Using Optimization to Detect Snowball Effects

by

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Abstract: In process plants with recycle streams some level control architectures are inoperable. Their use leads to large excursions in manipulated and/or controlled variables and this behavior has been termed the snowball effect. The snowball effect is a steady state phenomenon and it can be analyzed using steady state process models. In this paper a steady state mixed integer nonlinear programming (MINLP) approach is used to analyze for large excursions in process variables. This MINLP approach can be used to detect the likely occurrence of a snowball effect in a plant and to develop control architectures that can avoid this problem. The optimization-based approach is illustrated on a three-reactor three-distillation column plant taken from the literature.

Introduction

The design of plantwide control systems has received increasing attention in the last few years. Tighter plant designs, due to such considerations as energy integration and reduced emissions, are leading to more challenging control problems. Several authors have proposed approaches to the problem of configuring plantwide control systems. These approaches range from those based on optimization[1-3] to those that are heuristic in nature[4]. In all plantwide control designs, it is necessary to control variables that are non-self regulating in nature. The most common process example of such variables is liquid level in a vessel. Buckley[5] was the first to address the problem of controlling inventory in a plant. If one considers only controlling liquid inventories, then controlling liquid levels can result in problems with other variables in the process. These problems have been labeled as snowball effects by Luyben and co-workers[4,6].

Luyben and Luyben[6] presented a control study of a three-reactor/three-distillation tower process that is shown in Fig. 1. Most control schemes for this plant were found to be inoperable, and these schemes exhibited the snowball effect. As discussed by Luyben et.al.[4] the snowball effect arises in systems with recycle flows when small changes in one variable result in extremely large changes in other process variables. Their results indicate that in designing a plantwide control system, liquid level loops need to be configured carefully so that a snowball effect does not occur. Luyben et.al.[4] point out that the snowball effect is essentially a steady state phenomenon. Thus, whether or not it is likely to occur can be analyzed using a steady state model that includes integrating variables. This paper proposes an approach, using mixed integer nonlinear programming (MINLP) on steady state process models coupled with a model for the integrating variables, that can detect whether the snowball effect is likely to occur in a process. Once a potential snowball problem is detected, then a second MINLP optimization can be solved to determine which additional variables need to be controlled to avoid the snowball problem. Using the results of the optimization one can systematically select level control systems together with any additional variables that need to be controlled to avoid snowball effects.

This paper is organized as follows. First the development of the steady state model used is discussed. Next the MINLP optimization approach is discussed and applied to the three-reactor/three-distillation tower process[6]. It is shown that snowball effects will occur in this plant. Then, a second optimization problem is proposed to determine if additional variables can be controlled to avoid snowball effects. Finally conclusions are presented.

Development of Steady State Model

The steady state model used for the snowball analysis consists of two parts. The measurement vector, y, is separated into y_N, for non-integrating measurements, and y_I for the integrating measurements. For y_N a typical nonlinear steady state process model is used:

$$0 = f(x,u,d_j) \qquad (1)$$

$$y_N = g(x,u,d_j) \qquad (2)$$

where x is the state vector, u is the vector of manipulated variables and d_j is the disturbance being considered. The y_I measurements are not included in a steady state model. Here they are included and it is assumed that a linearized model for their rate of change is acceptable for analyzing snowball effects. This model can be developed from a linearized dynamic model using the approach published by Arkun and Downs[7]. Alternatively it can be approximated as done by Mc Avoy and Miller[8]. The model for y_I has the form:

$$\dot{y}_I = K_I u + d_{j,I} \qquad (3)$$

where $d_{j,I}$ is the effect of the disturbance on the rate of change of the integrating measurements.

In order to use Eqns. 1 to 3 to analyze for snowball effects, the plant under consideration is assumed to have only integrating poles, and no right half plane poles. If the plant has right half plane poles then it must be stabilized to use the approach given below. The problem that is solved involves controlling at least all of the integrating variables in the plant. The approach taken is similar to that presented by Mc Avoy[3] for synthesizing plantwide control systems. Control of y_I requires that:

$$\dot{y}_I = K_I u + d_{j,I} = 0 \qquad (4)$$

Equation 4 assumes steady state control in which $\dot{y}_I = 0$, and in the optimization approach discussed below u is assumed to be a valve movement. In analyzing for potential snowball effects all potential disturbances need to be considered, one at a time.

Optimization-Based Analysis of the Snowball Effect

The optimization problem solved to detect the snowball effect involves determining which manipulated u's should be used to control the y_I's for a given disturbance, and whether any product measurements exceed reasonable bounds due to the control effort applied. One measure of how good a particular level control architecture is can be taken to be how much the manipulated valves it uses have to move from their original steady state positions when d_j occurs. A system that requires large changes in valve positions is deemed inferior to one requiring smaller changes. In formulating an objective function for detecting the snowball effect, both positive and negative changes in valve movement are penalized. To account for both changes, u is re-written in terms of ν^+ and ν^- as:

$$u = v^+ - v^- \qquad (5)$$

where the elements of ν^+ and ν^- are all positive. To emphasize that valve movements are being considered, the symbol ν is used in place of u. It is assumed that the ν's all have the same units, e.g. between 0 and 100%. Then, an optimization problem to detect the snowball effect can be formulated as shown in Eqn. 6. In Eqn. 6 $v^+_{k,\max}$ and $v^-_{k,\max}$ are the maximum changes permitted for the valve movements away from their steady state values, $\Delta y_{\min}$ and $\Delta y_{\max}$ are the minimum and maximum allowable changes in the product measurements, κ is equal to the number of valves in the plant, and M is equal to the number of integrating measurements. The objective function is the sum of the absolute values of the movements of all of the valves used for controlling the integrating variables. The first equality constraint involves control of the integrating variables, Eqn. 4. The second equality constraint enforces steady state. The first inequality constraints involve product measurements. These constraints enforce reasonable limits on the excursions of these measurements after an upset. How to choose these limits is discussed below. The next 2 constraints deal with saturation of the manipulated variables. If a valve is selected $(z_k^+, z_k^- \neq 0)$, then it is constrained not to saturate either open or closed.

$$
\begin{aligned}
&\min_{v^+, v^-, z^+, z^-} \quad \sum_{k=1}^{k} (v_k^+ + v_k^-) \\
&s.t. \\
&K_I(v^+ - v^-) + d_{j,I} = 0 \\
&0 = f(x, v^+ - v^-, d_j) \\
&\Delta y_{\min} \le \Delta g(x, v^+ - v^-, d_j) \le \Delta y_{\max} \\
&n_k^+ \le z_k^+ v_{k,\max}^+ \ \ (k = 1:k) \\
&v_k^- \le z_k^- v_{k,\max}^- \ \ (k = 1:k) \\
&\sum_{k=1}^{k} (z_k^+ + z_k^-) = M \qquad\qquad (6) \\
&v_k^+, v_k^- \ge 0 \\
&z_k^+, z_k^- \in \{0,1\}
\end{aligned}
$$

It can be noted that in Eqn. 6 the integer variables appear in a linear manner. The solution of Eqn. 6 gives the M manipulated variables that have to move the least in order to keep the y_I measurements at their setpoints. If Eqn. 6 has a feasible solution then one can conclude that there is a control structure for the integrating variables that does not have a snowball problem for the plant under consideration. Integer cuts can be used to generate additional feasible control architectures for the integrating variables by ruling out earlier solutions. The application of Eqn. 6 to a plant shown in Fig. 1 is discussed next.

Application of Optimization Methodology

For th e process shown in Fig. 1, there are 9 integrating liquid level measurements, 3 each for the reactors, reflux accumulators, and reboilers. The steady state considered here is similar to that given by Luyben and Luyben [6] in their Table 12. However, their flows do not material balance exactly, and their plant model is not exactly at steady state. Flows were changed slightly from their results so that the plant started at steady state. Since stream densities are independent of composition, it is straightforward to develop Eqn. 3 for the nine integrating levels in this process. For example for reactor 1 the following model can be used:

$$A_1 c\dot{l}_1 = F_{OA} + D_1 + D_3 - F_1 \qquad (7)$$

where A_1 is the cross sectional area, c is the molal density and the right hand side consists of the various flows into and out of the reactor. Since $\dot{l}$ is set to 0, one can use ±1 for the gains in the first row of Eqn. 3, i.e. the $1/A_1c$ in each gain can be factored out. Then these gains can be scaled in terms of % flow. The product measurements consist of the mole fraction of C in the distillate from tower 2, y_{2C}, and the mole fraction of F in the bottoms from tower 3, x_{3F}. There are potentially 19 manipulated flows in the plant, but depending on the disturbance not all can be used. Changes in the fresh feed of A were used as a disturbance by Luyben and Luyben[6], and its elimination results in 18 manipulated variables. Three disturbances, given in reference[6], are considered here, and they are: 1. a 20% step change in feed composition of A; 2. a 50% step change in the specific reaction rate in the first reactor; and 3. a 20% step change in the feed flow of A. Since disturbances 1 and 2 do not involve flow changes, they are simpler to analyze than disturbance 3. For disturbances 1 and 2 control of y_I does not require any changes in u. All the manipulated variables, except the makeup of B and D (fod and fob), are constrained to be within 0 and twice their steady state values. The two makeup streams are constrained to be within ±50. Product mole fractions are constrained to be within ±.02. The reason for the somewhat loose specification on these bounds is that level control only cannot be expected to yield tight control of product composition. Rather what one is looking for is very large excursions in these variables which in turn will cause a snowball effect when one attempts to tightly control them. Note that one could add other variables to be constrained in the formulation such as reactor compositions. The second optimization problem discussed below does consider tighter control of the product variables.

For disturbances 1 and 3 no feasible solution to Eqn. 6 is found. Table 1 gives results for all three disturbances where it can be seen that extremely large changes in both the distillate composition in tower 2 and the bottoms composition in tower 3 occur for disturbances 1 and 3. The results for disturbance 3 are for a particular level configuration, but they are typical of what is calculated for other level schemes. By contrast disturbance 2 yields a feasible solution to Eqn. 6. The compositions of A and B in reactor 1 change significantly for disturbance 2 since it involves a 50% increase in the kinetic constant for reactor 1, but the product compositions are hardly affected. Actually it is not necessary to analyze all disturbances, since lack of feasibility for ***any*** disturbance indicates a potential snowball effect. For the Luyben and Luyben plant one can conclude that a snowball problem is likely. The optimization results indicate that one could not operate the plant by controlling only the 9 liquid levels when disturbance 1 or 3 occurs. If the plant can be operated in these cases, additional variables need to be controlled. To determine whether the snowball problem can be avoided a second optimization problem, discussed next, can be solved.

Additional Optimization Problem

To determine if the snowball problem can be avoided, additional integer variables, ζ, can be added to Eqn. 6 as follows:

$$
\begin{aligned}
&\min_{v^+,v^-,z^+,z^-,z} \quad \sum_{k=1}^{k}(v_k^+ + v_k^-) + m\sum_{j=1}^{J} z_j \\
&s.t. \\
&K_I(v^+ - v^-) + d_{j,I} = 0 \\
&0 = f(x, v^+ - v^-, d_j) \\
&\Delta y^*_{\min}(1 - z) \le \Delta g(x, v^+ - v^-, d_j) \le \Delta y^*_{\max}(1 - z) \\
&n_k^+ \le z_k^+ v_{k,\max}^+ \ (k = 1:k) \\
&v_k^- \le z_k^- v_{k,\max}^- \ (k = 1:k) \\
&\sum_{k=1}^{k}(z_k^+ + z_k^-) = M + \sum_{j=1}^{J} z_j \\
&v_k^+, v_k^- \ge 0 \\
&z_k^+, z_k^-, z_j \in \{0,1\} \\
&m = scalar
\end{aligned}
\tag{8}
$$

Eqn. 8 allows for additional non-integrating measurements, y*, to be controlled in order to achieve feasibility. The y* measurements include product measurements as well as other key measurements such as reactor compositions. If an additional measurement is chosen, then its ζ_j is 1. If v^+ and v^- are scaled in the range 0-100, then choosing m to be large, e.g. 1000, forces the optimization to limit the number of additional measurements that are controlled for feasibility. For measurements of product variables very tight constraints can be used for $\Delta y^*_{\min}$ and $\Delta y^*_{\max}$ since these constraints reflect how one would like the plant to operate. One could even specify that certain measurements need to be controlled exactly to steady state. Some engineering judgement is involved in the specification of bounds on the process measurements. Eqn. 8 is a difficult MINLP problem whose solution is currently under investigation. Since Eqn. 8 involves a larger number of integer variables than Eqn. 6 and some of these integer variables appear in the objective function its is more difficult to solve than Eqn. 6 is. The solution of Eqn. 8 yields plantwide architectures that avoid snowball problems.

Some preliminary results on the solution of Eqn. 8 have been calculated. If the fresh feed of A, F_{OA}, is a disturbance then it appears that no feasible solution of Eqn. 8 can be found. When F_{OA} changes too many light components escape in the bottom of tower 1 and these components exit in the distillate from tower 2, lowering the composition of C in this stream. Two feasible solutions of Eqn. 8 have been found and one is the same as scheme 1c presented by Luyben and Luyben. The second solution is similar, but it does not adhere to the rule of fixing a flow in every recycle loop. Results for the application of Eqn. 8 to the Luyben and Luyben process will be presented at the conference.

Conclusions

An optimization-based approach to detecting the snowball effect in plantwide control designs has been presented. The approach makes use of a steady state model and it involves solving a MINLP problem. The results of this problem indicated whether snowball effects are likely to occur in a particular plant. If such problems are likely, then one can solve a second problem to determine which additional variables need to be controlled to avoid the snowball effect. Preliminary results on a three-reactor/three-distillation tower process have been presented. The optimization-based approach holds promise as a systematic method for determining plantwide control architectures that avoid snowball problems.

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Table 1 Results for Solving Equation 6

Case	**Mol. Fract. C Tower-2**	**Mol. Fract. F Tower-3**
Base	0.9713	0.9980
disturbance 1	0.7762	0.8115
disturbance 2	0.9716	0.9980
disturbance 3	0.2398	0.3798

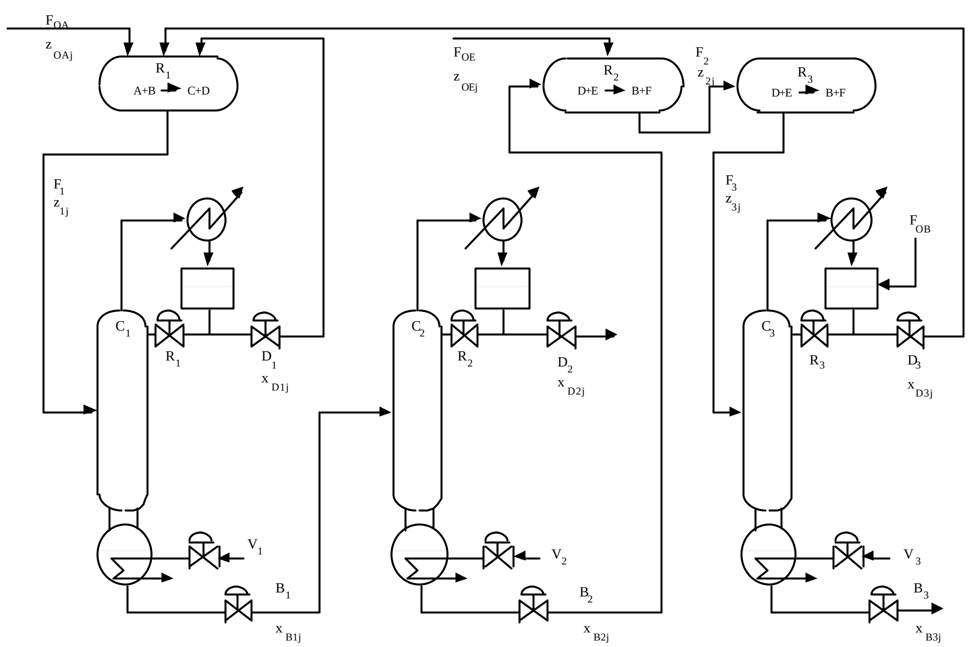

Figure 1 Luyben and Luyben Plant