PROCESS ANALYSIS AND OPTIMIZATION

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Contents

Summary

This chapter is intended as a brief overview of chemical process flowsheeting, optimization and analysis. It is intended for graduate students in engineering and science. It is also intended as a quick introduction for researchers who need to use process analysis tools. For the expert, it is intended as a quick refresher. It covers basic flowsheeting, solution of systems of nonlinear equations arising from the process models associated with the process units represented in the flowsheet and optimization. The latter introduces both unconstrained and constrained optimization.

1. Introduction

A web search through Google (www.google.com, August 1, 2005) on "What is process analysis?" gave the following results:

i. Simply a method of mathematically describing a complex phenomenon as the net result of a number of different processes. The rate concept more specifically assumes that the changes in the state of a system with time can be systematically treated as the sum of the rates of the individual processes acting on the system.

ii. www.erc.montana.edu/Res-Lib99-SW/glossary/geng.html

iii. First step of a release life cycle that includes reviewing and developing baselines for the current environment and identifying the high-level business processes and requirements to be addressed. It also includes assessing organization and network readiness, identifying current business processes, assessing the module as delivered by PeopleSoft, and confirming the scope of the release.

iv. www.umkc.edu/registrar/sis/glossary.asp

v. The systematic examination of a process to understand the process in order to develop ideas for improvement of the process. www.fiu.edu/~pie/sec8appglossary.htm

vi. Process analysis, one of the seven primary modes of exposition, either gives directions about how to do something (directive) or provides information on how something happened (informative). www.pearsoned.ca/text/ flachmann4/ gloss_iframe.html

While the above definitions pertain to several disciplines, in chemical engineering, item (iv) comes closest to our definition of process analysis. In other words in process analysis we try to do a systematic and thorough study of a chemical process in order to understand the relationship among the possibly many process variables. Although some of the relationships are observable, for most processes our understanding of the relationships is rather limited. Various mathematical formulae (commonly referred to as process models) have been developed to mimic the observed relationships. With these process models, we are equipped to devise ways to systematically improve the process using process optimization concepts. This is done by appropriately setting values of a subset of the process variables at levels that would make another subset of process variables attain their desired values.

This chapter discusses process analysis and optimization in the context of (a) the analysis of the structure of the flowsheet which is a representation of the connections among the various process units, (b) solution of the process models in the flowsheet and (c) optimization of the flowsheet. Comprehensive discussions of these issues can be found in [1] [2] [3].

A process analysis and optimization model may be cast as

$$\min_{x,u} f(x,u) \tag{1}$$

$$\varphi_i(x,u) = 0 \qquad i = 1,...,m \tag{2}$$

$$\psi_j(x,u) \le 0 \qquad j = 1,..., p \tag{3}$$

Here we assume that $f(x,u)$, $\varphi_i(x,u)$ and $\psi_j(x,u)$ are twice continuously differentiable functions. $f(x,u)$ is more commonly referred to as the performance objective (e.g. profit); it is a measure of how good the design is. The set $\{\varphi_i(x,u)\}$ usually denotes material and energy balances while the set $\{\psi_j(x,u)\}$ represents process constraints such as safety (e.g. limits on reaction pressure), environmental limitations (e.g. limits on purge rate of waste), and process specifications (e.g. product purity). In addition x is an n_x- vector of state variables (for example concentration and temperature), and u is an n_u-vector of decision variables (for example feed concentration and reactor size). Sometimes the model is more conveniently expressed as

$$\min_{z} f(z) \tag{4}$$

$$\varphi_i(z) = 0 \qquad i = 1,...,m \tag{5}$$

$$\psi_j(z) \le 0 \qquad j = 1,..., p \tag{6}$$

where $z = [x,u]$.

2. Steady State Simulation of a Chemical Process

Steady state simulation is a necessary part of process optimization since calculation of the performance objective function requires knowledge of the state variable values of some of the process streams. In short, steady state simulation involves the solution of Eq. (5). If the latter also depended on time, then we would be dealing with *dynamic* simulation.

2.1 Structure of Process Flowsheets

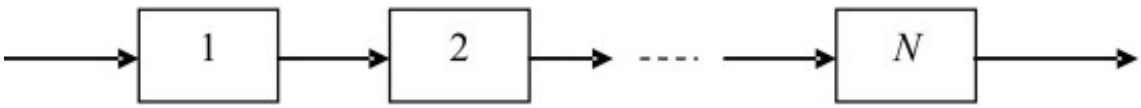

Figure 1: Sequential flowsheet

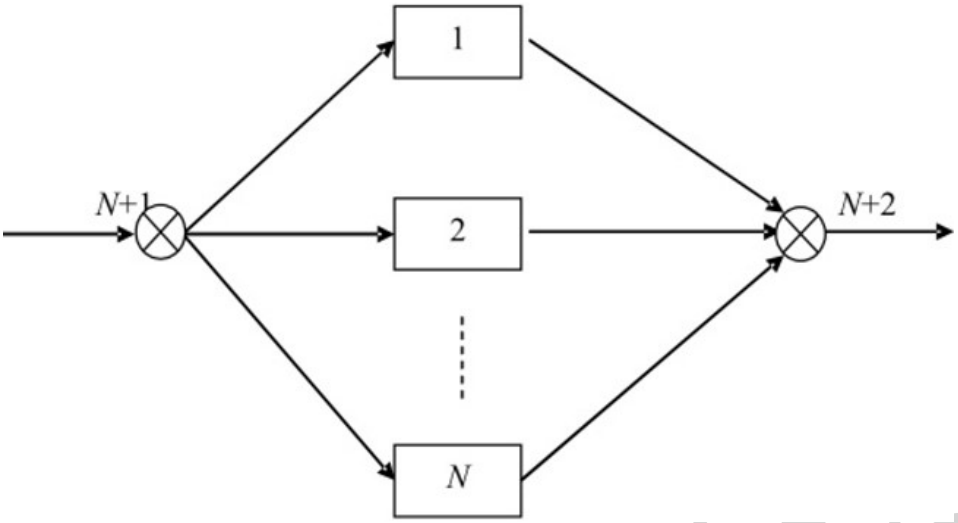

Figure 2: Parallel flowsheet

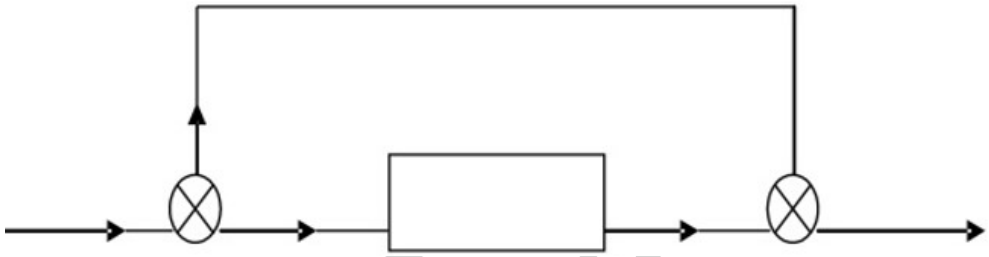

Figure 3: Flowsheet with bypass

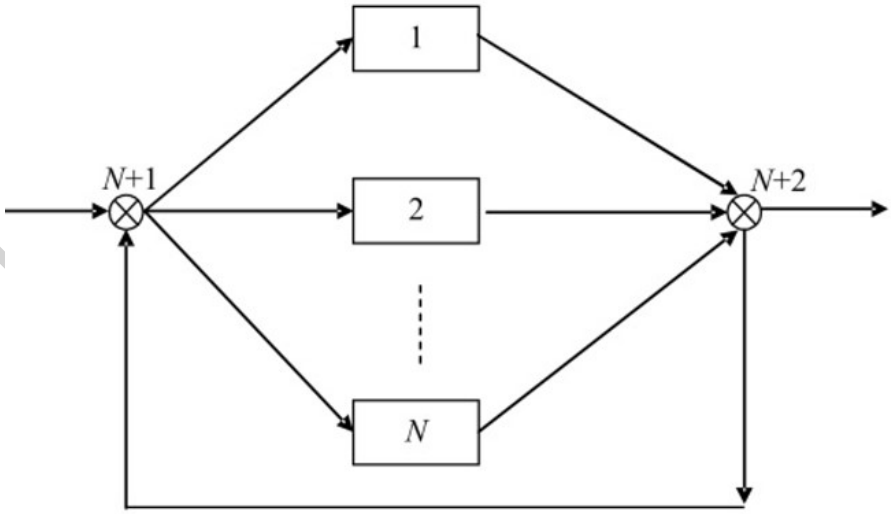

Figure 4: Parallel flowsheet with recycle

A process flowsheet is a representation of the various processing units and their interconnections with each other through material and energy flows. Examples of process units are chemical reactors, distillation columns, pumps, valves, decanters, heat exchangers, mixers, flash units, condensers, evaporators and crystallization units. Each process unit is represented as a block in the flowsheet. There are several flowsheet

configurations that are possible. Each configuration is some combination of the following basic configurations: sequential (Fig. 1), parallel (Fig. 2), bypass (Fig. 3) and recycle (Fig. 4). A flowsheet is *open-loop* (Figs. 1 to 3) if it does not contain recycles. Otherwise the flowsheet is *closed-loop* (Fig. 4).

2.2 Process Model Representation of Flowsheet

The simplest flowsheet consists of just one process unit. An example is a simple flash unit (Fig. 5) [1] for separating a mixture of (1) benzene, (2) toluene and (3) o-xylene into an overhead vapor product (richer in benzene and toluene) and a bottom liquid product richer in o-xylene. The total feed flowrate is denoted as F (in an appropriate unit such as kg/mol). The feed compositions (mole fractions) are in the vector zz and the individual flowrates (in kg-mol/hr) are in the vector f .The feed temperature is T_{feed} . The vapor product has a flowrate V and composition yz , while the liquid product has a flowrate L and composition xz . In addition the flash unit is at a temperature of T and pressure P with a steady heat input of Q . A value of $Q = 0$ corresponds to an adiabatic flash; $T =$ *fixed constant* corresponds to an isothermal flash; and $P =$ *fixed constant* is an isobaric flash. The vectors are defined as,

$$zz = \begin{bmatrix} zz_1 \\ zz_2 \\ zz_3 \end{bmatrix},\ yz = \begin{bmatrix} yz_1 \\ yz_2 \\ yz_3 \end{bmatrix},\ xz = \begin{bmatrix} xz_1 \\ xz_2 \\ xz_3 \end{bmatrix},\ f = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

Consider a flowsheet that consists of N process units (blocks) such that the *k*-th block has n^k input and m^k output streams. For the flowsheet in Fig. 5, there is only one process unit. Therefore $N = 1$; the first block is the flash unit with $n^1 = 1$ and $m^1 = 2$. For a standard heat exchanger unit, $n^k = m^k = 2$. Let $x_i^{(k)}$ and $y_j^{(k)}$ be vectors of state variables associated with the *i*-th inlet and the *j*-th outlet streams of the *k*-th block, respectively. Let $\dim x_i^{(k)} = n_i^k$. Define the super vectors $x^{(k)} = (x_1^{(k)}, ..., x_{n_k}^{(k)})$ and $y^{(k)} = (y_1^{(k)}, ..., y_{m_k}^{(k)})$.

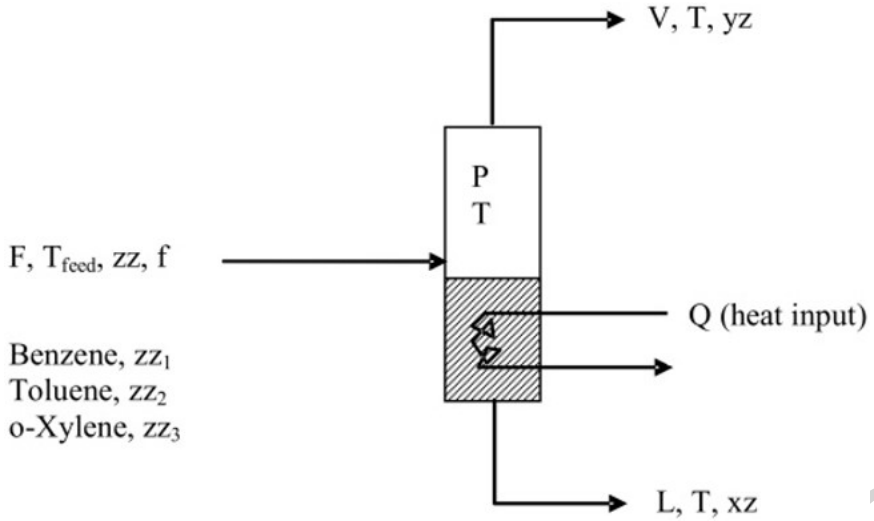

Figure 5: Flash unit with one input stream and two output streams

Component	Flowrate (kg-mol/hr)	Boiling Point (K)
Benzene (1)	30	353
Toluene (2)	50	383
o-Xylene (3)	40	418

Table 1: Data for flowsheet in Fig. 5

For the simple flowsheet in Fig. 5, there is only one block with one inlet stream and two outlet streams. Therefore the appropriate definitions are as follows:

$$x_1^{(1)} = \begin{bmatrix} zz_1 \\ zz_2 \\ zz_3 \\ F \\ T_{feed} \\ P_{feed} \end{bmatrix} \quad y_1^{(1)} = \begin{bmatrix} yz_1 \\ yz_2 \\ yz_3 \\ V \\ T \\ P \end{bmatrix} \quad y_2^{(1)} = \begin{bmatrix} xz_1 \\ xz_2 \\ xz_3 \\ L \\ T \\ P \end{bmatrix} \quad \dim x_1^{(1)} = n_1^{(1)} = 6$$

$$x^{(1)} = \begin{bmatrix} zz_1 \\ zz_2 \\ zz_3 \\ F \\ T_{feed} \\ P_{feed} \end{bmatrix} \qquad y^{(1)} = \begin{bmatrix} yz_1 \\ yz_2 \\ yz_3 \\ V \\ T \\ P \\ xz_1 \\ xz_2 \\ xz_3 \\ L \end{bmatrix}$$

The process model of a flowsheet consists of two parts, namely the models of the separate blocks and the model of the flowsheet structure. The process model of the *k*-th block is of the form

$$y_i^{(k)} = f_i^{(k)}(x^{(k)}, u^{(k)}) \qquad i = 1, ..., m_k \tag{7}$$

where $u^{(k)}$ is a vector of decision variables of block k. It consists of design variables and control variables. Note that the process model in Eq. (7) is a member of the equality constraints set in Eq. (2). For steady state simulation, $u^{(k)}$ is held constant. The flowsheet structure model consists of connection equations given as

$$x_i^{(k)} = y_j^{(p_k)} \qquad i \in Q_k, \quad k = 1, ..., N \tag{8}$$

where Q_k is a set of indices of inlet streams of the k-th block. The equation reflects the fact that the j-th output of the p_k-th block is the i-th input of the k-th block. Substituting the expression for $y_i^{(k)}$ from Eq. (7) into Eq. (8) we obtain a set of nonlinear equations

$$x_i^{(k)} = f_j^{(p_k)}(x^{(p_k)}, u^{(p_k)}) \qquad i = Q_k \quad k = 1, ..., N \tag{9}$$

Thus the steady state simulation is reduced to solving a set of nonlinear equations in Eq. (9) with respect to $x_i^{(k)}$. The set contains M variables such that

$$M = \sum_{k=1}^{N} \sum_{i \in Q_k} n_i^k$$

This is the equation-oriented approach. In the general case the set of nonlinear equations Eq. (9) can contain several hundreds variables and equations. For illustration consider the flowsheet in Fig. 6. Suppose blocks 1 to N are CSTRs (continuous stirred tank

reactors), block $(N+1)$ is a simple splitter, and block $(N+2)$ is a mixer. Here $n^k = m^k = 1$ $(k = 1,\ldots,N)$, $n^{N+1} = 1$, $m^{N+1} = 2$, $n^{N+2} = 2$, and $m^{N+2} = 1$. We will suppose that components of the vectors $x^{(k)}$ and $y^{(k)}$ are material and energy streams and all the vectors have the same dimension n. The process model of each CSTR is of the general form Eq. (7). The other process models are as follows.

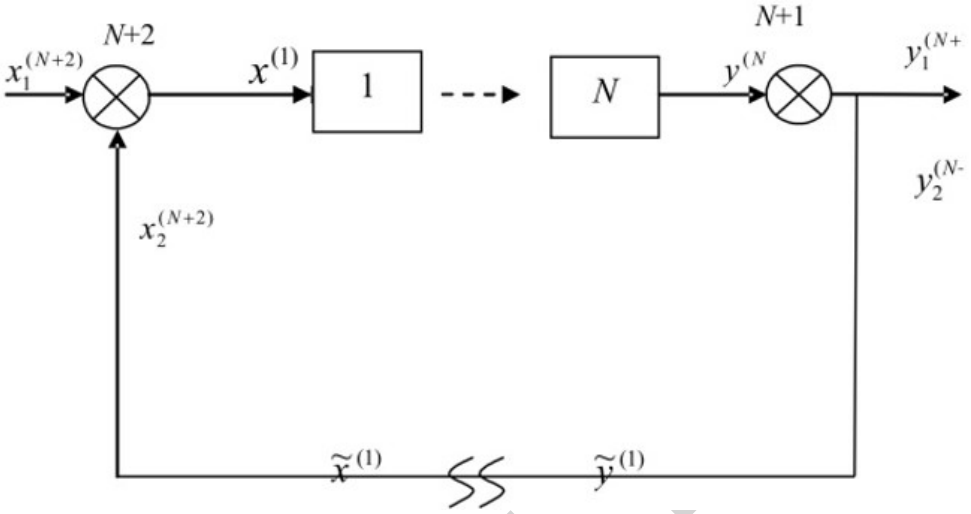

Figure 6: Flowsheet blocks with recycle

Splitter

$$y_1^{(N+1)} = (1-\alpha)y^{(N)}$$
$$y_2^{(N+1)} = \alpha y^{(N)} \qquad (10)$$

where α is the split fraction.

Mixer

$$y^{(N+2)} = x_1^{(N+2)} + x_2^{(N+2)} \qquad (11)$$

Connection equations

$$x^{(k)} = y^{(k-1)} \quad (k = 2,\ldots,N; \quad x^{(1)} = y^{(N+2)}; x_2^{(N+2)} = y_2^{(N+1)}) \qquad (12)$$

The simulation of the flowsheet is reduced to the simultaneous solution of the set of equations in Eq. (7), Eq. (10), Eq. (11) and Eq. (12). If we substitute Eq. (7) into Eq. (10) and Eq. (11) into Eq. (12) we obtain a set of M equations with M variables, where

$$M = Nn \qquad (13)$$

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