Abstract: Starting from the equations describing the equivalent dynamics of ordinary differential equations (ODEs), an equivalent dynamical differential algebraic equation (DAE) system is derived. It is shown that a procedure similar to the one available for ODEs can be used to construct an equivalent DAE system as well. The proposed method is shown to work with a class of discontinuous DAE systems typified by an ideal gas-liquid system and a soft drink manufacturing process.

Keywords: Sliding mode, Equivalent dynamics, Hybrid system, Singular system, Multiple forcing functions, Discontinuous system, Soft drink process.

1. INTRODUCTION

Simulation is a popular method to assess the safety of processes. This approach becomes even more important in difficult processes, such as those, for example, described by DAEs and discontinuities.

Discontinuous dynamical systems occur reasonably frequently in real life, see for example, the works of Mosterman et al. (1997), Moudgalya and Jaguste (2001) and Agrawal et al. (2002). These authors articulate the need to understand such systems and to solve them efficiently. Dynamical systems are generally modelled by DAEs. In view of this discussion, it is not surprising that discontinuous DAE systems occur reasonably often.

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. Although discontinuous systems made of DAEs also are known to possess this property (Moudgalya and Jaguste 2001), there exists no mathematical treatment of these systems.

Most of the time, DAEs are converted into ODEs for analysis and numerical solution. Brenan et al. (1996) argue why it is better to treat the DAEs directly. Vora et al. (2002) 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, at times it may be difficult to convert the DAEs into ODEs.

This study proposes a method for treating discontinuous DAEs in the DAE framework itself. This is illustrated with a simple gas-liquid system (Moudgalya and Ryali 2001) and a more complicated soft drink process.
2. AN IDEAL GAS-LIQUID SYSTEM IN SLIDING MOTION

Consider the ideal gas-liquid system studied by Moudgalya and Ryali (2001), with two phases in the tank and one outlet (see Fig. 1).

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 liquid level in the tank, 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)
\[
\begin{align*}
\frac{dM_G}{dt} & = F_G, \\
\frac{dM_L}{dt} & = F_L - L, \\
0 & = V - \left( M_G \frac{RT}{P} + \frac{M_L}{\rho_L} \right), \\
0 & = L - k_Lx(P - P_{out}).
\end{align*}
\]

Else If \( \frac{M_L}{\rho_L} < V_d \) (gas model)
\[
\begin{align*}
\frac{dM_G}{dt} & = F_G - G, \\
\frac{dM_L}{dt} & = F_L, \\
0 & = V - \left( M_G \frac{RT}{P} + \frac{M_L}{\rho_L} \right), \\
0 & = G - k_Gx(P - P_{out}).
\end{align*}
\]

The system keeps switching between these two models. The symbols are the same as the ones used by Agrawal et al. (2002).

Through substitution, a system of ODEs with two forcing functions is arrived 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
\[
f^+ = \begin{bmatrix} F_G \\ F_L - k_Lx \left( \frac{M_G RT}{V - \frac{M_L}{\rho_L}} - P_{out} \right) \end{bmatrix},
\]
with the switching function \( \varphi(M_G, M_L) > 0 \) and when the gas comes out, it is
\[
f^- = \begin{bmatrix} F_G - k_Gx \left( \frac{M_G RT}{V - \frac{M_L}{\rho_L}} - P_{out} \right) \end{bmatrix},
\]
with \( \varphi(M_G, M_L) < 0 \). 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 reaches the sliding mode, characterised by the following equivalent dynamics (Filippov 1988),
\[
\frac{d}{dt} \begin{bmatrix} M_G \\ M_L \end{bmatrix} = f_0,
\]
\[
f_0 = \alpha f^+ + (1 - \alpha) f^-, \quad 0 \leq \alpha \leq 1,
\]
\[
\alpha = \frac{\langle \nabla \varphi, f^- \rangle - \langle \nabla \varphi, f^+ \rangle}{\langle \nabla \varphi, f^- \rangle - \langle \nabla \varphi, f^+ \rangle},
\]
with the following specific values,
\[
f_0 = \begin{bmatrix} c_2 - c_1 M_G \\ 0 \end{bmatrix},
\]
\[
c_1 = \frac{k_{Gx}RT}{V - V_d} > 0,
\]
\[
c_2 = \left( \frac{F_G}{k_Gx} + \frac{F_L}{k_Lx} + P_{out} \right) k_Gx.
\]

They have shown that the behaviour of the equivalent system (16) is in exact agreement with the numerical solution of discontinuous system, (9).

3. TOWARDS EQUIVALENT DYNAMICS FOR DAES IN SLIDING MOTION

Although the DAEs can be converted into ODEs in the case of a simple system, such as the one discussed above, this may not be possible in a general case. An example in case is the High Density Polyethylene reactor (Moudgalya and Jaguste 2001) described by two DAE models consisting of 15 and 12 equations. This problem could become worse if more chemical components are present. In situations like these, we may not be able to convert the DAEs into ODEs by simple substitution. For the reasons discussed in Section 1 also, we may want to handle the DAEs directly. These reasons have motivated us to consider the construction of equivalent dynamics described by DAEs.

We begin with the equivalent dynamic description available from the ODE approach. Substituting
for \( f^+ \) and \( f^- \), respectively from (10) and (11) and making use of (14), (13) becomes
\[
\frac{dM_G}{dt} = \alpha F_G + (1- \alpha)F_G - \alpha k_G x \frac{M_GRT}{V - \frac{M_G}{\rho_G}} - P_{out},
\]
(17)
\[
\frac{dM_L}{dt} = \alpha F_L - \alpha k_L x \frac{M_GRT}{V - \frac{M_G}{\rho_L}} - P_{out} + (1- \alpha)F_L.
\]
(18)
From (3) or (7) we get,
\[
P = \frac{M_GRT}{V - \frac{M_G}{\rho_L}},
\]
(19)
and from (4), (8) we get,
\[
L = k_L x (P - P_{out}),
\]
(20)
\[
G = k_G x (P - P_{out}),
\]
(21)
using which, (17) and (18) become
\[
\frac{dM_G}{dt} = \alpha F_G + (1- \alpha)F_G - (1- \alpha)G,
\]
(22)
\[
\frac{dM_L}{dt} = \alpha F_L - \alpha L + (1- \alpha)F_L.
\]
(23)
While the substitutions indicated by (20) and (21) occur only once, that indicated by (19) has been used twice. This observation will be used in the subsequent discussion. We rewrite the above equations and order them in a way suitable for further discussion:
\[
\frac{dM_G}{dt} = \alpha F_G + (1- \alpha)(F_G - G),
\]
(24)
\[
\frac{dM_L}{dt} = \alpha (F_L - L) + (1- \alpha)F_L,
\]
(25)
\[
0 = V - \left( \frac{M_GRT}{P} + \frac{M_L}{\rho_L} \right),
\]
(26)
\[
0 = L - k_L x (P - P_{out}),
\]
(27)
\[
0 = G - k_G x (P - P_{out}).
\]
(28)
This set of DAEs describes the equivalent dynamics of the gas-liquid system in sliding motion. It is identical to the one obtained by Moudgalya and Ryali (2001). This can be verified by straightforward substitution of algebraic variables in differential equations.

The above set of equations can also be derived directly from (1) – (8), as described next. If we add \( \alpha \) times the equation set (1) – (2) with (1 – \( \alpha \)) times the set (5) – (6), we get the differential equation set (24) – (25). We augment this with all the algebraic constraints present in (1) – (8). Note that the volume constraint given by (3) and (7) indicates the same equation and hence needs to be included only once. This corresponds to (19) being used twice in the substitution process that has helped arrive at (22) and (23).

The mathematical formulation of this procedure is straightforward: (1) Form an equivalent dynamical system by combining ODEs only. (2) Augment the above system with algebraic constraints. In the next section, we present a Filippov like procedure to combine the entire DAE sets.

4. EQUIVALENT DAEs IN SLIDING

We would like to find out whether the Filippov’s method of multiplying the entire set of ODEs by \( \alpha \) can be extended to the entire set of DAEs as well. That is, we would like to multiply each equation in (1) to (4) by \( \alpha \) and add to \((1- \alpha)\) times the corresponding equation in the gas model. One can easily check that this procedure will give rise to (24) to (26).

Thus we can extend Filippov’s procedure to the entire DAE set only if we have equations that describe the chosen phenomenon in both the models. This motivates us to define the missing equations. As no liquid flows out of the system during the gas model, one may be tempted to use \( L = 0 \) as the liquid flow equation in the gas model. Unfortunately, such a combination would produce an equation different from (4) and hence will violate the derivation of equations (24) – (28): recall that to derive this equivalent dynamics, we have used (4).

Then we ask the question, “With what equation can we combine (4) so that it comes out unchanged?” The answer is obvious: combine it with an equation of the form \( 0 = 0 \). Similarly, (8) can be combined with the equation \( 0 = 0 \).

We present the mathematical formulation of this second approach now. Suppose the following discontinuous DAEs are in a sliding state.
\[
\frac{dy}{dt} = f(y, z),
\]
(29)
\[
0 = g(y, z),
\]
(30)
where, \( f, g \in \mathbb{R}^n \); \( y, z \in \mathbb{R}^n \) and
\[
f = \begin{cases} f^+(y, z), & \varphi(y, z) > 0, \\ f^-(y, z), & \varphi(y, z) < 0, \end{cases}
\]
(31)
\[
g = \begin{cases} g^+(y, z), & \varphi(y, z) > 0, \\ g^-(y, z), & \varphi(y, z) < 0. \end{cases}
\]
(32)
With the usual vector notation
\[
F^\pm = (f^\pm, g^\pm) = (f^\pm(y, z), g^\pm(y, z)),
\]
(33)
we get the following equivalent dynamics:

$$\begin{bmatrix} \frac{dy}{dt} \\ 0 \end{bmatrix} = F_0$$

(34)

where,

$$F_0 = \alpha F^+ + (1-\alpha)F^-, \quad 0 \leq \alpha \leq 1$$

(35)

$$\alpha = \frac{\langle \nabla \phi, (f^-_G, g^-) \rangle - \langle \nabla \phi, (f^+_G, g^+) \rangle}{\langle \nabla \phi, (f^-_G, g^-) \rangle}.$$ 

(36)

One can see this procedure to be identical to the one proposed by Filippov for ODEs.

Note that this method of combining the equations is not generic because it requires domain knowledge. For example, we have to combine the liquid flow equation with the corresponding liquid flow equation only. Unfortunately, it is not clear how to overcome this requirement. It is noteworthy, however, that Filippov’s approach also has this restriction implicitly. For example, we combine the two equations corresponding to $dM_G/dt$ only - we do not combine the equation corresponding to $dM_G/dt$ in one model with that corresponding to $dM_L/dt$ in the other.

5. APPLICATION

In order to test this equivalent DAE dynamic approach, we have modelled a realistic DAE system, possibly applicable in soft drink manufacturing. 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.

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 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. Each model of the system is shown in Table 1. 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 discontinuous system is integrated using the state of the art DAE integrator, DASSL (Brenan et al. 1996), using the algorithm in Fig. 2. The parameters in Table 2 are used in this simulation. In Table 2, initial conditions (left) and DASSL parameters (right) are given. The results are plotted in Fig. 3 and 4 with dotted lines. Sliding motion is observed in this simulation.

while the model is to be integrated do
if the acid model is applicable then
repeat
if gas model was used previously then
re-initialize 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-initialize the gas model
end if
integrate the gas model
until the gas model is invalid
end if
end while

Fig. 2. Pseudo-code to integrate soft drink process

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>$\nu_0$</td>
<td>0.433/400 l/mole/s</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>1640 atm/mole frac</td>
</tr>
</tbody>
</table>

Table 3. Initial conditions and DASSL parameters

<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>
<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>

We next solve this system using the proposed equivalent dynamic approach. One can check that these DAEs cannot be reduced to ODEs through substitution. The missing equations in columns 2 and 3 of Table 1 are represented by an equation of the form $0 = 0$. The equivalent DAE dynamic approach is then applied to this system: find $\alpha$ times the equations in column 2 and $1 - \alpha$ times the corresponding equations in column 3 to arrive at the following equations:

$$\frac{dM_1}{dt} = \alpha(G - L_1)F_1 - G - r,$$ 

(37)

$$\frac{dM_2}{dt} = -\alpha L_2 + F_2 - r,$$ 

(38)

$$\frac{dM_3}{dt} = -\alpha L_3 + r,$$ 

(39)
Table 1. Discontinuous DAE model for CO₂ mixing in soft-drink process with 
\[ \varphi = \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} - V_d. \]

<table>
<thead>
<tr>
<th>Model</th>
<th>Acid Model ((F^+, \varphi &gt; 0))</th>
<th>Gas Model ((F^-, \varphi &lt; 0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂ balance</td>
<td>[ \frac{dM_1}{dt} = F_1 - L_1 - r ]</td>
<td>[ \frac{dM_1}{dt} = F_1 - G - r ]</td>
</tr>
<tr>
<td>H₂O balance</td>
<td>[ \frac{dM_2}{dt} = F_2 - L_2 - r ]</td>
<td>[ \frac{dM_1}{dt} = F_2 - r ]</td>
</tr>
<tr>
<td>H₂CO₃ balance</td>
<td>[ \frac{dM_3}{dt} = -L_3 + r ]</td>
<td>[ \frac{dM_3}{dt} = r ]</td>
</tr>
<tr>
<td>Acid outflow</td>
<td>0 = L_1 + L_2 + L_3 - k_{L,x}(P - P_{out})</td>
<td>0 = 0</td>
</tr>
<tr>
<td>H₂O outflow</td>
<td>0 = ( \frac{M_1 + M_2 + M_3}{M_4} ) - ( \frac{L_1 + L_2 + L_3}{L_3} )</td>
<td>0 = 0</td>
</tr>
<tr>
<td>H₂CO₃ in outflow</td>
<td>0 = ( \frac{M_2 + M_3}{M_4} )</td>
<td>0 = 0</td>
</tr>
<tr>
<td>Gas outflow</td>
<td>0 = 0</td>
<td>0 = 0</td>
</tr>
<tr>
<td>Gas-liquid equilibrium</td>
<td>0 = ( P - \frac{M_1 + M_2 + M_3}{\sigma M_1} )</td>
<td>0 = ( P - \frac{M_1 + M_2 + M_3}{\sigma M_1} )</td>
</tr>
<tr>
<td>CO₂ in the reactor</td>
<td>0 = ( M_1 - (M_2 + M_3) )</td>
<td>0 = ( M_1 - (M_2 + M_3) )</td>
</tr>
<tr>
<td>Volume constraint</td>
<td>0 = ( V - \left( \frac{M_1 RT}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} \right) )</td>
<td>0 = ( V - \left( \frac{M_1 RT}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} \right) )</td>
</tr>
</tbody>
</table>

\[ 0 = \frac{M_2}{M_1 + M_2 + M_3} \left( \frac{L_2}{L_1 + L_2 + L_3} \right), \quad (40) \]
\[ 0 = \frac{M_2}{M_1 + M_2 + M_3} \left( \frac{L_3}{L_1 + L_2 + L_3} \right), \quad (41) \]
\[ 0 = L_1 + L_2 + L_3 - k_{L,x}(P - P_{out}), \quad (42) \]
\[ 0 = G - k_{G,x}(P - P_{out}), \quad (43) \]
\[ 0 = M_1 - (M_2 + M_3), \quad (44) \]
\[ 0 = P - \frac{\sigma M_1}{M_1 + M_2 + M_3}, \quad (45) \]
\[ 0 = V - \left( \frac{M_1 RT}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} \right), \quad (46) \]

where, \( \alpha \) can be found on substitution of \( F^+ \) and \( F^- \) from Table 1 in (36) as
\[ \alpha = \frac{F_2 \rho_a + r(\rho_L - \rho_a)}{L_2 \rho_a + L_3 \rho_L}. \quad (47) \]

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, which is found during simulation of discontinuous system. These results are plotted with solid lines in Fig. 3 and in the former, the total holdup of the three components inside the reactor (CO₂, H₂O, H₂CO₃) are plotted; in the latter, from the top, fraction of the gas dissolved in liquid, acid concentration and CO₂ concentration, respectively, in the liquid phase are plotted.

6. CONCLUSIONS

It is shown that an equivalent dynamic description consisting of DAEs can be obtained for a class of discontinuous DAEs. Two methods have been proposed towards this end. The first method combines only the ODEs and augments them with algebraic constraints. The second method is more Filippov-like in the sense that the algebraic equations also participate in the combining step.

Simulation of a discontinuous DAE system is expensive because of the frequent initialisations and the associated startup problems. Moreover, one is also constrained to take small steps because of difficulties, such as, discontinuity sticking (Moudgalaya and Ryali 2001). The equivalent dynamic formulation overcomes these difficulties: the proposed method is several orders of magnitude more efficient than the discontinuous method.
Fig. 4. Dotted line: discontinuous system. Solid line: equivalent dynamics.

NOMENCLATURE

Roman Symbols

- $F^\pm$: Augmented forcing functions for DAEs
- $F_1$: Flow-rate of CO$_2$ in feed mole/s
- $F_2$: Flow-rate of water in feed mole/s
- $F_G$: Gas feed rate, mol/s
- $F_L$: Liquid feed rate, mol/s
- $f^\pm$: Forcing function
- $G$: Gas outflow rate, mol/s and subscript to indicate gas
- $g^\pm$: 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 kmole/hr
- $L_2$: Water outflow in acid model mole/s
- $L_3$: H$_2$CO$_3$ outflow in acid model mole/s
- $M_G$: Gas holdup in the system, mol
- $M_{CO_2}$: Moles of CO$_2$ in reactor mole
- $M_{H_2CO_3}$: Moles of H$_2$CO$_3$ in reactor mole
- $M_C$: Moles of CO$_2$ in acid model mole
- $M_H$: Moles of H$_2$CO$_3$ in reactor mole
- $M_L$: Moles of CO$_2$ in liquid phase mole
- $P$: Pressure atm
- $P_{out}$: Outlet pressure atm
- $R$: Gas constant l atm/mole/K
- $r$: H$_2$CO$_3$ formation rate $= \frac{\kappa_c M_a M_b}{V}$ mole/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 moles/l
- $\rho_a$: Molar density of acid moles/l
- $\kappa_c$: Rate constant l/mol/s
- $\varphi$: Switch function

REFERENCES


