16th European Symposium on Computer Aided Process Engineering
and 9th International Symposium on Process Systems Engineering
W. Marquardt, C. Pantelides (Editors)

Equivalent dynamic solution of an industrial HDPE slurry reactor

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Abstract

A discontinuous industrial High Density Polyethylene (HDPE) reactor system, described by 15 Differential Algebraic Equations (DAEs) and 12 DAEs, has been numerically solved in this work. This system is characterised by frequent switches between these two sets of DAEs, making the numerical solution expensive. Using an extension of Filippov's regularisation approach, we obtain an equivalent, continuous, dynamic model of the discontinuous system. The equivalent dynamic solution is several orders of magnitude faster than the discontinuous solution.

1. Introduction

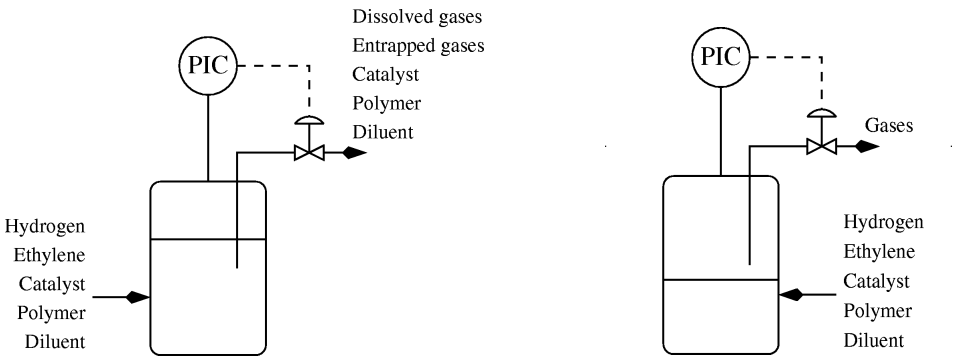
Discontinuous systems are especially common in man made technologies. An example of this is the sliding mode controller. This approach is present in process industry as well. Moudgalya and Jaguste [1] have reported a realistic discontinuous slurry process to produce HDPE. Moudgalya et al. [2] have reported that such discontinuities can be used to understand fundamental mechanisms, to improve mixing, to enhance heat transfer coefficients and to produce stable two phase flows. Numerical solution of these systems, however, is expensive owing to frequent switches. This is especially true when DAEs are present, thanks to frequent initialisations. Moudgalya and Ryali [3] show that these systems exhibit discontinuity sticking, with small step sizes being the solution. Finally, in optimisation processes, designed to tune model parameters [1], a complete simulation has to be carried out for every objective function evaluation. All of the above observations point to the necessity of an efficient integration procedure for such discontinuous processes. In this report, we present the equivalent dynamic solution to the HDPE reactor system studied by [1] and compare its performance with the discontinuous solution.

2. Discontinuous HDPE Model

In an industrial slurry process, studied in detail by [1], ethylene is polymerised into HDPE in a well mixed reactor in the presence of hydrogen and a Ziegler Natta catalyst dispersed in a diluent, a schematic of which is shown in Fig. 1. The slurry level in this figure is given by $ML_4/\rho + ML_5$, where, the variables are as defined in [1]. First define the switching function φ as follows:

$$\varphi = \frac{ML_4}{\rho} + ML_5 - V_d \tag{1}$$

We obtain the following slurry model when $\varphi > 0$ (Fig. 1(a)):



(a) Slurry model (b) Gas model

Figure 1. A schematic of HDPE reactor, described by slurry and gas models

$$\frac{dM_1}{dt} = F_1 - L_1 - r_1 \tag{2}$$

$$\frac{dM_2}{dt} = F_2 - L_2 - r_2 \tag{3}$$

$$\frac{dML_3}{dt} = F_3 - L_3 \tag{4}$$

$$\frac{dML_4}{dt} = F_4 - L_4 + \frac{28r_2}{1000} \tag{5}$$

$$\frac{dML_5}{dt} = F_5 - L_5 \tag{6}$$

$$\frac{ML_1}{\frac{ML_4}{\rho}+ML_5} = \frac{L_1}{\frac{L_4}{\rho}+L_5} \tag{7}$$

$$\frac{ML_2}{\frac{ML_4}{\rho}+ML_5} = \frac{L_2}{\frac{L_4}{\rho}+L_5} \tag{8}$$

$$\frac{ML_3}{\frac{ML_4}{\rho}+ML_5} = \frac{L_3}{\frac{L_4}{\rho}+L_5} \tag{9}$$

$$\frac{ML_4}{\frac{ML_4}{\rho}+ML_5} = \frac{L_4}{\frac{L_4}{\rho}+L_5} \tag{10}$$

$$\frac{L_4}{\rho} + L_5 = 0.2268C_v\sqrt{\frac{P-P_{out}}{g_s}} \tag{11}$$

When $\varphi < 0$ (Fig. 1(b)), the system is modelled by

$$\frac{dM_1}{dt} = F_1 - G_1 - r_1 \tag{12}$$

$$\frac{dM_2}{dt} = F_2 - G_2 - r_2 \tag{13}$$

$$\frac{dML_3}{dt} = F_3 \tag{14}$$

$$\frac{dML_4}{dt} = F_4 + \frac{28r_2}{1000} \tag{15}$$

$$\frac{dML_5}{dt} = F_5 \tag{16}$$

$$\frac{MG_1}{MG_2} = \frac{G_1}{G_2} \tag{17}$$

$$(G_1 + G_2)\frac{RT}{P} = 0.2268C_v\sqrt{\frac{P-P_{out}}{g_g}} \tag{18}$$

The following equations are applicable, whatever the value of φ is:

$$ML_1 + MG_1 = M_1 \tag{19}$$

$$ML_2 + MG_2 = M_2 \tag{20}$$

$$\frac{\alpha_1 MG_1}{(MG_1+MG_2)\frac{RT}{P}} = \frac{ML_1}{\frac{ML_4}{\rho}+ML_5} \tag{21}$$

$$\frac{\eta\alpha_2 MG_2}{(MG_1+MG_2)\frac{RT}{P}} = \frac{ML_2}{\frac{ML_4}{\rho}+ML_5} \tag{22}$$

$$(MG_1 + MG_2)\frac{RT}{P} + \frac{ML_4}{\rho} + ML_5 = V \tag{23}$$

In the above model, the subscripts 1 to 5, respectively, denote hydrogen, ethylene, catalyst, polymer and diluent. F, L and G, respectively, stand for inflow rate of feed and outflow rates of slurry and gases. M denotes the total holdup in the reactor, while, ML and MG, respectively, denote the holdup in the slurry and the gas phases. All the symbols used above have the same meaning as in [1], except for g_s and g_g, which now denote the densities of the slurry and the gas streams flowing out of the reactor through the control valve. A proportional integral controller is used to control this system. For further details, the reader is referred to [1]. This system is solved with the help of DASSL [4] using the procedure of [1]. Pressure in the reactor, ethylene concentration in the gas phase and the slurry level, as functions of time, are shown in Fig. 2. After initial swings, the slurry level in the reactor settles down at the level of the dip tube. As gas and slurry leave the reactor alternatively, the applicable model also keeps changing [1].

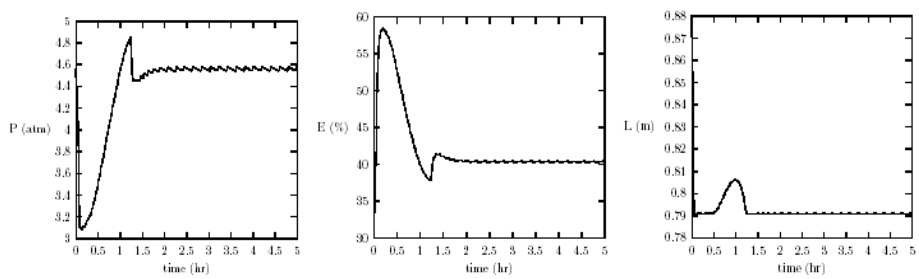


Figure 2. Pressure, ethylene and slurry level in HDPE reactor

A mathematical idealisation of this is referred to as sliding. The procedure to handle ODE systems in sliding mode is well known [5].

3. Equivalent Dynamics

In this section, we first state the results available for a class of discontinuous, index-1 DAE systems, while in sliding mode [6,7], and then apply them to the HDPE reactor under discussion. Consider a discontinuous system described by the following equations:

If $\varphi(y)>0$,

$$\frac{dy}{dt} = f^{+}(y, z_1, z_2) \tag{24}$$

$$0 = g(y, z_1) \tag{25}$$

$$0 = h^{+}(y, z_1, z_2) \tag{26}$$

Else if $\varphi(y)<0$

$$\frac{dy}{dt} = f^{-}(y, z_1, z_3) \tag{27}$$

$$0 = g(y, z_1) \tag{28}$$

$$0 = h^{-}(y, z_1, z_3) \tag{29}$$

Here, $z_1(t) \in R^j, z_2(t) \in R^k$ and $z_3(t) \in R^l$ with $j+k+l=m$. We also have, $f^{+}:R^{n+j+k} \rightarrow R^n$, $f^{-}:R^{n+j+l} \rightarrow R^n$, $g:R^{n+j} \rightarrow R^j$, $h^{+}:R^{n+j+k} \rightarrow R^k$ and $h^{+}:R^{n+j+k} \rightarrow R^k$. Note that in the region where $\varphi(y)>0$, the system consists of $n\psi$ 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.

In the HDPE system, Eq. (2) to (6) are denoted by Eq. (24); Eq. (7) to (11) are denoted by Eq. (26); Eq. (12) to (16) are denoted by Eq. (27); Eq. (17) and (18) are denoted by Eq. (29). Finally, the vector g that appears in Eq. (25) and (28) stands for Eq. (19) to (23). If the system reaches sliding mode, the equivalent dynamics can be described by [6,7],

$$\frac{dy}{dt} = \alpha f^{+}(y, z_1, z_2) + (1-\alpha) f^{-}(y, z_1, z_3) \tag{30}$$

$$0 = g(y, z_1) \tag{31}$$

$$0 = h^{+}(y, z_1, z_2) \tag{32}$$

$$0 = h^{-}(y, z_1, z_3) \tag{33}$$

Where, α is calculated as follows:

$$\alpha=\frac{(\Delta\varphi, f^{-})}{(\Delta\varphi, f^{-})-(\Delta\varphi, f^{+})} \tag{34}$$

We now apply this approach to the HDPE reactor system [8]:

$$\Delta\varphi=(0,0,0,\frac{1}{\rho},1) \tag{35}$$

$$(\Delta\varphi, f^{+}) = \frac{1}{\rho}(F_4 - L_4 + \frac{28r_2}{1000}) + F_5 - L_5 \tag{36}$$

$$(\Delta\varphi, f^{-}) = \frac{1}{\rho}(F_4 + \frac{28r_2}{1000}) + F_5 \tag{37}$$

Substituting these in Eq. (34), we obtain

$$\alpha = \frac{F_4+28r_2/1000+\rho F_5}{L_4+\rho L_5} \tag{38}$$

In order to complete the description of the sliding model, we need to calculate only Eq. (30). We obtain the following:

$$\frac{dM_1}{dt} = F_1 - G_1 - r_1 + \alpha(G_1 - L_1) \tag{39}$$

$$\frac{dM_2}{dt} = F_2 - G_2 - r_2 + \alpha(G_2 - L_2) \tag{40}$$

$$\frac{dML_3}{dt} = F_3 - \alpha L_3 \tag{41}$$

$$\frac{dML_4}{dt} = F_4 + \frac{28r_2}{1000} - \alpha L_4 \tag{42}$$

$$\frac{dML_5}{dt} = F_5 - \alpha L_5 \tag{43}$$

The equivalent dynamic system is solved by DASSL, using the same integration parameters as in the discontinuous system. Unlike before, however, there are no discontinuities now. We get results identical to the ones in Fig. 2.

The comparison of two approaches, namely, integration of discontinuous and the equivalent dynamic models was carried out in a Mac PowerBook G4, with a 667 MHz processor, 512 MB RAM, operating with Mac OS X, version 10.2.8. The time taken by the equivalent dynamic approach for the dassl parameter of dtout is taken as the metric for comparison. The number of times the discontinuous method required for different dtout values is shown in Fig. 3. Note that we are justified in choosing a fixed value of dtout for the equivalent dynamic system, as there are no discontinuities in it, whereas, one has to choose small values for the discontinuous system, owing to discontinuity sticking. The equivalent dynamic model is several orders of magnitude more efficient than the discontinuous model. As a matter of fact, one can even argue that it is not fair to compare the two models.

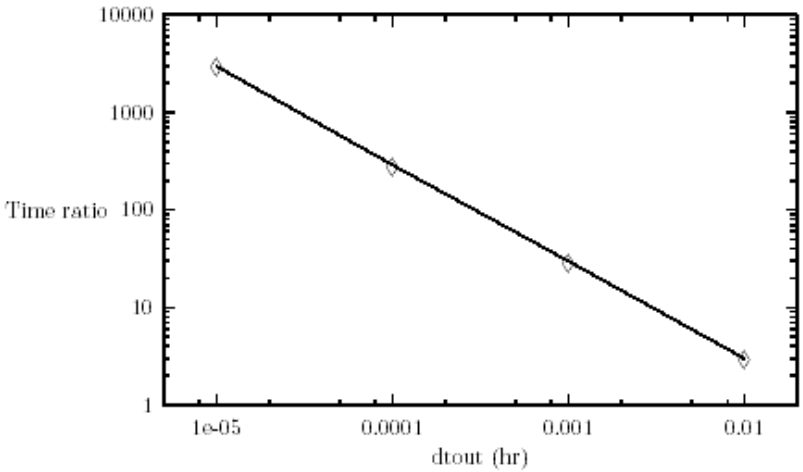


Figure 3. Ratio of time taken by discontinuous model for different dtout values to time taken by equivalent dynamic model with dtout=0.01hr

4. Conclusion

Using the extension of Filippov's regularisation procedure, an equivalent dynamic model of a discontinuous HDPE reactor system, modelled by 15 DAEs and 12 DAEs is obtained. Numerical solution of the equivalent dynamic system is identical to the one obtained through the integration of the discontinuous system. As the proposed method converts a discontinuous system into a continuous one on the sliding surface, it is several orders of magnitude more efficient than the one involving discontinuous models. This is of immense value, especially, when DAEs are to be integrated as a part of an optimisation process.

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