Sliding Motion of Discontinuous Dynamical Systems Described by Semi-Implicit Index One Differential Algebraic Equations

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Abstract

We have proposed an approach to derive a continuous system of differential algebraic equations (DAE) of index one that is dynamically equivalent to a discontinuous index one DAE system. This involves augmenting the convex combination of the ordinary differential equations with the algebraic equations from individual models. This result is proved by using the implicit function theorem. This procedure is illustrated with the help of an ideal gas-liquid system in which the algebraic variables can be expressed as explicit functions of differential variables. It is also demonstrated with an example from a soft-drink manufacturing process, in which, it is difficult to express the algebraic variables as explicit functions of differential variables. Through computer simulation, it is shown that the equivalent dynamic DAE system and the discontinuous DAE system have identical solutions. The proposed method is several orders of magnitude more efficient than the procedure that works with the discontinuous system of DAEs.

Key words: Sliding mode, Equivalent dynamics, Hybrid system, Singular system, Multiple forcing functions, Discontinuous system.

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1 Introduction

Discontinuous systems often exhibit the property of *sliding*, a state, in which the resultant of the forcing functions is used to drive the system. This is also known as equivalent dynamics. This is a reasonably well understood phenomenon for systems made up of ODEs. Some of the early works in this area are by Filippov (1960) and André and Seibert (1960).

Such systems have been reported in various fields, such as, resource allocation (Kunniyur and Srikant, 1999), spring mass system (Filippov, 1988), evaporator and cam follower (Mosterman et al., 1997), to name a few. A realistic industrial problem that has this characteristic is presented by Moudgalya and Jaguste (2001). This class of systems has been studied in detail by Moudgalya and coworkers (Moudgalya and Ryali, 2001; Moudgalya, 2001; Moudgalya et al., 2003; Agrawal and Moudgalya, 2004; Agrawal et al., 2004). In all of the above examples, the analysis has been carried out on ODEs only, although, discontinuous DAEs also may have this property (Agrawal et al., 2003; Moudgalya and Jaguste, 2001).

Brenan et al. (1996) argue that it is better to treat the DAEs directly as opposed to converting them into ODEs. Rao et al. (2003) demonstrate with an example that it is possible for a simple controller designed using a DAE control theory to work better than an advanced controller designed through the ODE route. Moreover, it may not be easy to convert the DAEs into ODEs all the time.

In this paper, we present a systematic approach for the study of discontinuous systems made up of index-1 DAEs. We summarise the existing theory on the sliding phenomenon. Then we present the well studied ideal gas-liquid system of Moudgalya and Ryali (2001) in DAE perspective. We also show how this approach can be extended to a class of DAE systems that are difficult to convert to ODEs by substitution: It is illustrated with an example of mixing $CO_2$ and an acid, which has a potential for use in soft-drink manufacturing.

2 Sliding Motion of ODE Systems

Consider the following system of ODEs with a discontinuous right hand side

\[
\frac{dy}{dt} = f(y)
\]

where for each $t > 0$, the state vector $y(t) \in \mathbb{R}^n$, $f : G \rightarrow \mathbb{R}^n$ is a piecewise continuous function with domain $G \subset \mathbb{R}^n$ and $\mathcal{M}$ is a set (of measure zero) of
points of discontinuity of $f$. Here, the discontinuities occur mainly in the state variable $y$ rather than in the temporal variable $t$. The system is completely described by (1) outside of a sufficiently small $\delta$-neighbourhood of the set of discontinuity $\mathcal{M}$. Nevertheless, in the $\delta$-neighbourhood of $\mathcal{M}$, the standard definition of solution for ODEs may not be even applicable. Filippov (1960) proposed a regularisation method which is known in literature as Filippov’s regularisation in which the discontinuous right hand side of (1) is replaced by a differential inclusion, i.e.,

$$\frac{dy}{dt} \in F(y). \quad (2)$$

Here, $F(y)$ is the smallest closed convex set containing all the limit values of $f(y^*)$ for $y^* \notin \mathcal{M}, y^* \rightarrow y$. More precisely, we write $F$ as

$$F(y) = \bigcap_{\delta > 0} \bigcap_{\zeta(M) = 0} \text{conv} f((y(t) + \delta B) \setminus \mathcal{M}),$$

where, $B$ is a unit ball in $\mathbb{R}^n$, \setminus is the set difference operator, $\zeta$ is the Lebesgue-measurable set and $\text{conv}$ is the closed convex hull (closure of set of all possible convex combinations). The set $F$ is effectively the convex hull of values of $f$ at points near $y(t)$, while ignoring the behaviour of $f$ on the surface of discontinuity $\mathcal{M}$. Although we use autonomous systems for simplicity of exposition, there is no difficulty in extending these results for non-autonomous system of ODEs.

**Definition 1** A vector valued function $y(t)$ is said to be a solution of (1) if it is absolutely continuous and $y$ satisfies (2) almost everywhere.

We restrict ourselves to a case where $f(y)$ is discontinuous on a smooth $(n-1)$ dimensional surface $S$, given by the set of all points $y$, such that $\varphi(y) = 0$. $S$ is called a switching surface and it separates its neighbourhood in the $y$-space into domains $G^+$ and $G^-$, where

$$G^+ = \{ y \in \mathbb{R}^n : \varphi(y) > 0 \}$$

and

$$G^- = \{ y \in \mathbb{R}^n : \varphi(y) < 0 \}.$$  

Thus, we consider the following system of differential equations:

$$\frac{dy}{dt} = f^+(y), \quad y \in G^+, \text{ a. e. } t > 0,$$

$$\frac{dy}{dt} = f^-(y), \quad y \in G^-, \text{ a. e. } t > 0,$$

where, $f|_{G^\pm} = f^\pm$ and a. e. is an abbreviation of “almost every”. For fixed $t$ and for $y^*$ approaching the point $u \in S$ from the domain $G^+$ and $G^-$, let

$$\lim_{y^* \in G^- \rightarrow u} f^- = f^-_0(u)$$

and

$$\lim_{y^* \in G^+ \rightarrow u} f^+ = f^+_0(u).$$

Then the set $F(u)$ is the line segment $l$ joining the end points of the vectors $f^-_0(u)$ and $f^+_0(u)$ with $u \in S$. In case this line segment $l$ is on one side of the
tangent plane \( P \) to the switching surface \( S \) at \( u \) for \( t \in (t_0, t_1) \), the solutions pass from one side of the surface to the other side for \( t \in (t_0, t_1) \), i.e., from \( G^- \) to \( G^+ \) or vice versa. Therefore, the solution of (3) satisfies it everywhere except for the points on the discontinuity surface \( S \). In the other case, when the line segment \( l \) intersects the tangent plane \( P \), i.e., the solutions approach \( S \) from both the sides, the standard notion of solution is not suitable as there is no indication of how a solution which has reached \( S \) can be continued. Nevertheless, using Filippov’s regularisation, if the intersection point between \( l \) and \( P \) is the endpoint of a vector, say \( f_0(u) \), then \( f_0 \) determines the velocity of the motion \( \frac{du}{dt} = f_0(u) \) along the surface \( S \) at \( u \). Now, from (2), \( y(t) \) satisfies

\[
\frac{dy}{dt} = f_0(y),
\]

where, \( f_0 \) is a linear combination of \( f_0^+ \) and \( f_0^- \) and hence, it is a solution of (1). Note that \( f_0 \) is a particular selection from \( F(u) \). If \( f_0 \neq f_0^- \) and \( f_0 \neq f_0^+ \), then a solution of (4) is called the sliding solution.

**Definition 2 (André and Seibert (1960); Hung et al. (1993))** A point \( u \) on the switching surface \( S \) is called an end point if there are solution trajectories reaching \( u \) from both sides of \( S \).

Assume that the switching surface \( S \) is \( C^1 \) and \( \nabla \varphi \neq 0 \). Then the unit normal \( \hat{n} \) at \( u \in S \) directed towards \( G^+ \) is denoted by \( \hat{n} = \frac{\nabla \varphi}{|\nabla \varphi|} \), where, \( |\nabla \varphi| \) is the standard Euclidean norm. Let \( f_N^+ \) and \( f_N^- \), respectively, be the projection of the vectors \( f_0^+(u) \) and \( f_0^-(u) \) onto the normal \( \hat{n} \) to the surface \( S \) at \( u \), i.e.,

\[
f_{N}^\pm = \langle \hat{n}, f_0^\pm \rangle = \frac{\langle \nabla \varphi, f_0^\pm \rangle}{|\nabla \varphi|}, \tag{5}
\]

where \( \langle \ldots \rangle \) denotes the Euclidean inner product. If the vectors \( f^+ \) and \( f^- \) are directed to the surface from both sides, \( i.e., \) \( f_N^+ < 0 \) and \( f_N^- > 0 \) at \( u \in S \), all solutions near the surface \( S \) approach it from both sides, as \( t \) increases. Thus, we have the following result.

**Theorem 1 (André and Seibert (1960); Filippov (1988))** A point \( u \) on \( C^1 \) switching surface \( S \) with \( \nabla \varphi \neq 0 \) is an end point if \( \langle \nabla \varphi, f_0^+ \rangle < 0 \) and \( \langle \nabla \varphi, f_0^- \rangle > 0 \).

**Definition 3 (Hung et al. (1993))** If every point in the switching surface \( S \) (or a part \( S_1 \) of the switching surface \( S \)) is an end point, then \( S \) (or \( S_1 \)) is called a sliding surface.

**Remark 1** As the sliding surface is a switching surface with trajectories reaching from both sides of it, a trajectory that leaves it (because of the switch) will return immediately. In other words, once a trajectory reaches the sliding surface, it will stay on it.
Now coming back to the system given by (4), since the line segment \( l \) joining the end points \( f_0^+ \) and \( f_0^- \) can be written as a convex combination of \( f_0^+ \) and \( f_0^- \), we have the equation for \( l \) as

\[
f_0 = \alpha f_0^+ + (1 - \alpha) f_0^-, \quad 0 \leq \alpha \leq 1.
\]  
(6)

Note that as \( f_0 \) is the intersection point of \( l \) and the tangent plane \( P \) at \( u \in S \), \( f_0 = \alpha f_0^+ + (1 - \alpha) f_0^- \) for some \( \alpha \in [0, 1] \). In order to compute \( \alpha \), we observe that the normal component \( f_N \) of \( f_0 \) vanishes, i.e.,

\[
f_0^N = 0 \Rightarrow \alpha f_0^N + (1 - \alpha) f_0^- = 0.
\]

Hence,

\[
\alpha = \frac{f_0^-}{f_0^+ - f_0^-}.
\]  
(7)

Using (5) in (7), we obtain

\[
\alpha = \frac{\langle \nabla \varphi, f_0^- \rangle}{\langle \nabla \varphi, f_0^+ \rangle - \langle \nabla \varphi, f_0^- \rangle}.
\]  
(8)

A pictorial illustration of these ideas is presented in Fig. 1. For details, see Filippov (1988). To illustrate these ideas, we next present a summary of the ideal gas-liquid system studied by Moudgalya and Ryali (2001).
3 Sliding Motion of an Ideal Gas-Liquid System Described by ODEs

Consider the ideal gas-liquid system studied by Moudgalya and Ryali (2001), with two phases in the tank and one outlet (see Fig. 2). In the left figure, as the outlet tube dips into it, the liquid comes out. As the gas is sent in but not removed, the pressure builds up and hence, the liquid outflow increases with an eventual dropping of liquid level in the tank. When the level falls below the dip tube, the gas starts coming out. If on the other hand, the liquid level is below the dip tube, as in the right figure, gas only flows out; the liquid level rises and eventually reaches the dip tube. There are two DAE models that describe these two situations.

If $\frac{M_L}{\rho_L} > V_d$ (liquid model)

\[
\frac{dM_G}{dt} = F_G, \\
\frac{dM_L}{dt} = F_L - L, \\
0 = V - \left(M_G \frac{RT}{P} + \frac{M_L}{\rho_L}\right), \\
0 = L - k_L x (P - P_{out}).
\]

Else If $\frac{M_L}{\rho_L} < V_d$ (gas model)

\[
\frac{dM_G}{dt} = F_G - G, \\
\frac{dM_L}{dt} = F_L, \\
0 = V - \left(M_G \frac{RT}{P} + \frac{M_L}{\rho_L}\right), \\
0 = G - k_G x (P - P_{out}).
\]
The system keeps switching between these two models.

Moudgalya and Ryali (2001) use a substitution procedure to reduce these DAEs into ODEs. From (11), get an expression for \( P \) as

\[
P = \frac{M_G RT}{V - \frac{M_L}{\rho_L}}.
\]

Substituting (17) in (12), we find that

\[
L = k_L x \left( \frac{M_G RT}{V - \frac{M_L}{\rho_L}} - P_{\text{out}} \right).
\]

Using (17) in (16), we obtain a similar expression for \( G \). On substitution of \( L \) and \( G \), respectively, in (10) and (13), we arrive at

\[
\frac{d}{dt} \begin{bmatrix} M_G \\ M_L \end{bmatrix} = f,
\]

where, \( f \) takes one of the two expressions \( f^+ \) or \( f^- \). When the liquid flows out of the system, the forcing function is

\[
f^+ = \begin{bmatrix} F_G \\ F_L - k_L x \left( \frac{M_G RT}{V - \frac{M_L}{\rho_L}} - P_{\text{out}} \right) \end{bmatrix},
\]

with the switching function \( \varphi(M_G, M_L) > 0 \). When the gas comes out, it is

\[
f^- = \begin{bmatrix} F_G - k_G x \left( \frac{M_G RT}{V - \frac{M_L}{\rho_L}} - P_{\text{out}} \right) \\ F_L \end{bmatrix},
\]

with \( \varphi(M_G, M_L) < 0 \). Here, the switching function \( \varphi \) is given by

\[
\varphi(M_G, M_L) = M_L - \rho_L V_d.
\]

It is shown by Moudgalya and Ryali (2001) that this system (19) reaches the sliding mode, characterised by the following equivalent dynamics,

\[
\frac{d}{dt} \begin{bmatrix} M_G \\ M_L \end{bmatrix} = f_0,
\]

\[
f_0 = \alpha f^+_0 + (1 - \alpha) f^-_0, \ 0 \leq \alpha \leq 1
\]
with the following specific values:

\[ \alpha = \frac{F_L}{k_L x \left( \frac{M_G R T}{V \frac{M_L}{\rho_L}} - P_{out} \right)}, \]

\[ f_0 = \begin{bmatrix} c_2 - c_1 M_G \\ 0 \end{bmatrix}, \]

\[ c_1 = \frac{k_G x R T}{V - \frac{M_L}{\rho_L}} = \frac{k_G x R T}{V - V_d}, \]

\[ c_2 = \left( \frac{F_G}{k_G x} + \frac{F_L}{k_L x} + P_{out} \right) k_G x. \]

Moudgalya (2001) interprets (24) as the forcing function for a mixer in which the gas and the liquid phases get mixed and come out. Equivalently, if we observe the system for any interval of time, the liquid and the gas come out for \( \alpha \) and \( 1 - \alpha \) fractions of the interval, respectively.

4 Sliding Motion of Discontinuous Index-1 DAE Systems

In this section, we consider the following system of DAEs:

\[ \frac{dy}{dt} = f(y, z), \]

\[ 0 = g(y, z), \]  \hspace{1cm} (25) \hspace{1cm} (26)

where for each \( t > 0 \), the state vectors \( y(t) \in \mathbb{R}^n \) and \( z(t) \in \mathbb{R}^m \), \( f : \mathbb{R}^{n+m} \to \mathbb{R}^n \) and \( g : \mathbb{R}^{n+m} \to \mathbb{R}^m \). We restrict our attention to index one DAEs, in which, the Jacobian of \( g \) with respect to \( z \) is nonsingular.

Suppose this DAE system has a discontinuous right hand side. The vector valued functions \( f : \Omega \to \mathbb{R}^n \) and \( g : \Omega \to \mathbb{R}^m \) are piecewise continuous with domain \( \Omega \subset \mathbb{R}^{n+m} \). Let \( \mathcal{M} \) be a set (of measure zero) of points of discontinuity of \( f \) and \( g \). To be more specific, let \( f \) and \( g \) be discontinuous on an \( (n-1) \)-dimensional surface \( S = \{ y \in \mathbb{R}^n : \varphi(y) = 0 \} \). We call \( S \) as a switching surface since it separates its neighbourhood in \( y \)-space into domains \( G^+ \) and \( G^- \), where \( G^+ = \{ (y, z) \in \mathbb{R}^{n+m} : \varphi(y) > 0 \} \) and \( G^- = \{ (y, z) \in \mathbb{R}^{n+m} : \varphi(y) < 0 \} \). Therefore, we rewrite the system (25) – (26) as

\[ \frac{dy}{dt} = \begin{cases} f^+(y, z) & (y, z) \in G^+, \text{ a. e. } t > 0, \\ f^-(y, z) & (y, z) \in G^-, \text{ a. e. } t > 0, \end{cases} \]  \hspace{1cm} (27)
and

\[
0 = \begin{cases} 
  g^+(y, z) & (y, z) \in G^+, \; \text{a. e. } t > 0, \\
  g^-(y, z) & (y, z) \in G^-, \; \text{a. e. } t > 0,
\end{cases}
\]  \tag{28}

where, \( f|_{G^\pm} = f^\pm \) and \( g|_{G^\pm} = g^\pm \).

As the system of DAEs considered in this work is of index one, we now assume that in each of \( G^+ \) and \( G^- \), the systems are DAE of index one. Therefore, by the well known implicit function theorem (Apostol, 1992, pp. 374-375), \( z \) can be written as a function of \( y \), that is, \( z = \psi^\pm(y) \), satisfying \( g^\pm(y, \psi^\pm(y)) = 0 \).

Let on \( G^\pm, z = \psi^\pm(y) \). Then, we substitute \( z = \psi^\pm(y) \) to obtain

\[
\frac{dy}{dt} = \begin{cases} 
  f^+(y, \psi^+(y)) & (y, z) \in G^+, \; \text{a. e. } t > 0, \\
  f^-(y, \psi^-(y)) & (y, z) \in G^-, \; \text{a. e. } t > 0,
\end{cases}
\]  \tag{29}

**Definition 4** The system (27) – (28) is in sliding mode if the corresponding system of ODEs (29) is in sliding mode, i.e., if \( \langle \nabla \varphi, f^+_0 \rangle < 0 \) and \( \langle \nabla \varphi, f^-_0 \rangle > 0 \), where

\[
f^\pm_0 = \lim_{y \in G^\pm \to u \in S} f^\pm(y, \psi^\pm(y)).
\]

Thus, using Filippov’s regularisation, we arrive at the following system of ODEs

\[
\frac{dy}{dt} = f_0(y),
\]

where,

\[
f_0 = \alpha f^+_0 + (1 - \alpha) f^-_0, \; 0 \leq \alpha \leq 1
\]

and \( \alpha \) as in (8). Note that \( \psi^\pm \) satisfy

\[
g^+(y, \psi^+(y)) = 0
\]

and

\[
g^-(y, \psi^-(y)) = 0.
\]

We next extend the notion of sliding to systems in which it is not easy to express the algebraic variables as explicit functions of the differential variables. We restrict our attention on index-1 DAE systems that have the following form:
If $\varphi(y) > 0$,
\[
\frac{dy}{dt} = f^+(y, z_1, z_2), \quad (30)
\]
\[
0 = g(y, z_1), \quad (31)
\]
\[
0 = h^+(y, z_1, z_2). \quad (32)
\]

Else If $\varphi(y) < 0$,
\[
\frac{dy}{dt} = f^-(y, z_1, z_3), \quad (33)
\]
\[
0 = g(y, z_1), \quad (34)
\]
\[
0 = h^-(y, z_1, z_3). \quad (35)
\]

Here, $z_1(t) \in \mathbb{R}^j$, $z_2(t) \in \mathbb{R}^k$ and $z_3(t) \in \mathbb{R}^l$ with $j + k + l = m$. We also have, $f^+ : \mathbb{R}^{n+j+k} \to \mathbb{R}^n$, $f^- : \mathbb{R}^{n+j+l} \to \mathbb{R}^n$, $g : \mathbb{R}^{n+j} \to \mathbb{R}^j$, $h^+ : \mathbb{R}^{n+j+k} \to \mathbb{R}^k$ and $h^- : \mathbb{R}^{n+j+l} \to \mathbb{R}^l$. Note that in the region where $\varphi(y) > 0$, the system consists of $n$ differential equations and $j + k$ algebraic equations while in the region $\varphi(y) < 0$, we have a system with $n$ differential equations and $j + l$ algebraic equations. One can check that in the air-water system, (11) or (15) corresponds to (31) or (34), (12) corresponds to (32) and (16) corresponds to (35). Similar systems have been studied by others (Agrawal et al., 2003; Moudgalya and Jaguste, 2001).

We next derive the equivalent dynamics of the system described by (30) to (35).

As it is an index 1 system, the Jacobians $[\partial g/\partial z_1]$, $[\partial h^+/\partial z_2]$ and $[\partial h^-/\partial z_3]$ are invertible. Then the implicit function theorem guarantees

1. a function $\phi$ such that $z_1 = \phi(y)$ and
   \[
   g(y, \phi(y)) = 0, \quad (36)
   \]
2. a function $\psi^+(y, z_1)$ such that $z_2 = \psi^+(y, z_1)$, i.e., $z_2 = \psi^+(y, \phi(y))$ and
   \[
   h^+(y, \phi(y), \psi^+(y, \phi(y))) = 0, \quad (37)
   \]
3. and a function $\psi^-$ such that $z_3 = \psi^-(y, \phi(y))$ and
   \[
   h^-(y, \phi(y), \psi^-(y, \phi(y))) = 0. \quad (38)
   \]

Therefore, we obtain
\[
\frac{dy}{dt} = \begin{cases} 
    f^+(y, \phi(y), \psi^+(y, \phi(y))), & \text{if } \varphi(y) > 0 \\
    f^-(y, \phi(y), \psi^-(y, \phi(y))), & \text{if } \varphi(y) < 0.
\end{cases} \quad (39)
\]
As this discontinuous system has only one unknown, namely, $y$, we know how to regularise it. Using Definition 4, the system (30)–(35) is in sliding mode, if the corresponding ODE (39) is in sliding mode. That is, if $\langle \nabla \varphi, f^+_0 \rangle < 0$ and $\langle \nabla \varphi, f^-_0 \rangle > 0$, where,

$$f^+_0 = \lim_{y^* \in G^+ \rightarrow u} f^+(y^*, \phi(y^*), \psi^+(y^*, \phi(y^*))$$

and

$$f^-_0 = \lim_{y^* \in G^- \rightarrow u} f^-(y^*, \phi(y^*), \psi^-(y^*, \phi(y^*))$$

Using Filippov’s procedure, we arrive at an equivalent dynamic model described by

$$\frac{dy}{dt} = \alpha f^+_0 (y, \phi(y), \psi^+(y, \phi(y))) + (1 - \alpha) f^-_0 (y, \phi(y), \psi^-(y, \phi(y))). \quad (40)$$

Note that (40) together with (36) – (38) yields the following system:

$$\frac{dy}{dt} = \alpha f^+ (y, z_1, z_2) + (1 - \alpha) f^- (y, z_1, z_3), \quad (41)$$

$$0 = g(y, z_1), \quad (42)$$

$$0 = h^+(y, z_1, z_2), \quad (43)$$

$$0 = h^-(y, z_1, z_3). \quad (44)$$

Thus, we arrive at the following theorem.

**Theorem 2** Assume that the Jacobians $[\partial g/\partial z_1]$, $[\partial h^+/\partial z_2]$ and $[\partial h^-/\partial z_3]$ are invertible. Further, for some $t^*$ such that $t > t^*$, assume that the system (42)–(44) is in sliding mode. Then, the system described by (30) – (35) is dynamically equivalent in the sense of Filippov to the system (41) – (44).

We first check that this approach works when $\phi$, $\psi^+$ and $\psi^-$ can be explicitly found. We turn to the ideal gas-liquid system, which belongs to this class. Using these explicit functions we had derived an equivalent dynamic description given by (23). The use of the above theorem, on the other hand, yields the following system:

$$\frac{dM_G}{dt} = \alpha F_G + (1 - \alpha)(F_G - G), \quad (45)$$

$$\frac{dM_L}{dt} = \alpha (F_L - L) + (1 - \alpha)F_L, \quad (46)$$

$$0 = V - \left( M_G \frac{RT}{P} + \frac{M_L}{\rho_L} \right), \quad (47)$$

$$0 = L - k_L x(P - P_{out}), \quad (48)$$

$$0 = G - k_G x(P - P_{out}). \quad (49)$$
We see that (47) – (49) correspond to (42) – (44) in order. This set of DAEs describes the equivalent dynamics of the gas-liquid system in sliding motion.

It is easy to check that this system is identical to the one given by (23): We begin with the equivalent dynamic description available from the ODE approach. Substituting for \(f^+\) and \(f^-\), respectively from (20) and (21), and making use of (24), (23) becomes

\[
\frac{dM_G}{dt} = \alpha F_G + (1 - \alpha)F_G - (1 - \alpha)k_G x \left( \frac{M_G RT}{V - \frac{ML}{\rho_L}} - P_{out} \right), \quad (50)
\]

\[
\frac{dM_L}{dt} = \alpha F_L - \alpha k_L x \left( \frac{M_G RT}{V - \frac{ML}{\rho_L}} - P_{out} \right) + (1 - \alpha)F_L. \quad (51)
\]

Using (11) or (15), (12) and (16), we arrive at

\[
\frac{dM_G}{dt} = \alpha F_G + (1 - \alpha)F_G - (1 - \alpha)G, \quad (52)
\]

\[
\frac{dM_L}{dt} = \alpha F_L - \alpha F_L + (1 - \alpha)F_L. \quad (53)
\]

The sliding model given by (45) – (49) is nothing but the above equations, along with the substitutions indicated therein.

While the substitutions indicated by (12) and (16) occur only once, that indicated by (11) or (15) has been used twice. This observation will be used in the subsequent discussion.

This approach of going through the ODE route works only when \(\phi, \psi^+\) and \(\psi^-\) can be obtained explicitly. It is not difficult to visualise a situation where this is not possible. This difficulty arises in the soft-drink mixing process of Agrawal et al. (2003) and in the HDPE system presented by Moudgalaya and Jaguste (2001). Through substitution alone, these cannot be reduced to explicit ODE systems. If differentiation is attempted as a way to convert the DAEs into ODEs, some hidden dynamics may result and the applicability of Filippov’s approach is not clear. Brenan et al. (1996) give several other reasons why dealing with DAEs directly is better than the differentiation route. Rao et al. (2003) demonstrate through an example that it is possible for a simple controller designed using a DAE control theory to work better than an advanced controller designed through the ODE route.

In view of this remark, we will explore different ways of arriving at the equivalent dynamic DAE model for the ideal gas-liquid system directly, i.e., without going through the ODE route.

If we add \(\alpha\) times the equation set (9) – (10) with \((1 - \alpha)\) times the set (13) – (14), we get the differential equation set (45) – (46). We augment this
with all the algebraic constraints present in (9) – (16). Note that the volume constraint given by (11) or (15) indicates the same equation and hence needs to be included only once. This corresponds to (11) or (15) being used twice in the substitution process that has helped arrive at (52) and (53).

The mathematical formulation of this procedure is straight forward:

(1) Form an equivalent dynamical system by combining ODEs only.
(2) Augment the above system with algebraic constraints and without repetitions.

This approach is especially useful when the algebraic variables cannot be expressed as explicit functions of the differential variables, as explained in the next section.

5 A Soft-Drink Production System

In order to test this equivalent DAE dynamic approach, we have modelled a realistic DAE system, possibly applicable in soft-drink manufacturing (Agrawal et al., 2003). It is well known that soft-drinks have CO$_2$ and sugar syrup. Let CO$_2$ and syrup be fed into a mixing tank and withdrawn through a single outlet. As in the ideal gas liquid system, the model that is to be used to describe the gas outflow is referred to as the gas model, while the corresponding model for acid outflow is referred to as the acid model, both consisting of DAEs. Note that

$$CO_2 + H_2O \rightarrow H_2CO_3.$$  

The following assumptions are made to formulate this interesting process:

(1) The system is described by the three components: CO$_2$, H$_2$O and H$_2$CO$_3$.
(2) Intermediate ionization reactions and dissociation of H$_2$CO$_3$ are ignored.
(3) No gas bubbles in the liquid phase.
(4) The valve dynamics are ignored.
(5) Fluid out-flow is proportional to the difference of tank pressure and outlet pressure.
(6) The temperature, outlet pressure, feed outflow rates, valve opening, and valve coefficients, are all constant.

Although this system also has a reaction taking place, its behaviour is similar to that of the air-water system.

The model that is to be used to describe the gas outflow is referred as the gas model while the corresponding model for acid outflow is referred as acid model.
Both of these models is made up of DAEs. Differential equations are required to capture the dynamics. Outflow rate, equilibrium relation, volume constraints and mass balance of the components give rise to algebraic equations. Thus, the process is modelled by two systems of DAEs and at any instant, one of these two is used.

The two models, namely, gas and acid models, have different number of variables. This is because the liquid phase (acid) consists of $H_2CO_3$, $H_2O$ and $CO_2$ while the gas phase has only $CO_2$ as component. Consequently, the two models are described by different number of equations.

Carbon dioxide, water and carbonic acid are referred with subscript 1, 2 and 3, respectively. $F, L$ and $G$, respectively, represent feed inflow, liquid outflow, and gas outflow. $M$ denotes total holdup, while $M_l$ and $M_g$ denote moles of $CO_2$ in liquid and gas phases, respectively. The liquid phase or acid outflow mode of the system is modelled using following DAEs:

\[
\frac{dM_1}{dt} = F_1 - L_1 - r, \tag{54}
\]
\[
\frac{dM_2}{dt} = F_2 - L_2 - r, \tag{55}
\]
\[
\frac{dM_3}{dt} = -L_3 + r, \tag{56}
\]
\[
0 = \frac{M_2}{M_1 + M_2 + M_3} - \frac{L_2}{L_1 + L_2 + L_3}, \tag{57}
\]
\[
0 = \frac{M_3}{M_1 + M_2 + M_3} - \frac{L_3}{L_1 + L_2 + L_3}, \tag{58}
\]
\[
0 = L_1 + L_2 + L_3 - k_L x(P - P_{out}), \tag{59}
\]
\[
0 = M_1 - (M_g + M_l), \tag{60}
\]
\[
0 = P - \frac{\sigma M_l}{M_1 + M_2 + M_3}. \tag{61}
\]

Fig. 3. $CO_2$ mixing using the features of ideal gas-liquid system
and

\[ 0 = V - \left( \frac{M_1 RT}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} \right), \quad (62) \]

where

\[ r = \kappa_c M_1 M_2, \quad (63) \]

and, \( \kappa_c \) is the rate constant. First three equations (54) - (56) are the mass balance of the three components in the reactor. Here, \( r \) is the rate of formation of \( H_2CO_3 \) given in (63). Equations (57) and (58) state that the concentration inside the tank is the same as that in the outflow stream. The acid outflow is given in (59), where \( k_L \) denotes the valve coefficient for liquid flow and \( x \) is the valve opening. The outflow stream has dissolved carbon dioxide, unreacted water and carbonic acid. \( P \) is the reactor pressure. \( M_1 \) in (60) is the total holdup of carbon dioxide in gas and liquid phase. Henry’s law is used to describe the gas liquid equilibrium in (61). The two phase system is constrained by volume of the reactor in (62). The acid outflow mode activates when \( \varphi \) attains nonnegative value. Here, \( \varphi \) is the difference of acid volume (liquid phase) and the volume of the reactor below the outflow tube, \( V_d \):

\[ \varphi = \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} - V_d. \quad (64) \]

As soon as liquid level falls below the outflow tube or \( \varphi < 0 \), the gas outflow starts. As a result \( \varphi \) in (64) changes sign from positive to negative. The equations presented below together with (60) - (62) formulate the system in gas outflow mode.

\[ \frac{dM_1}{dt} = F_1 - G - r, \quad (65) \]

\[ \frac{dM_2}{dt} = F_2 - r, \quad (66) \]

\[ \frac{dM_3}{dt} = r, \quad (67) \]

and

\[ G = k_G x (P - P_{out}). \quad (68) \]

The mass balance of gas in two phases (60), gas-liquid equilibrium (61) and volume constraint (62) are applicable for the gas model also. The molar outflow rate of gas is given in (68); here, \( k_G \) is the valve coefficient for gas flow.

The gas and the acid models have different number of variables. This is because the acid phase consists of \( H_2CO_3 \), \( H_2O \) and dissolved \( CO_2 \), while the gas
Table 1
Incidence matrix of the algebraic variables in the acid model: variable vs. equation number

<table>
<thead>
<tr>
<th></th>
<th>(L_2)</th>
<th>(L_3)</th>
<th>(L_1)</th>
<th>(M_g)</th>
<th>(M_l)</th>
<th>(P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>57</td>
<td>(\otimes)</td>
<td>(\times)</td>
<td>(\times)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>58</td>
<td>(\times)</td>
<td>(\otimes)</td>
<td>(\times)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>59</td>
<td>(\times)</td>
<td>(\times)</td>
<td>(\otimes)</td>
<td>(\times)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td></td>
<td>(\otimes)</td>
<td>(\times)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>61</td>
<td></td>
<td>(\otimes)</td>
<td>(\times)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>62</td>
<td></td>
<td></td>
<td></td>
<td>(\otimes)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**while** the model is to be integrated **do**

**if** the acid model is applicable **then**

**repeat**

**if** gas model was used previously **then**

re-initialise the acid model

**end if**

integrate the acid model

**until** the acid model is invalid

**else**

**repeat**

**if** acid model was used before **then**

re-initialise the gas model

**end if**

integrate the gas model

**until** the gas model is invalid

**end if**

**end while**

Fig. 4. Pseudo-code to integrate soft-drink process using discontinuous model

phase has only \(CO_2\). Acid model is described by 3 ODEs and 6 algebraic equations and gas model is described by 3 ODEs and 4 algebraic equations. The solvability of the acid and the gas models is tested using the incidence matrix analysis proposed by Moudgalya (2001). Both the models are found to be index-1 DAEs. The incidence matrix of the algebraic equations in acid model is as shown in Table 1. The variables are depicted by \(\times\) and output of the equation is assigned by \(\otimes\). It shows every variable is assigned an output of some equation and every equation and every variable gets this assignment once and no more. Hence, the acid model is a solvable index-1 DAE system. The test is straightforward for gas model too.
Table 2
Soft-drink process parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_L$</td>
<td>50 mol/l</td>
</tr>
<tr>
<td>$\rho_a$</td>
<td>16 mol/l</td>
</tr>
<tr>
<td>$V$</td>
<td>10 l</td>
</tr>
<tr>
<td>$V_d$</td>
<td>2.25 l</td>
</tr>
<tr>
<td>$T$</td>
<td>293 K</td>
</tr>
<tr>
<td>$P_{out}$</td>
<td>1 atm</td>
</tr>
<tr>
<td>$x$</td>
<td>1.0</td>
</tr>
<tr>
<td>$k_L$</td>
<td>2.5 l/atm/s</td>
</tr>
<tr>
<td>$k_G$</td>
<td>3.0 l/atm/s</td>
</tr>
<tr>
<td>$F_1$</td>
<td>5.5 mol/s</td>
</tr>
<tr>
<td>$F_2$</td>
<td>7.5 mol/s</td>
</tr>
<tr>
<td>$\kappa_c$</td>
<td>$0.433/4000$ l/mole/s</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>1640 atm/mole frac</td>
</tr>
</tbody>
</table>

Table 3
Initial conditions

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Gas</td>
</tr>
<tr>
<td>$M_1$</td>
<td>0.72 mol</td>
</tr>
<tr>
<td>$M_2$</td>
<td>95.0 mol</td>
</tr>
<tr>
<td>$M_3$</td>
<td>0.0 mol</td>
</tr>
</tbody>
</table>

Table 4
DASSL parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>rtol</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>atol</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>$10^{-4}$</td>
</tr>
</tbody>
</table>

The discontinuous system is integrated using the state of the art DAE integrator, DASSL Brenan et al. (1996), using the algorithm in Fig. 4. The process is characterised by the parameters in Table 2. Initial conditions and DASSL parameters are given in Tables 3 and 4, respectively.
The results are plotted in Fig. 5 and 6 with dotted lines: in the former, the total holdup of the three components inside the reactor (CO$_2$, H$_2$O, H$_2$CO$_3$) are plotted; in the latter, from the top, fraction of the gas dissolved in liquid, acid concentration and CO$_2$ concentration, respectively, in the liquid phase are plotted. The system reaches sliding mode at approximately $t = 46s$.

We next solve this system using the proposed equivalent dynamic approach. One can check that it is difficult to reduce these DAEs to ODEs through substitution.

We first calculate $\alpha$ as explained in (7)-(8). We obtain from (64)

$$\nabla \varphi = \left( \frac{\partial \varphi}{\partial M_1}, \frac{\partial \varphi}{\partial M_2}, \frac{\partial \varphi}{\partial M_3} \right) = \left( 0, \frac{1}{\rho_L}, \frac{1}{\rho_a} \right)$$

$f_0^+$ is given by (54)-(56) while $f_0^-$ is given by (65)-(67). We obtain,

$$\langle \nabla \varphi, f_0^+ \rangle = \frac{1}{\rho_L} (F_2 - L_2 - r) + \frac{1}{\rho_a} (-L_3 + r)$$

$$\langle \nabla \varphi, f_0^- \rangle = \frac{1}{\rho_L} (F_2 - r) + \frac{r}{\rho_a}$$

Using (8), we obtain the following expression for $\alpha$:

$$\alpha = \frac{F_2 \rho_a + r(\rho_L - \rho_a)}{L_2 \rho_a + L_3 \rho_L}.$$  \hspace{1cm} (69)

The equivalent dynamic equations, indicated by (41)-(44) are obtained as,

$$\frac{dM_1}{dt} = \alpha (G - L_1) + F_1 - G - r,$$ \hspace{1cm} (70)

$$\frac{dM_2}{dt} = -\alpha L_2 + F_2 - r,$$ \hspace{1cm} (71)

$$\frac{dM_3}{dt} = -\alpha L_3 + r,$$ \hspace{1cm} (72)

$$0 = \frac{M_2}{M_1 + M_2 + M_3} - \left( \frac{L_2}{L_1 + L_2 + L_3} \right),$$ \hspace{1cm} (73)

$$0 = \frac{M_3}{M_1 + M_2 + M_3} - \left( \frac{L_3}{L_1 + L_2 + L_3} \right),$$ \hspace{1cm} (74)

$$0 = L_1 + L_2 + L_3 - k_L x (P - P_{out}),$$ \hspace{1cm} (75)

$$0 = G - k_G x (P - P_{out}),$$ \hspace{1cm} (76)

$$0 = M_1 - (M_g + M_l),$$ \hspace{1cm} (77)

$$0 = P - \frac{\sigma M_l}{M_1 + M_2 + M_3},$$ \hspace{1cm} (78)

$$0 = V - \left( \frac{M_1 RT}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} \right),$$ \hspace{1cm} (79)
The equivalent DAE system is also of index 1. It is integrated using DASSL with initial conditions obtained at the beginning of the sliding motion. The onset of sliding is detected by checking at the points of discontinuity, for the satisfaction of the conditions $\langle \nabla \varphi, f^+_0 \rangle < 0$ and $\langle \nabla \varphi, f^-_0 \rangle > 0$, see Theorem 1 and Definition 3. The same conditions have to be satisfied for the system to continue in the state of sliding.

Simulation of a discontinuous DAE system is expensive because of frequent initializations and the associated startup problems. Moreover, one is also constrained to take small steps because of discontinuity sticking in the gas model, while the system is in sliding mode (Moudgalya and Ryali, 2001): When the gas model is used, no matter how small a step size is used, the inflow of liquid will raise the liquid level above the dip tube and invalidate the assumption of the validity of the gas model. As in the equivalent dynamic formulation, we deal with only a continuous DAE system, the above problems do not exist. The proposed method can be several orders of magnitude more efficient than the discontinuous method. We noticed that the computation speed had improved by a factor of over 10,000 times in a typical simulation.

Although not reported here, this approach has been found to work well (Nigam et al., 2006) also in the discontinuous HDPE slurry reactor system presented by Moudgalya and Jaguste (2001).

The reader should note that no feedback controller has been used in this study. In case the speed of response is not acceptable, a feedback control structure, as reported in Moudgalya and Jaguste (2001), could be used.

6 Conclusions

In this work, we presented examples of discontinuous DAE systems that have the property of sliding. Integrating such systems is a numerically expensive proposition because of frequent initialisations. This difficulty is compounded by the fact that one is forced to take small steps, owing to the discontinuity sticking.

It is shown in this work that an equivalent dynamic description consisting of DAEs can be obtained for a class of discontinuous DAEs. This method combines only the ODEs and augments them with algebraic constraints.

Numerical solution of the equivalent dynamic system gives results identical to the ones obtained through the integration of the discontinuous system. As the proposed method converts a discontinuous system into a continuous one on the sliding surface $S$, it is several orders of magnitude more efficient than the
Fig. 5. Comparison of solution of discontinuous (dotted lines) and equivalent dynamic models (solid line)

one involving discontinuous models. This is of immense value in differential algebraic systems, where we have seen a speed factor of the order of 10,000.
Fig. 6. Comparison of solution of discontinuous (dotted lines) and equivalent dynamic models (solid line)
Nomenclature

Roman Symbols

$F^±$  Augmented forcing functions for DAEs
$F_1$  Flow-rate of $CO_2$ in feed, mol/s
$F_2$  Flow-rate of water in feed, mol/s
$F_G$  Gas feed rate, mol/s
$F_L$  Liquid feed rate, mol/s
$f^±$  Forcing function
$G$  Gas outflow rate, mol/s and subscript to indicate gas
$g^±$  Vector of algebraic constraints
$k_L$  Valve coefficient for gas flow
$k_G$  Valve coefficient for liquid flow
$L$  Liquid outflow rate, mol/s and subscript to indicate liquid
$L_1$  $CO_2$ outflow in acid model, mol/s
$L_2$  Water outflow in acid model, mol/s
$L_3$  $H_2CO_3$ outflow in acid model, mol/s
$M_1$  Moles of $CO_2$ in reactor, mol
$M_2$  Moles of water in reactor, mol
$M_3$  Moles of $H_2CO_3$ in reactor, mol
$M_G$  Gas holdup in the ideal system, mol
$M_L$  Liquid holdup in the ideal system, mol
$M_g$  Moles of $CO_2$ in gas phase, mol
$M_l$  Moles of $CO_2$ in liquid phase, mol
$P$  Pressure, atm
$P_{out}$  Outlet pressure, atm
$R$  Gas constant, l atm/mol/K
$r$  $H_2CO_3$ formation rate $= \kappa e^{\frac{M_1 M_2}{1}}$, mol/l/s
\( T \) Temperature in the reactor, K
\( \Delta t \) integration interval, s
\( V \) Volume of the reactor, l
\( V_d \) Volume below the dip tube, l
\( x \) Valve opening

**Greek symbols**

\( \sigma \) Henry’s constant for \( CO_2 \), atm/mole frac
\( \rho_L \) Molar density of water, mol/l
\( \rho_a \) Molar density of acid, mol/l
\( \kappa_c \) Rate constant, 1/mol/s
\( \varphi \) Switch function

**References**


