A Definition for Plantwide Controllability

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Abstract

Chemical process synthesis typically accounts for model uncertainty by ensuring process flexibility. However, ensuring process flexibility does not guarantee steady-state robust feasibility (i.e., the existence of a plantwide control system to maintain the process at a desired steady state in the presence of uncertainty). We show, through examples, that the difference between process flexibility and steady-state robust feasibility can be observed at three levels of severity. A definition for plantwide controllability that guarantees steady-state robust feasibility is proposed.

Keywords

Flexibility, Controllability, Plantwide control, Steady-State robust feasibility

Introduction

A minimum requirement for process synthesis is to design an operable process. A process is operable if there exists a plantwide control system to maintain the process at a desired steady state in the presence of uncertainty. Considering uncertainty explicitly during process synthesis is important for many reasons. For example, models used for process synthesis are rarely perfect and assumptions made during process synthesis may not hold exactly. As a result, the process may not be operable if the uncertainty is not properly accounted for.

Researchers have proposed using various process flexibility conditions during process synthesis to ensure that there exist feasible steady-state operating conditions in the presence of uncertainty. In general, these conditions are independent of plantwide control systems. Grossmann and co-workers (Swaney and Grossmann, 1985a,b, etc.), for example, have developed several methods to deal with uncertainty optimally. More recent work in this area has been by Pistikopoulos and co-workers (Pistikopoulos, 1995; Georgiadis and Pistikopoulos, 1999, etc.) who focus on combining more than one operability characteristics during synthesis—such as flexibility, controllability and reliability. In this paper, we will show that ensuring process flexibility does not guarantee the existence of a plantwide control system. In fact, we identify three cases in which the process design satisfies the process flexibility conditions although the process is not plantwide controllable at the desired steady state.

Controllability is generally considered after a process has been synthesized. Many tools have been proposed to study process controllability issues (Lee et al., 1991; Braatz et al., 1991; Braatz and Morari, 1994; Skogestad and Wolff, 1992, etc.). However, most of the tools assume a fixed control structure (i.e., a fixed set of controlled variables and manipulated variables) and focus on the controller synthesis. The plantwide controllability definition proposed in this paper does not assume a fixed control structure.

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Process Flexibility

Process flexibility is defined by Grossmann and Swaney (Swaney and Grossmann, 1985a) as "the ability of a design to tolerate and adjust to variations in conditions which may be encountered during operation." Mathematically, this definition means that, for each allowable value of p and d, there exist allowable values of u and y such that the following is feasible:

$$\begin{cases} f(u,d,y,x,p) & = 0 \\ g(u,d,y,x,p) & \leq 0 \end{cases} \tag{1}$$

where x are the design variables, u are the manipulated variables, d are the disturbances, y are the outputs and p are the system parameters. The equation set, f, corresponds to all the energy and material balances and other algebraic equations (e.g., vapor-liquid relations), while g corresponds to the process constraints for the system (e.g., input and output constraints). Notice that for simplicity, we have only considered the parametric uncertainty and ignored the structural uncertainty.

This process flexibility definition assumes that both u and y can be adjusted based on the values of d and p to ensure (1) is feasible. However, in practice, both d and p are rarely known exactly. A common strategy is to adjust u to maintain some of the outputs at desired setpoints via a plantwide control system, an aspect not considered by the process flexibility definition. Therefore, we would expect that ensuring process flexibility is not sufficient to guarantee the steady-state robust feasibility, defined below.

Steady-State Robust Feasibility: A process is robustly feasible at steady state if there exists a plantwide control system so that (1) is feasible for all allowable values of p and d.

Plantwide Controllability

We propose a definition for plantwide controllability which explicitly considers the plantwide control system. In this definition, the steady-state relations for the plantwide control system are represented by $h(u, d, y, x, p, r) = 0$, where r represents the setpoints for a set of controlled variables.

Steady-State Plantwide Controllability: A process is plantwide controllable at steady state if there exist h and r such that the following is feasible for all allowable values of d and p:

$$\begin{cases} f(u, d, y, x, p) & = 0 \\ g(u, d, y, x, p) & \leq 0 \\ h(u, d, y, x, p, r) & = 0 \end{cases} \quad (2)$$

Notice that h and r are not unique. For fixed h and r, the plantwide controllability reduces to the conventional controllability.

Comparing the process flexibility condition (1) and the proposed plantwide controllability condition (2), it should be clear that ensuring process flexibility is a necessary but not a sufficient condition to guarantee steady-state plantwide controllability (i.e., a design which satisfies the process flexibility condition may not be steady-state plantwide controllable). In fact, there are three cases where (2) is not feasible even if (1) is feasible:

- Case 1: The steady-state plantwide controllability is not guaranteed for a fixed set of controlled variables at fixed setpoints (i.e., h and r are fixed). However, the steady-state plantwide controllability may be restored by simply choosing alternative setpoints.
- Case 2: The steady-state plantwide controllability is not guaranteed for a fixed set of controlled variables regardless of their setpoints (i.e., h is fixed but r is not). The steady-state plantwide controllability may be restored by choosing an alternative set of controlled variables.
- Case 3: The steady-state plantwide controllability is not guaranteed regardless of the controlled variable set and their setpoints (i.e., both h and r are not fixed). The steady-state plantwide controllability can only be restored through process retrofits or redesign.

We illustrate the first two cases using the Hydrodealkylation of Toluene (HDA) process and the third case using a reactor-separator-recycle (RSR) process.

HDA Process—Cases 1 and 2

We assume that the reactions involved in this process are

Rxn 1 $Toluene + Hydrogen \rightarrow Benzene + Methane$

Rxn 2 $2Benzene \leftrightarrow Diphenyl + Hydrogen$

Parameter	Reaction 1	Reaction 2
Rate constant	6×10^{14}	7.6×10^{14}
ΔH_{rxn} (kJ/kgmol)	-42,000	8,100
Activation Energy (kJ/kgmol)	220,000	130,000

Table 1: Kinetic parameters for the HDA process: units for reaction 1 rate constants are $\frac{(ft^3)^{1/2}}{lbmol^{1/2}-hr}$ while the units for reaction 2 rate constants are $\frac{ft^3}{lbmol-hr}$.

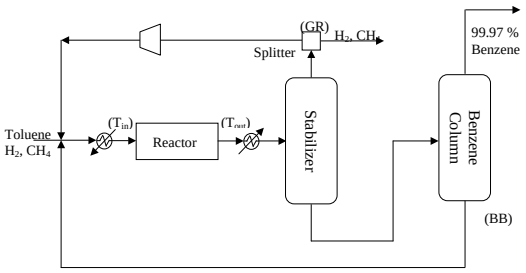

Figure 1: Simplified flowsheet for HDA process.

Both reactions are elementary and the nominal values of the kinetic parameters for these reactions are summarized in Table 1. To study the effect of model uncertainty, we assume a 50% uncertainty in the rate constant for Reaction 1.

The flowsheet of the HDA process (Figure 1) is simplified by assuming that diphenyl is recycled to extinction and that there is no impurity in the feed stream nor any by-product other than diphenyl. The stabilizer is also assumed to yield a perfect split. Finally, fixing the pressure in the benzene column (P = 2 atm) and the fresh feed flowrates, there are four degrees of freedom—one for the reactor, two for the benzene column, and one for the gas recycle splitter.

Constraints for this process include a benzene product purity constraint (99.97%), flooding and weeping constraints for the benzene column (2000 and 500 kgmol/hr respectively (Kister, 1989)), and a maximum reactor outlet temperature (700 deg C) to prevent coking.

In the following sections, we present designs for Cases 1 and 2. Both designs consist of a 54 stage benzene column with the feed entering at the 38th stage and a reactor diameter fixed at 3.05 meters. However, the reactor length in the two designs differs.

Case 1: Infeasible at Fixed Setpoints

Consider the process with a reactor length of 24.4 meters. We can verify that this design satisfies condition (1) by fixing the benzene bottoms composition and gas recycle ratio at 0.05% and 88% and decreasing the reac-

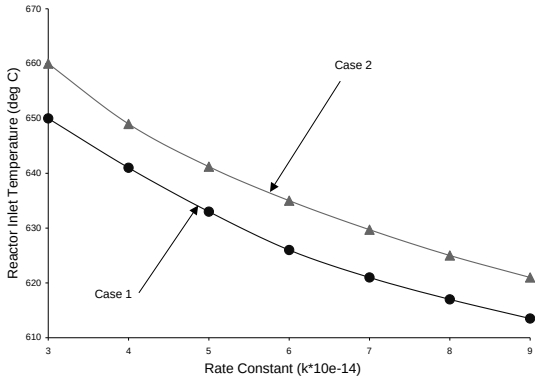

Figure 2: Reactor inlet temperature setpoint as function of the rate constant for the designs in Cases 1 and 2.

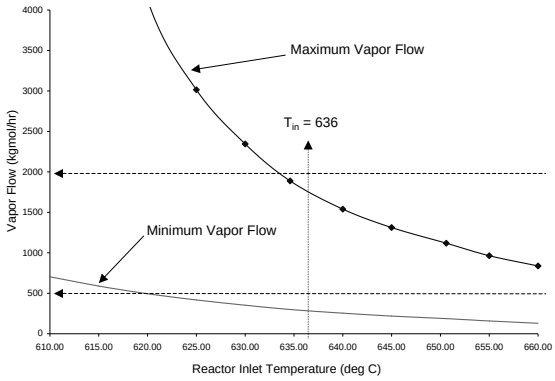

Figure 3: Minimum and maximum column vapor flows as functions of reactor inlet temperature setpoint with gas recycle setpoint of 88% and benzene bottoms composition setpoint of 0.05%.

tor inlet temperature with increasing values of the rate constant as shown in Figure 2. The maximum vapor flow, minimum vapor flow and maximum reactor outlet temperature obtained when following this trajectory are 1800 kgmol/hr, 1300 kgmol/hr and 689 deg C respectively. Since there exist steady-state operating conditions which satisfy all process constraints despite the uncertainty, this design satisfies condition (1).

However, to change the reactor inlet temperature setpoint according to this trajectory, exact values of the rate constant are needed. Since this is usually not the case in practice, we instead control the reactor inlet temperature, benzene product purity, benzene bottoms composition, and gas recycle ratio setpoints at 636 deg C, 99.97%, 0.05%, and 88%, respectively. Note that since we are only interested in the steady-state plantwide controllability, we merely need to select a set of controlled variables and their setpoints. Figure 3 shows

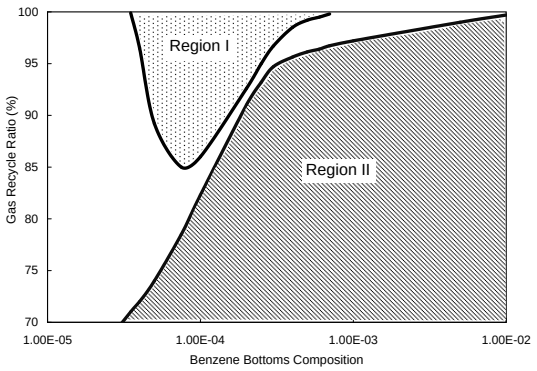

Figure 4: Feasibility regions for the design in Case 2.

that, for this reactor inlet temperature setpoint, the minimum vapor flow is less than the weeping constraint of 500 kgmol/hr. Therefore, the design with the proposed plantwide control system is not feasible at the specified setpoints although condition (1) is satisfied. In fact, no setpoint for the reactor inlet temperature would satisfy both flooding and weeping limits in this case.

Steady-state plantwide controllability can be restored to this process by choosing alternative setpoints. For example, changing the benzene bottoms composition setpoint to 0.01% and the reactor inlet temperature to 649 deg C would guarantee that all process constraints are satisfied.

Case 2: Infeasible for Fixed Controlled Variables

With a reactor of length 18 meters, the design still satisfies condition (1) (Figure 2 for Case 2). The maximum and minimum vapor flows in this case are 1900 and 1400 kgmol/hr while the maximum reactor outlet temperature is 695 deg C. However, steady-state plantwide controllability is still not guaranteed since the rate constant is not known exactly in practice.

Suppose we choose the benzene bottoms composition, gas recycle ratio, reactor inlet temperature and the benzene product purity as controlled variables. Figure 4 then maps the regions in which the flooding, weeping and reactor outlet temperature constraints are satisfied for different gas recycle ratios and benzene bottoms compositions setpoints. In this diagram, Region I corresponds to the setpoints which satisfy the flooding and weeping constraints, while Region II corresponds to the setpoints which satisfy the flooding and the reactor outlet temperature constraints. Since Region I and II do not overlap, there does not exist a gas recycle ratio and benzene bottoms composition setpoint satisfying all process constraints. This controlled variable set is therefore not feasible regardless of the setpoints.

Steady-state plantwide controllability can be restored to this system, by choosing an alternative set of con-

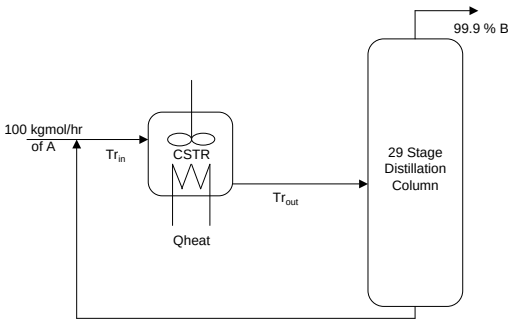

Figure 5: Reactor-Separator-Recycle process.

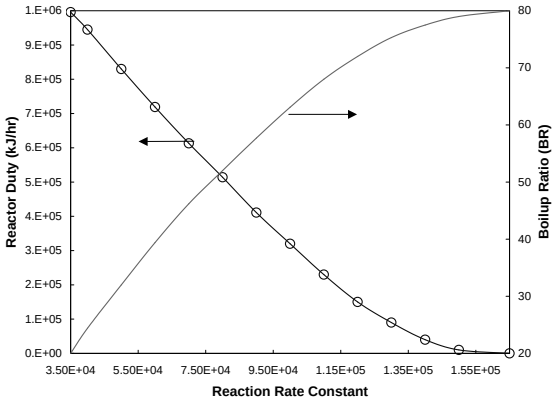

Figure 6: Reactor duty and reboil ratio setpoints as functions of the rate constant.

trolled variables. This can be accomplished, for example, by using the reboil duty (with a setpoint of 3×10^6 kJ/hr) instead of the benzene bottoms composition as a controlled variable.

Case 3: RSR Process

Determining a HDA design that is infeasible for all steady-state control structures requires the evaluation of all controlled variable alternatives and setpoints. To illustrate this third case without the associated complexity, we use a simpler process with one less degree of freedom—a reactor-separator-recycle (RSR) process (Figure 5).

The reactor in this process is a CSTR with a volume of 0.6 m^3, while the separator is a 29-stage distillation column with the feed entering at the 15th stage. The reaction is $A \rightarrow B$ with elementary kinetics. The activation energy and heat of reaction are 5×10^4 and -8.5×10^3 kJ/kgmol, respectively, while the nominal value of the rate constant, k_r, is 10^5. The effects of uncertainty are studied by assuming that the actual rate constant could be any value between $k_{rmin} = 3.5 \times 10^4$ and $k_{rmax} = 1.65 \times 10^5$.

Constraints for this process include flooding and weeping limits (12000 kgmol/hr and 3000 kgmol/hr, respectively) for the distillation column, a minimum reactor feed temperature ($Tr_{in} \geq 55$ deg C), a maximum reactor effluent temperature ($Tr_{out} \leq 117.5$ deg C), and a product purity constraint in the distillate of 99.9% B. We can verify that condition (1) is satisfied for this design by choosing setpoints according to the rate constant as shown in Figure 6: The maximum and minimum vapor flows in the column are 12000 and 7000 kgmol/hr, respectively, the minimum reactor feed temperature is 65 deg C and the maximum reactor effluent temperature is 114 deg C.

However, choosing setpoints in this fashion assumes that the rate constant is known exactly. Since this may not be the case in practice, the question is: Can we synthesize a plantwide control system such that all constraints can be satisfied for all possible values of the rate constant? For this system, we have to choose three controlled variables—two for the distillation column and one for the reactor. Choosing the product purity of B as one controlled variable, we are left with selecting two more controlled variables. Controlled variable alternatives for the reactor include the reactor duty and the reactor effluent temperature while controlled variable alternatives for the stripping section of the distillation column include the reboil ratio, the reboil duty and the bottoms composition of A.

With the reactor effluent temperature as the controlled variable for the reactor, there are two important limits. When the reaction rate constant is at the minimum possible value (i.e., $k_r = k_{rmin}$), a reactor effluent temperature setpoint greater than 114 deg C is required to ensure that the maximum vapor flow in the column would be less than 12000 kgmol/hr. On the other hand, when the rate constant is at the maximum possible value (i.e., $k_r = k_{rmax}$), a reactor effluent temperature setpoint less than 109 deg C is necessary to satisfy the weeping constraint. Since there does not exist a reactor effluent temperature setpoint satisfying both the flooding and weeping constraints for all possible values of the rate constant, any controlled variable set with the reactor effluent temperature would not be feasible and can be eliminated. The only controlled variable alternative remaining for the reactor is the reactor duty. Note that the reactor duty setpoint has to be less than 10^6 kJ/mol to satisfy the reactor effluent temperature constraint. With the product purity and reactor duty as controlled variables, we now discuss three alternatives with the bottoms composition of A, reboil ratio, or reboil duty as the other controlled variable.

For the controlled variable set with the bottoms composition of A, the setpoints for which the flooding and weeping constraints are satisfied are shown in Figure 7.

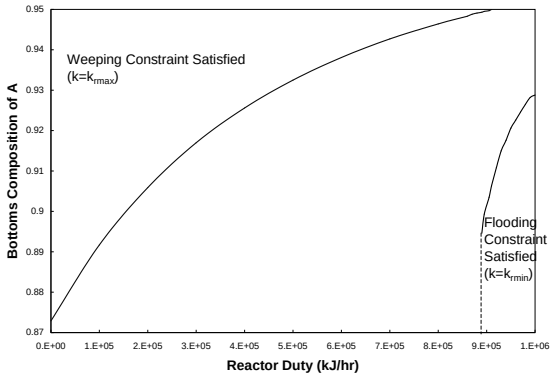

Figure 7: Feasibility regions with reactor duty and bottoms composition as controlled variables.

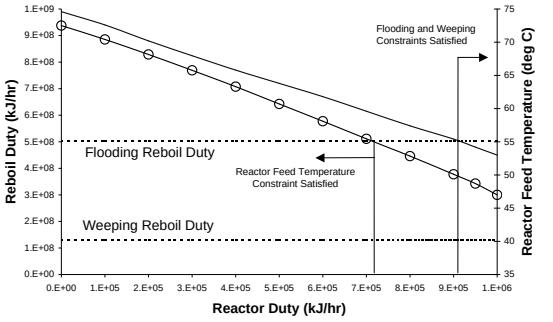

Figure 8: Feasibility regions with reactor duty and reboiler duty as controlled variables (minimum reactor feed temperature plotted by circles).

Since there do not exist setpoints which satisfy both the constraints, this controlled variable alternative is also not feasible. A graph similar to Figure 7 is obtained when using the reboil ratio instead of the bottoms composition of A and therefore, the controlled variable set with reboil ratio and reactor duty is also not feasible.

The final alternative to be studied utilizes the reactor duty, reboil duty and the product purity of B as controlled variables. With this controlled variable set, Figure 8 indicates that for reactor duties greater than 9×10^5 kJ/hr, there exist reboiler duty setpoints which satisfy both the flooding and weeping constraints. However, these setpoints are yet again infeasible since the minimum reactor feed temperature is below 55 deg C at these operating conditions.

From this discussion, it should be apparent that although this design satisfies condition (1), there may not exist a set of controlled variables and corresponding setpoints which would satisfy all process constraints for the given uncertainty. It should be emphasized that we only explored the obvious controlled variable alternatives and that we did not explore all possible alternatives (e.g., control of tray temperature, control of a variable that is a function of the column composition profile, etc.). While the steady-state plantwide controllability can be restored to designs corresponding to cases 1 and 2 with relatively small modifications, processes which fall in this third case have no recourse but for a major redesign or retrofit.

Conclusions

In this paper, we showed that ensuring process flexibility does not guarantee steady-state robust feasibility. A definition for steady-state plantwide controllability that ensures steady-state robust feasibility is proposed. The difference between this definition of plantwide controllability and the conventional controllability definition is that plantwide controllability does not assume a fixed controlled structure.

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