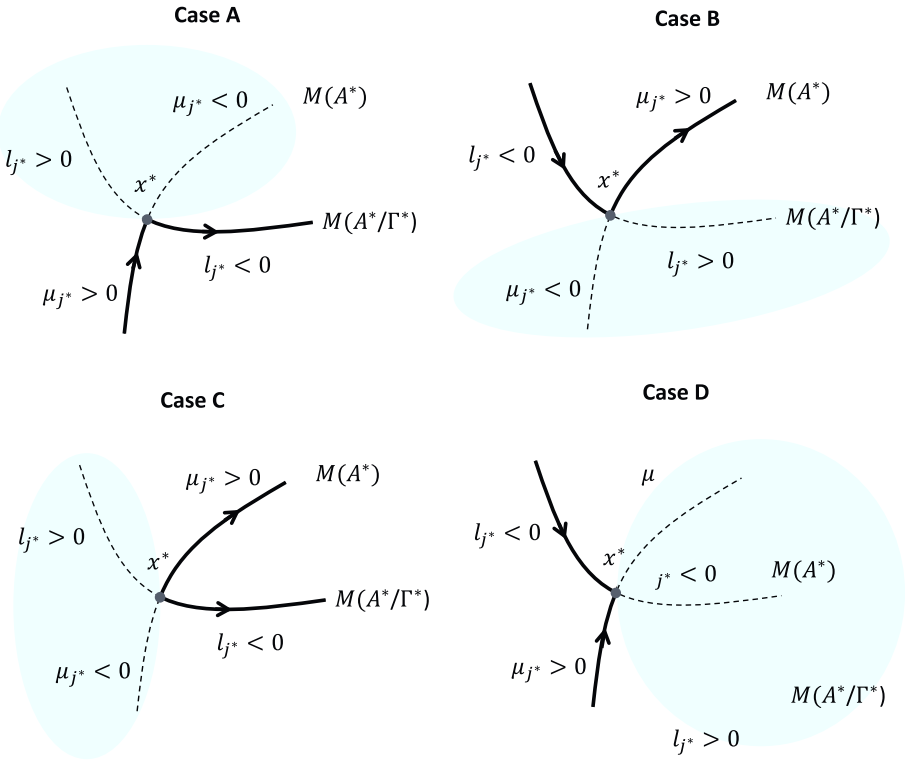

FIGURE 1 Four cases of mode switching when TC holds. Solid lines refer to solutions fulfilling all inequality constraints (4a), while dashed lines refer to solutions with the j^*-th inequality constraint (4a) violated. The arrows represent the direction of time

$$\Gamma^* = \{ j^* \} \neq \emptyset, \tag{17}$$

while the other conditions in Theorem 3.3 still hold.

For a given Γ^*, we consider modes $M(\mathcal{A}^*)$ and $M(\mathcal{A}^* \setminus \Gamma^*)$. From Theorem 3.2, each mode is still an index-1 DAE system, and therefore their solutions, denoted as $y^{\mathcal{A}^*}(t)$ and $y^{\mathcal{A}^* \setminus \Gamma^*}(t)$, are locally well-posed. Without loss of generality, we shift the initial time to $t = t^*$ with initial states $(x^{*\top}, z^{*\top})^\top$.

Because $\mu_{j^*}^{\mathcal{A}^*}(t^*) = l_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) = 0$ and the equality constraint $\mu_{j^*}(t) = 0$ ($l_{j^*}(y(t)) = 0$) are not included in the definitions of mode $M(\mathcal{A}^*)$ ($M(\mathcal{A}^* \setminus \Gamma^*)$), it is possible that inequality constraints $\mu_{j^*}(t) \geq 0$ ($-l_{j^*}(y(t)) \geq 0$) of complementarity conditions may be violated along the solution trajectory $y^{\mathcal{A}^*}(t)$ ($y^{\mathcal{A}^* \setminus \Gamma^*}(t)$) for t near t^*.

The motivation of imposing TC is to use first-order time gradients to ensure the change of signs of $\mu_{j^*}^{\mathcal{A}^*}(t)$ and $l_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t)\right)$ at $t = t^*$ where SCC fails, so that SCC is violated only at $t = t^*$. Under TC, we will show that the local solution of mode $M(\mathcal{A}^*)$ for $t \in (t^* - \epsilon, t^*]$ and the local solution of $M(\mathcal{A}^* \setminus \Gamma^*)$ for $t \in [t^*, t^* + \epsilon)$ (or change the direction of time) can be linked together to construct a local solution of CS for t near t^*. Moreover, under SOSC this local solution is a local solution of the original OCDE. If TC is violated, one may obtain multiple solutions starting from the same initial point $(x^{*\top}, z^{*\top})^\top$, or more complicated phenomena may happen. In particular, by assigning different signs to $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*)$ and $\dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right)$, four cases of mode switching are obtained as shown in Figure 1.

Case A: $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) < 0$, $\dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) < 0$. In this case, the solution trajectory of mode $M(\mathcal{A}^*)$ fulfills inequality constraint $u_{j^*}(t) \geq 0$, for $t \in [t^* - \epsilon, t^*)$, while the solution of mode $M(\mathcal{A}^* \setminus \Gamma^*)$ fulfills inequality constraint $l_{j^*}(y(t)) \leq 0$, for $t \in [t^*, t^* + \epsilon)$. Therefore, if one links the solution of mode $M(\mathcal{A}^*)$ for $t \in (t^* - \epsilon, t^*]$, and the solution of $M(\mathcal{A}^* \setminus \Gamma^*)$ at KKT point y^* for $t \in [t^*, t^* + \epsilon)$, a solution of the CS (6) can be obtained.

Case B: $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) > 0$, $\dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) > 0$. This case is analogous to case A by inverting the direction of time.

Case C: $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) > 0$, $\dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) < 0$. In this case, both inequality constraints $u_{j^*}(t) \geq 0$ and $l_{j^*}(y(t)) \leq 0$ will get fulfilled for modes $M(\mathcal{A}^*)$ and $M(\mathcal{A}^* \setminus \Gamma^*)$, for $t \in [t^*, t^* + \epsilon)$. Therefore, CS (6) does not have a unique solution starting from KKT point y^*.

Case D: $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) < 0$, $\dot{l}_{j^*}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t^*)\right) > 0$. This case is analogous to case C by inverting the direction of time.

Although case C and D are possible in general, by imposing TC (11), we exclude cases C and D. Case C corresponds to the situation that the local solutions of OCDE and the derived CS are not locally unique. Case D corresponds to the situation where a local solutions of OCDE and the derived CS may not exist. Because case C and D result in non-regular solutions, they are excluded from our discussion. To our experience, the encountered examples are mainly of case A and B. However, a mathematical example of case C and D is shown in Example 1 of the supplemental material.

In the language of parametric optimization, case A and B refer to deactivation and activation of inequality constraints $l_{j^*}(x(t), z(t)) \leq 0$ along the solution trajectory of CS, respectively. Because of the activation/deactivation of inequality constraints, the solution trajectory of CS contains discontinuous derivatives.

We have shown that mode switching fulfills all complementarity constraints, as well as KKT conditions, for a small time interval containing the switching time. Next we show that under SOSC at $t = t^*$, for $t \in I_T$ the solutions of $M(\mathcal{A}^* \setminus \Gamma^*)$ to $M(\mathcal{A}^*)$ correspond not only to KKT points, but also to a local minimum. Therefore, we conclude in

Theorem 3.4 that a mode switch of the derived CS leads to a local solution of OCDE, that is, a local solution of OCDE exists. Local uniqueness property of OCDE, when SCC is violated, is a more challenging topic and not covered in this article.

Theorem 3.4 *Assume that for KKT point* $(x^{*\top}, z^{*\top}, \lambda^{*\top}, \mu^{*\top})^\top$, *LICQ and SOSC hold, while SCC is violated for the* j^**-th inequality constraint, that is,* $\Gamma^* = \{j^*\}$. *If TC holds with* $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) < 0$ ($\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) > 0$), *then there exists an* $\epsilon > 0$ *such that*: (1) $z^{\mathcal{A}^*}(t)$ *are local minima of* $P\left(x^{\mathcal{A}^*}(t)\right)$, $t \in (t^* - \epsilon, t^*]$ ($t \in [t^*, t^* + \epsilon)$), (2) $z^{\mathcal{A}^* \setminus \Gamma^*}(t)$ *are local minima of* $P\left(x^{\mathcal{A}^* \setminus \Gamma^*}(t)\right)$, $t \in [t^*, t^* + \epsilon)$ ($t \in (t^* - \epsilon, t^*]$).

Proof. We prove only the case $\dot{u}_{j^*}^{\mathcal{A}^*}(t^*) < 0$ (cf. case A in Figure 1, that is, mode switch from $M(\mathcal{A}^*)$ to $M(\mathcal{A}^* \setminus \Gamma^*)$. We aim to apply Lemma 3.2, for $t = t^*$, $t \in (t^* - \epsilon, t^*)$ and $t \in (t^*, t^* + \epsilon)$, separately. This proof follows similarly to Theorem 2.1.[24]

At $t = t^*$, from Lemma 3.2, KKT point y^* is a local minimizer of $P(x^*)$. Moreover, $z^{\mathcal{A}^*}(t^*) = z^{\mathcal{A}^* \setminus \Gamma^*}(t^*) = z^*$. So (1) and (2) hold at $t = t^*$.

At $t \in (t^* - \epsilon, t^*)$, because of TC, SCC holds for solution trajectory $y^{\mathcal{A}^*}(t)$, $\forall t \in (t^* - \epsilon, t^*)$. Therefore, the active (binding) set $\mathcal{A}\left(y^{\mathcal{A}^*}(t)\right) = \mathcal{A}^*$ is unchanged for $t \in (t^* - \epsilon, t^*)$, given ϵ sufficiently small. Recalling Lemma 3.2, we aim to prove that SOSC holds for $\forall t \in (t^* - \epsilon, t^*)$, i.e.

$$s^\top \nabla_z^2 L\left(y^{\mathcal{A}^*}(t)\right) s > 0, \tag{18}$$

for all $s \in \mathbb{R}^m \setminus \{0\}$ satisfying

$$\begin{aligned} &\nabla_z l_j\left(y^{\mathcal{A}^*}(t)\right) s = 0, j \in \mathcal{A}^*, \\ &\nabla_z h_i\left(y^{\mathcal{A}^*}(t)\right) s = 0, i \in \mathcal{I}. \end{aligned} \tag{19}$$

Assume now that SOSC (18), (19) does not hold for $t \in (t^* - \epsilon, t^*)$, namely for $\epsilon^k \to 0$, we can always find $t^k \in (t^* - \epsilon^k, t^*)$ such that there exists a $s^k \neq 0$, s^k satisfying Equation (19) and $s^{k\top} \nabla_z^2 L\left(y^{\mathcal{A}^*}(t^k)\right) s^k \leq 0$. Without loss of generality, take all $\|s^k\| = 1$ and select a convergent sub-sequence s^κ of s^k with $s^\kappa \to \bar{s}$. Then, we have $\bar{s}^\top \nabla_z^2 L\left(y^{\mathcal{A}^*}(t^*)\right) \bar{s} \leq 0$ with

$$\begin{aligned} &\nabla_z l_j\left(y^{\mathcal{A}^*}(t^*)\right) \bar{s} = 0, j \in \mathcal{A}^*, \\ &\nabla_z h_i\left(y^{\mathcal{A}^*}(t^*)\right) \bar{s} = 0, i \in \mathcal{I}, \end{aligned}$$

namely $\bar{s} \in Ker\left(E^{\mathcal{A}^*}\right)^\top = \Omega^+ \cap \Omega^- \subseteq \Omega^-$. This is to say that SOSC does not hold at $t = t^*$, which is a contradiction.

For $t \in (t^*, t^* + \epsilon)$, the active set $\mathcal{A}\left(y^{\mathcal{A}^* \setminus \Gamma^*}(t)\right) = \mathcal{A}^* \setminus \Gamma^*$. By using point (2) of Lemma 3.3, the result can be proven in a similar way, which is omitted here.

4 | NUMERICAL ALGORITHM

For initial points where SCC is fulfilled, and if the assumptions in Theorems 3.2 and 3.3 hold, local solution of OCDE (1) is well-posed and is the same as the local solution of a derived mode of CS (6). For initial points where SCC is violated, and if the assumptions in Theorems 3.2 and 3.4 hold, a local solution of OCDE can be constructed by sequentially connecting the local solutions of two derived modes of CS (6). So numerical methods for CS can be directly applied to obtain local solutions of OCDE. Numerical methods for CS can be roughly classified into event-tracking method, time-stepping method and smoothing method.[40,41] This section will present an event-tracking algorithm to solve OCDE. Recall that, functions $x(t)$ and $z(t)$ are called a local solution of OCDE (1) for the time interval I_T, if $\forall t \in I_T$, (i)

$$x(t) = x_0 + \int_{t_0}^{t} f(x(\tau), z(\tau)) d\tau,$$

(ii) $z(t)$ is a local minimizer of $P(x(t))$, cf. Section 2.1.

The event-tracking algorithm solves a sequence of DAE modes $M(\mathcal{S}_i)$, $i = 0, 1, \ldots$, and the event is determined by the time when SCC fails. We illustrate this procedure as follows. At $t = t_0$, we assume that a consistent initial point y_0 fulfilling Equations (7b)–(7e) is obtained, for example, by solving the lower-level optimization $P(x_0)$. Denote $\mathcal{S}_0 = \mathcal{A}(y_0)$ as the active set at $y(t_0) = y_0$. Without loss of generality, we can assume that SCC is fulfilled at y_0 (If SCC is violated at y_0, switching happens exactly at this point, cf. Theorem 3.4.). We thus integrate DAE system $M(\mathcal{S}_0)$ for a positive time interval without violating any inequality constraints (4a). If the conditions in Theorem 3.2 and 3.3 hold, $y^{\mathcal{S}_0}(t)$, $t \in [t_0, t_0 + \epsilon)$, is a locally unique solution of OCDE.

Denote

$$t_m(t_i, y_i, \mathcal{S}_i) := \inf\left\{ t_{i+1} \geq 0 \,\middle|\, \begin{bmatrix} \exists j^* \in \mathcal{S}_i \\ s.t. \\ \mu_{j^*}^{\mathcal{S}_i}(t_{i+1}) = 0 \end{bmatrix} \text{or} \begin{bmatrix} \exists j^* \in \mathcal{J} \setminus \mathcal{S}_i \\ s.t. \\ l_{j^*}\left(y^{\mathcal{S}_i}(t_{i+1})\right) = 0 \end{bmatrix} \right\} - t_i, i = 0, 1, \ldots, \tag{20}$$

as the minimum length of time interval, for which SCC is violated for the j^*-th constraint at $t_{i+1} = t_i + t_m(t_i, y_i, \mathcal{S}_i)$, $i = 0, 1, \ldots$. Hence, $t_1, t_2, \ldots$, denote switching time.

Starting from $i = 0$ and $\mathcal{S}_0$, mode $M(\mathcal{S}_0)$ with initial states y_0 is solved until switch time t_1. From the definition of $t_m(\cdot)$, one has $t_1 - t_0 = t_m(t_0, y_0, \mathcal{S}_0)$. Denote $y_1 = y^{\mathcal{S}_0}(t_1)$ as the states at time t_1, $\Gamma^* = \Gamma(y_1) = \{j^*\}$ as the index of the j^*-th constraint violating SCC, $\mathcal{A}^* = \mathcal{A}(y_1)$ as the active set at y_1. Choose

$$\mathcal{S}_1 \in \left\{\mathcal{S}_1 \neq \mathcal{S}_0 \mid \mathcal{S}_1 = \mathcal{A}^* \text{ or } \mathcal{S}_1 = \mathcal{A}^* \setminus \Gamma^*\right\}$$

so that $\mathcal{S}_1$ is different from $\mathcal{S}_0$. If the conditions in Theorem 3.4 hold, for $t \in [t_1, t_1 + \epsilon)$, the solution trajectory $y^{\mathcal{S}_1}(t)$ of mode $M(\mathcal{S}_1)$ starting from y_1 is a local solution of OCDE. Therefore, at $t = t_1$ one starts to solve mode $M(\mathcal{S}_1)$ until SCC is violated again at $t = t_2$. We assume that this procedure can be repeated until a given ending time $t_f > 0$ is reached. We summarize this solution procedure formally as the following algorithm.

Algorithm 1 An event-based algorithm to solve OCDE (1)

At $t = t^0$, compute $\left(z_0^\top, \lambda_0^\top, \mu_0^\top\right)^\top$, so that $y_0 = \left(x_0^\top, z_0^\top, \lambda_0^\top, \mu_0^\top\right)^\top$ is a KKT point of $P(x^0)$

$\mathcal{S}_0 \leftarrow \mathcal{A}(x_0, z_0)$

$i \leftarrow 0$

while $t \le t^f$ **do**

  Solve DAE mode $M(\mathcal{S}_i)$ with initial value y^i

  Compute the length of time integration $t_m(t_i, y_i, \mathcal{S}_i)$ in Equation (20)

  $t_{i+1} \leftarrow t_i + t_m(t_i, y_i, \mathcal{S}_i)$

  $\mathcal{A}^* \leftarrow \mathcal{A}\left(y^{\mathcal{S}_i}(t_{i+1})\right)$

  $\Gamma^* \leftarrow \Gamma\left(y^{\mathcal{S}_i}(t_{i+1})\right)$

  if LICQ, SOSC, TC hold **then**

    $\mathcal{S}_{i+1} \leftarrow \left\{\mathcal{A}^*, \mathcal{A}^* \backslash \Gamma^*\right\} \backslash \{\mathcal{S}_i\}$

    $y_{i+1} \leftarrow y^{\mathcal{S}_i}(t_{i+1})$

    $i \leftarrow i + 1$

  else

    Stop (failure)

  end if

end while

An important step in Algorithm 1 is to determine the minimum length of integration $t_m(t_i, y_i, \mathcal{S}_i)$, cf. Equation (20). Define

$$U^{\mathcal{S}_i}(y(t)) := \left(\underbrace{\ldots, u_j(t), \ldots}_{j \in \mathcal{S}_i}, \underbrace{\ldots, l_j(y(t)), \ldots}_{j \in \mathcal{J} \setminus \mathcal{S}_i} \right)^\top, i = 0, 1, \ldots. \tag{21}$$

For each mode $M(\mathcal{S}_i)$ initialized at y_i, $t_m(t_i, y_i, \mathcal{S}_i)$ can be numerically computed by monitoring the values of $U^{\mathcal{S}_i}(y(t))$ along the solution trajectory $y^{\mathcal{S}_i}(t)$. When any element of $U^{\mathcal{S}_i}(y(t))$ crosses zero at t_{i+1}, it indicates that SCC is violated at t_{i+1} and $t_m(t_i, y_i, \mathcal{S}_i) = t_{i+1} - t_i$ is obtained. In literature, $U^{\mathcal{S}_i}(y(t))$ are called event functions and an event happens if any element of $U^{\mathcal{S}_i}(y(t))$ crosses zero. Note that algorithms to locate the zeros of event functions $U^{\mathcal{S}_i}(y(t))$ for DAE system $M(\mathcal{S}_i)$ already exist (cf. the references in paper[4]).

Algorithm 1 is implemented as a numerical toolbox OCDES (OCDE Simulator, https://github.com/modsim/OCDES) in MATLAB environment (Figure 2). Users need to provide the symbolic formulation of OCDE (1) using MATLAB's symbolic variables and an initial condition x_0. Initial states z_0 with corresponding Lagrangian multipliers λ_0, μ_0 are first computed by calling NLP solver *fmincon* in MATLAB. Then derivatives in the formulation of mode $M(\mathcal{S}_0)$ are obtained by applying MATLAB symbolic toolbox. Symbolic expressions of mode $M(\mathcal{S}_0)$ can be constructed. M-files are then generated for evaluating the right-hand side of differential Equations (7a) and algebraic Equations (7b)–(7e) of mode $M(\mathcal{S}_0)$. Event functions $U^{\mathcal{S}_i}(y(t))$, defined in Equation (21), are also given to the integrator *ode15s* (cf. the paper of Shampine and Reichelt[42]) through the "events" option (Surely *ode15s* is just one choice and there may exist other suitable integrators.). To this point, one can start calling the integrator to solve mode $M(\mathcal{S}_0)$ until an element in $U^{\mathcal{S}_i}(y(t))$ changes its sign at $t = t_1$, that is, a switching is encountered. With updated index, initial condition and modes, the same procedure is evoked again. To detect non-regular systems, LICQ, SCC, SOSC and TC are also checked at the initial and switching times. The software implementation automates this procedure repeatedly until the specified end time t_f is reached.

5 | NUMERICAL EXAMPLES

We illustrate the approach and algorithm using a model for microbial cultivation and a single flash unit. Contrived numerical examples and a microbial example can be found in the Supplemental Material. All examples are computed using the toolbox OCDES which is published on GitHub.

5.1 | Microbial cultivation example

Dynamic flux balance analysis (DFBA) is an established modeling strategy to simulate microbial conversion processes. It enables a combined simulation of both intracellular and extracellular environments. A DFBA model contains two coupled parts, a dynamic part at the upper level for the extracellular environment and an optimization part at the lower level for the intracellular environment. For more technical details of DFBA please refer to the papers[43,20] and the references therein.

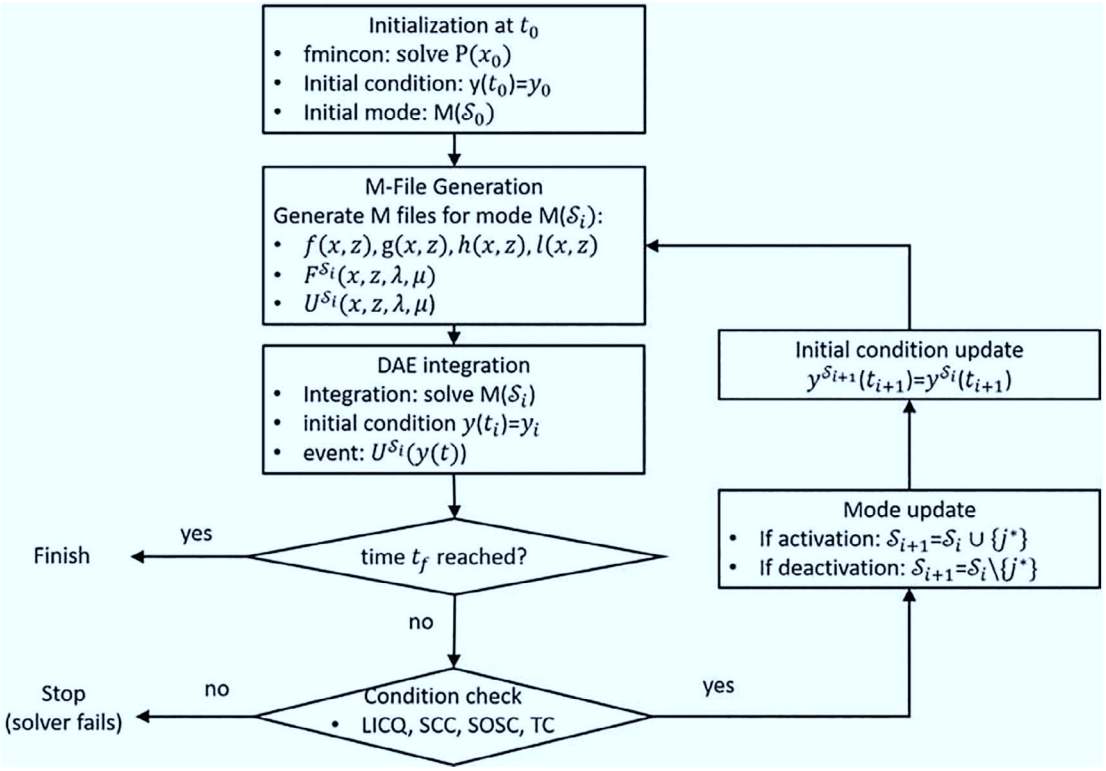

FIGURE 2 Software implementation of Algorithm 1 in MATLAB

This section presents an engineering application of DFBA in systems biotechnology, in which the central metabolic network of wild-type *Corynebacterium glutamicum* is considered. The central network model comprises 46 intracellular reactions and 49 metabolites, which enables the simulation of *C. glutamicum* growth on glucose as sole carbon and energy source. More technical modeling details and the DFBA method can be found in papers[43,20] and the references therein. To illustrate the basic idea, a simplified DFBA example can be found in the Supplemental Material.

The DFBA method results in the following OCDE system

$$\dot{c}_{Biomass}(t) = v_{biosynth}(t)\ c_{Biomass}(t),\ c_{Biomass}(0) = 1, \tag{22a}$$

$$\dot{c}_{GLC}(t) = -v_{GLC\_t\_PEP}(t)\ c_{Biomass}(t),\ c_{GLC}(0) = 20, \tag{22b}$$

$$(v(t),a(t)) \in \underset{\hat{v}\in\mathbb{R}^{46},\hat{a}\in\mathbb{R}^{104}}{\arg\max} \frac{\hat{v}_{ATPexcess}}{\hat{v}^\top \hat{v}} + \epsilon \hat{a}^\top \hat{a}, \tag{22c}$$

$$s.t. 0 \le \hat{a}, \tag{22d}$$

$$\hat{v} = E_a \hat{a}, \tag{22e}$$

$$\hat{v}_{GLC\_t\_PEP} = \frac{4.5\ c_{GLC}(t)}{c_{GLC}(t) + 1}. \tag{22f}$$

$c_{Biomass}(t)$ and $c_{GLC}(t)$ are the concentrations of biomass (g/l) and glucose (g/l) in the fluid medium. $v_{GLC\_t\_PEP}(t)$, $v_{ATPexcess}(t) \in \mathbb{R}$ are the glucose uptake flux and the flux of converting excess ATP to ADP, which are

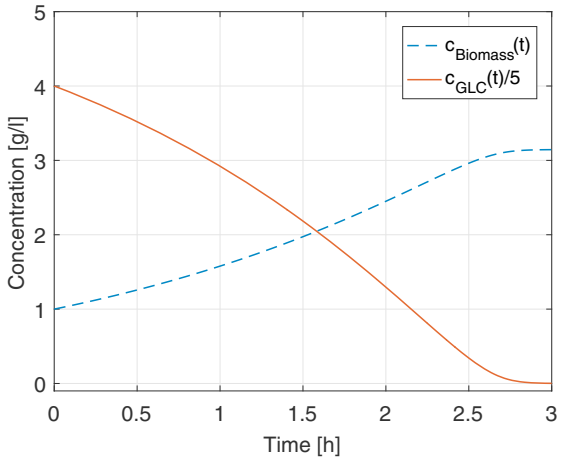

FIGURE 3 Extracellular concentrations $c_{Biomass}(t)$ and $c_{GLC}(t)$ of DFBA model (22) [Color figure can be viewed at wileyonlinelibrary.com]

elements of vector $v(t) \in \mathbb{R}^{46}$ in (mmol/g/hr) containing all flux variables. $E_a \in \mathbb{R}^{46\times 104}$ is a derived matrix containing all extreme rays. $\hat{a}\in\mathbb{R}^{104}$ are coefficients of extreme rays and the flux vector $\hat{v} = E_a\hat{a}$. ϵ is small positive number to avoid non-unique local solutions of a.[20] In comparison to the presented example,[20] a different cellular objective function is chosen, namely we take the assumption that cells have the goal to maximize ATP yield while minimizing enzyme usage (cf. Table 3[44]).

Because model (22) is an OCDE, we apply Algorithm 1 to solve it. Its solution is presented in Figures 3 and 4. The extracellular states

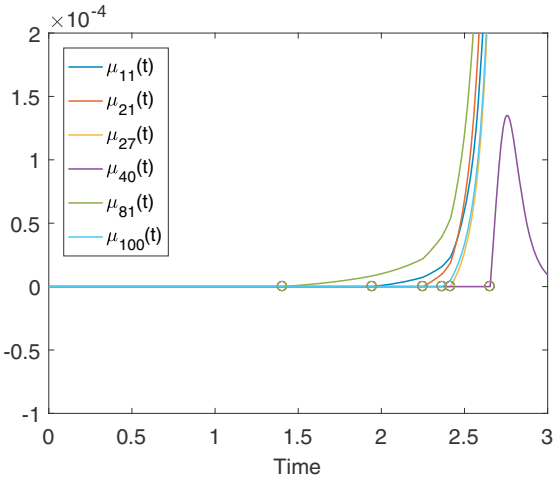

FIGURE 4 The values of Lagrangian multipliers (with switching points) along the solution trajectory [Color figure can be viewed at wileyonlinelibrary.com]

$c_{Biomass}(t)$ and $c_{GLC}(t)$ are presented in Figure 3. Figure 4 shows the values of selected Lagrangian multipliers, where small circle refers to the switching time. The computation is performed on a Windows 10 Computer with MATLAB version 2016b installed. The computation of this example takes 159.8 s.

5.2 | Vapor–liquid equilibrium example

Here we present an example in chemical engineering, in which a single-stage flash unit in vapor–liquid equilibrium, shown in Figure 5, is modeled by a nonlinear OCDE. The flash unit separates a binary mixture of acetone (1) and ethanol (2) into two phases. The flash unit is operated at constant temperature T = 338 K and pressure p = 101325 Pa. The dynamic model for a system with C components is given by

$$\dot{M}(t) = F_{in}(t) - V_{out}(t) - L_{out}(t), \tag{23a}$$

$$\dot{M}_i(t) = F_{in}(t)\cdot z_{i,in}(t) - V_{out}(t)\cdot y_i(t) - L_{out}(t)\cdot x_i(t), \quad i = 1,\ldots,C-1, \tag{23b}$$

$$M(t) = \sum_{i=1}^{C} M_i(t), \tag{23c}$$

$$0 = F_{in}(t) - V_{out}(t) - L_{out}(t), \tag{23d}$$

$$V_{out}(t) = \frac{M_V(t)}{M_V(t) + M_L(t)}\cdot(V_{out}(t) + L_{out}(t)), \tag{23e}$$

where $M(t)$ are the total moles of the system, $M_i(t) \in \mathbb{R}^C$ are the molar amounts of each component i. $F_{in}(t)$, $V_{out}(t)$ and $L_{out}(t)$ are the flow rate of the feed, vapor outlet and liquid outlet with molar composition $z_{i,in}(t) \in \mathbb{R}^C$, $y_i(t) \in \mathbb{R}^C$ and $x_i(t) \in \mathbb{R}^C$, respectively. $M_V(t)$ and $M_L(t)$ are the moles of the vapor and liquid phase, respectively. We assume that the vapor and liquid phase in the flash unit are in equilibrium to determine $M_V(t)$, $M_L(t)$, $y_i(t) \in \mathbb{R}^C$ and $x_i(t) \in \mathbb{R}^C$, respectively. Phase equilibrium at a given temperature T and pressure p is found at the global minimum of the Gibbs free energy.[45,46] The embedded optimization problem can be written as[47,48]

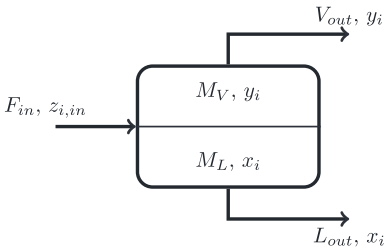

FIGURE 5 Illustration of single-stage flash unit

$$(M_V(t), M_L(t), \boldsymbol{x}(t), \boldsymbol{y}(t)) \in \arg\min_{\hat{M}_V, \hat{M}_L, \hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}} G^M = \hat{M}_V \sum_{i=1}^{C} \hat{y}_i \bar{G}_i^V + \hat{M}_L \sum_{i=1}^{C} \hat{x}_i \bar{G}_i^L \tag{24a}$$

$$\text{s.t.} \quad M_i(t) = \hat{M}_V \cdot \hat{y}_i + \hat{M}_L \cdot \hat{x}_i, \quad i = 1,\ldots,C, \tag{24b}$$

$$\sum_{i=1}^{C} M_i(t) = \hat{M}_V + \hat{M}_L, \tag{24c}$$

$$\sum_{i=1}^{C} \hat{y}_i - \sum_{i=1}^{C} \hat{x}_i = 0, \tag{24d}$$

$$\hat{M}_V \geq \epsilon, \quad \hat{M}_L \geq \epsilon, \tag{24e}$$

$$\hat{y}_i > 0, \quad \hat{x}_i > 0, \quad i = 1,\ldots,C, \tag{24f}$$

where G^M is the reduced Gibbs free energy of the mixture and $\bar{G}_i^V$ and $\bar{G}_i^L$ are the partial molar Gibbs free energies for each component in the respective phase. The equality constraints comprise C species mole balances, the overall mole balance and the closure conditions for the mole fractions. The inequality constraint become active if one phase vanishes, that is, the mixture is vapor only or liquid only. The partial molar Gibbs free energies are given by the following relations:

$$\begin{aligned} \bar{G}_i^V &= \ln\left(\frac{y_i \cdot p}{p_{i0}(T)}\right), \quad i = 1,\ldots,C, \\ \bar{G}_i^L &= \ln(x_i \cdot \gamma_i(T, \boldsymbol{x})), \quad i = 1,\ldots,C, \end{aligned}$$

where p_{i0} is the vapor pressure at given temperature T that is calculated using the extended Antoine equation and γ_i is the activity coefficient calculated with the NRTL model. Note that we introduce a small regularization term $\epsilon = 10^{-6}$ to ensure that the SOSC are fulfilled in the single-phase region. The first-order KKT conditions of optimization problem (24a) - (24f) are essentially equal to the ones discussed in literature[47,48] except for a small error in the mass balance caused by the introduced regularization term.

The number of phases present in the flash unit depends on the overall composition, temperature T and pressure p. While we set the

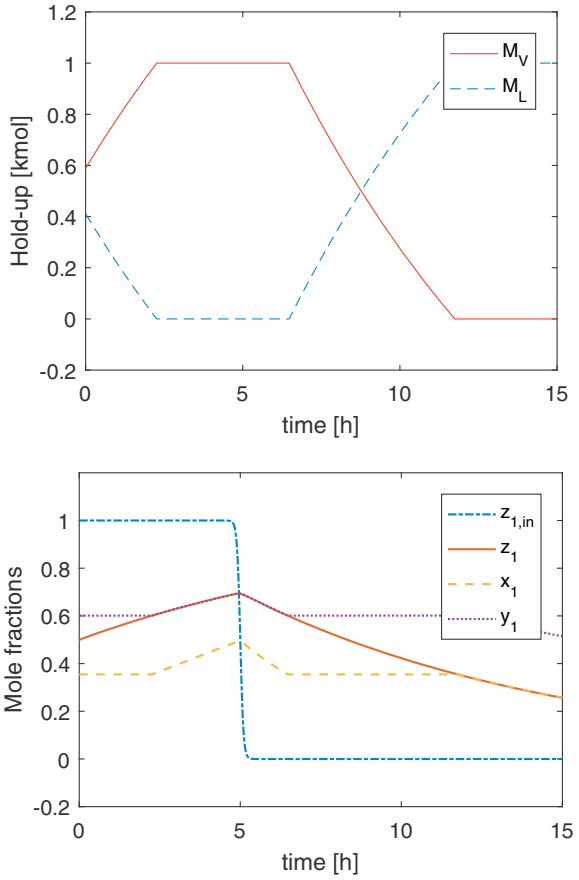

FIGURE 6 Dynamic simulation profiles. Active set changes after 2.26 hr, 6.47 hr, and 11.74 hr [Color figure can be viewed at wileyonlinelibrary.com]

latter to constant values, we use a feed with changing composition resulting in vanishing and reappearing phases:

$$\begin{aligned} F_{in}(t) &= 0.1\,\text{kmol}\,\text{h}^{-1} \\ z_{1,in}(t) &= 1-0.5\cdot(1+\tanh(10\cdot(t-5))) \\ z_{2,in}(t) &= 1-z_{1,in}, \end{aligned}$$

where t is the time in hours. The initial conditions are $M(t = 0) = 1$ kmol and $M_1(t = 0) = 0.5$ kmol. For a final simulation time of 15 hr, the simulation trajectories are given in Figure 6.

The upper plot shows the molar hold-ups of the vapor and liquid phase, respectively, while the lower plot shows the mole fractions of acetone. For the given simulation set-up, the simulation starts with a two-phase mixture, that is, the hold-up of both phases is greater than 0. The feed of essentially pure acetone ($z_{1,\,in} \approx 1$ for $t \ll 5$ hr) leads to an increase of the overall mole fraction of this component z_1. As a consequence, the liquid phase vanishes after approx. 2.26 hr and only vapor exists in the flash unit ($M_L = \epsilon$). After approx. 5 hr, the feed changes to pure ethanol ($z_{1,\,in} = 0$ for $t \gg 5$ hr) leading to a decrease of the overall composition of acetone z_1 and the reappearance of the liquid phase at $t \approx 6.47$ hr. After 11.74 hr, another switching point is detected indicating the disappearance of the vapor phase ($M_V = \epsilon$). The computation is performed on a Windows 10 Computer with MATLAB version 2016b installed. The entire computation of this example takes 4.02 seconds. The simulation time is much faster than the first example, because the problem size is smaller.

6 | CONCLUSIONS

We study the local well-posedness of OCDE under several classical local optimality conditions, including LICQ, SCC and SOSC. The KKT conditions are used to transform the OCDE into a CS. With the help of the derived CS, we show that: (a) a local solution of the original OCDE is locally well-posed, when LICQ, SCC and SOSC hold. In this case the local solution of OCDE is identical to an index-1 DAE mode of the derived CS. (b) A local solution of OCDE exists, when LICQ, SOSC and TC hold but SCC fails. In this case, the local solution can be constructed by mode switch. We propose a numerical algorithm, which is implemented in MATLAB as a toolbox. We present two contrived numerical examples and three engineering applications, two from systems biotechnology and one from a flash unit operation in chemical engineering.

The presented results can be extended in the following directions. First, OCDE requires the embedded optimization problem to be solved to global optimality, while the proposed conditions in this article ensure only local optimality. It is possible that a local minimizer of the embedded optimization problem loses global optimality along the solution trajectory by using the proposed method (Example 3 in the Supplemental Material). Second, only regular points and a special type of degenerated KKT points are considered. There exist other types of degenerated critical points[22] for the lower-level optimization problem, which have not been treated in this work. Third, for the case that SCC fails, the local uniqueness property of OCDE has not been established and multiple solutions seem to be possible. At the end, we assume LICQ condition in the article. But this seems to be a too-strong condition for typical DFBA models, see for example.[20] If LICQ is violated, Lagrange multipliers become non-unique and the derived DAE mode of CS becomes a non-deterministic system. Finally, the extension of the proposed analysis to treat local minima when LICQ fails is relevant to engineering applications and is challenging.

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ORCID

Xiao Zhao https://orcid.org/0000-0002-4083-3432
Stephan Noack https://orcid.org/0000-0001-9784-3626
Wolfgang Wiechert https://orcid.org/0000-0001-8501-0694
Alexander Mitsos https://orcid.org/0000-0003-0335-6566
Eric von Lieres https://orcid.org/0000-0002-0309-8408

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