CHAPTER 4

FLOWSHEET OPTIMIZATION

4.1 Introduction

In this chapter, the relationship between the different approaches to process flow sheeting, as well as describe their advantage and disadvantages will be discussed in length. Tools for simulating the model of which have to combine the properties and abilities to handle Fortran Language in this research is Aspen Plus, a commercial simulation package.

4.2 Flowsheet Optimization

For an optimization problem, objective function, constraint and optimization algorithm are considered crucial and taken into account.

1. Decision variables

Decision variables are those independent variables over which the engineer has some control. These can be continuous variables such as temperature or discrete (integer) variables such as number of stages in a column. Decision variables are also called design variables.

2. Objective function

An objective function is a mathematical function that, for the best values of the decision variables, reaches a minimum (or a maximum). Thus, the objective function is the measure of value or goodness for the optimization problem. If it is a profit, one searches for its maximum. If it is a cost, one searches for its minimum. There may be more than one objective function for a given optimization problem. There are different types of objective function depending on the needs and uses. Sometimes this objective function is referred as the "Economic Model".

For an economic point of view, the objective function could be:

- Minimize revenue
- Maximize net profit
- Maximize income
- Minimize time

For technology development point of view, the objective function could be:

- Maximize production rate
- Minimize production time
- Minimize energy consumption

The objective functions could be categorized into three types, (Edgar and Himmelblau, 1989)

1. The first category of objective function involves no capital costs at all but just operating costs and revenues. Such cases are often referred to as "supervisory control" problems and arise when capital costs are a fixed sum, i.e. the equipment is already in place. For this, one could not influence these costs by optimizing the operating variables.
2. The second category is optimization of capital equipment in circumstances where no operating costs are involved. Many mechanical design problems fall into this category.
3. The third category of objective functions includes both capital costs and operating costs. Such problems usually involve some capital expenditure in order to reduce operating costs or manufacturing additional products. Capital costs herein include the purchase price of the equipment plus a term for a return on the investment (Happel and Jordan, 1975). Both design variables and operating conditions could be optimized in such a problem, this type of objective function posses the greatest conceptual difficulty in formulation. The principal difficulty is that how to mesh the two types of costs in a sensible way so that the objective function comprised of terms with common unit.

3. Constraint

In every process there will be a constrain on limits of the process of which these constrain are values that indicates the ability and limit of the feasible path of the process. Constrains can be classified into two types as follows:

- **Inequality constrains**

Inequality constrains are constrains that indicate the limits due to design and other limits from:

Production : usage of equipment, storage space, maximum feed rate

Feedstock : limited amount, quality of feedstock, safety factors such as safe operating temperature

Other limits : maximum process pressure, minimum production rate

- **Equality constrains**

Equality constrains are constrains that indicates the limits of the process or its product such as the purity of the products, mass and energy balance. For example, a reaction may require a specific oxygen concentration in the combined feed to the reactor. The mole balance on the oxygen in the reactor feed is an equality constraint.

4. Optimization algorithm

The optimization algorithm uses the unit model and objective function to solve the problem. There is no single algorithm or method of optimization that can be efficiently applied to all problems. The method chosen for particular case depends on

(1) character of the objective function

(2) nature of the constrains

(3) number of dependant and independent variables.

Mathematically, the algorithm of the optimization problem using the process model and objective function can be formulated as following equation:

Maximize (or minimize) $\quad F(x,y) \quad$ (4.1)

Subject to

$$H(x,y) = 0$$
$$C(x,y) = 0$$
$$G(x,y) \geq 0$$

where F = objective function with respect to the freed variable, x.

H = Process simulation equation

C = Equality design constrains

G = Inequality design constrains

y = Process variables

The convergence methods available in Aspen Plus are SQP, Complex, Wegstein, Direct, Secant, Broyden, and Newton method. In this research the SQP method is used as the optimization.

Gallier and Kisala (1987) used process simulation package, ASPENPLUS, as the process model. The simulator was treated as a black-box and as an infeasible path optimization using the Successive Quadratic Programming (SQP) method. Gaines and Gaddy (1976); Ballman and Caddy (1977) also used process simulation package, PROPS, as the process model, although there was no evidence to date of this method being used in industry. Fatora and Ayala (1992) suggested the application of open equation based on models instead of closed form equation. A simultaneous equation solving and optimization software package manipulated the unknown such that the residual, R which was driven to zero. The implication of using open form equation based on modeling technology was far reaching. In industrial world, this equation had been used successfully when the proper mathematical tools had been available.

Gaines and Caddy (1976) compared effectiveness of three optimization algorithm, Complex Method, Pattern Search and Adaptive Random Search, and concluded that the Adaptive Random Search generally yielded larger changes in the independent variables than the rest.

Because of recent advances in optimization, such as the Successive Quadratic Programming (SQP) algorithm, it is now possible to solve process optimization problems more efficiently. The SQP algorithm is an infeasible path method: the equality or inequality constraints needed not be satisfied in each iteration. Rather, the constraints are converged while the objective function is converged to the optimal solution SQP, then, can be very efficient for solving highly constrained problems like those found in most literature (Bailey, 1993; Darby, 1988; Factora, 1992; Gallier, 1987; Wellons, 1994).

The application of process simulation package, such as Aspen Plus, for process modeling and optimization in chemical industry is studied in ammonia process (Gallier and Kisala, 1987) ASPENPLUS, process simulator was chosen as process model to illustrate the capability of process optimization using SQP optimization algorithm. There are three steps in performing the process optimization: identify the objective function, which in this case is to maximize the ammonia production from the process; identify the degrees of freedom for optimization; identify the constraints in this problem. There were three degrees of freedom and three constraints. They found the SQP method was very efficient at finding the optimum of the ammonia synthesis using later as a sample for testing.

The state-of-art of sequential quadratic programming (SQP) method could be used for flowsheet optimization for simultaneous convergence of optimization problems with constrains ,equality or inequality, and/or tear streams. The algorithm generally follows an infeasible path, i.e. constrains and tear streams are converged simultaneously with the optimization problem. However, it could be adjusted to follow a feasible path, i.e. converging the tear streams at each iteration of the optimization. The SQP was used for system-generated optimization convergence blocks. It has been recommended for user-generated convergence blocks as well.

Process optimization problems modeled within the modular simulation mode have a structure represented by Figure 4.1. Here, the modules relating to feed processing (FP), reaction (RX), recycle separation (RS), recycle processing (RP), and product recovery PR contain the modeling equation and procedures. The objective and constraint function are formulated in terms of unit and stream variables in the flowsheet and assumed to be an implicit functions of the decision variables, $\bar{x}$ which is subset of x. The objective function, f(x), represents processing cost, product yield, or overall profit. The product purity and operating limits are often represented by inequalities, g (x). The implicit design specification are represented by additional equality constraints, c(x)

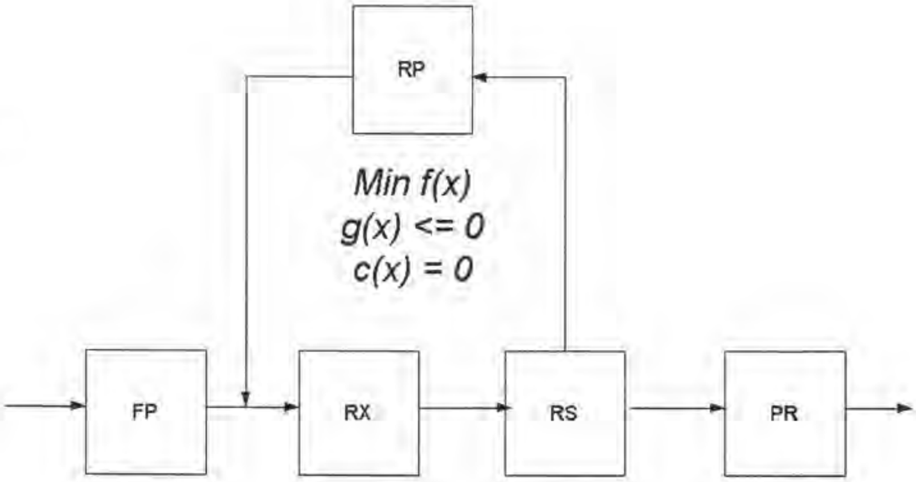

Figure 4.1 Structure of modular flowsheet optimization problem

The modular mode offers several advantages for flowsheet optimization. First, the flowsheet problem is relatively easy to be constructed or to be initiate, since numerical procedures that are tailored to each unit are being applied. Moreover, the flowsheet model is relatively easy to debug using process concepts intuitive to the process engineer. On the other hand, a draw back to using the modular mode for optimization is that unit models need to be solved repeatedly, and often, careful problem definition is required to prevent intermediate failure of these processing units.

Early attempts at applying optimization strategies within the modular mode were based on black-box implementations, and these were discouraging. In this simple approach, an optimization algorithm was tied around the process simulator as show in Figure 4.2

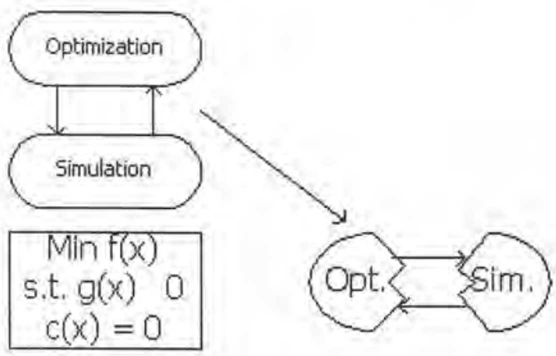

Figure 4.2 Evolving from the black-box (left) to the infeasible path approach using SQP

In this black-box mode, the entire flowsheet needs to be solved repeatedly and failure in flowsheet convergence is detrimental to the optimization. Moreover, as gradients are determined by finite differences, they are often corrupted with round off errors from flowsheet convergence. This has adverse effects on the optimization strategy. Typically, a flowsheet optimization with ten degrees of freedom requires the equivalent time of several hundred simulations with the black box implementation.

Since the mid 1980s, however, flowsheet optimization for the modular mode has become popular and widely used as an industrial tool. This has been made possibly by three advantageous factors in implementation:

1. The SQP strategy requires few function evaluations and performs very efficiently for process optimization problems with few function evaluations.
2. Intermediate convergence loops, such as recycle streams and specification can be incorporated as equality constraints in the optimization problem. This is particularly important for loops that were converged with slow fixed points methods in the flowsheet. The SQP, on the other hand, converges both equality and inequality constraints simultaneously under the optimization problem condition.
3. Since SQP is a Newton-type method, it could be incorporated within the modular simulation environment via an "equation solver block" frequently used for recycle convergence. As a result, the structure of the simulation environment and the unit operations blocks are unnecessary to be modified.

4.3 Optimization Modeling of Chemical Reactors

Optimization in the design and operation of a reactor focuses on formulating a suitable objective function plus a mathematical description of the reaction. Ideal reactors can be classified in various ways, but for our purposes here the most convenient classification is according to the mathematical description of the reactor, as listed In Table 4.1. Each of the reactor types In Table 4.1 can be expressed in terms of integral equations, or difference equations, as well. However, not all reactors can neatly fit into the classification in Table 4.1. The accuracy and precision of the mathematical description rest not only on the character of the mixing and the heat and mass transfer

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Table 4.1 Classification of reactors

Reactor type	Mathematical description (continuous variables)
Batch (well-mixed (CSTR), closed system)	Ordinary differential equations (unsteady state)
Semibatch (well-mixed (CSTR), open system)	Ordinary differential equations (unsteady state) Algebraic equation (steady state)
Continuous stirred tank reactors, individual or in series	Ordinary differential equations (unsteady state) Algebraic equation (steady state)
Plug flow reactor or in series	Partial differential equations in one spatial variable (unsteady state) Ordinary differential equations In the spatial variable (steady state)
Dispersion reactor	Partial differential equations (unsteady state and steady state) Ordinary differential equations In one spatial variable (steady state)

Other factors that must be considered in the modeling of reactors, factors that influence the number of equations and their degree of nonlinearly but not their form, are

1. The number an nature of the phases present In the reactor (gas, liquid, solid, and combinations thereof)

2. The way of supplying and removal of heat (adiabatic, heat exchange mechanism, etc.)

3. The geometric configuration (empty cylinder, packed bed, sphere, etc.)

4. Reaction features (exothermic, endothermic, reversible, irreversible, number of species, parallel, consecutive, chain, selectivity)

5. Stability

6. The catalyst characteristics

4.3.1 Objective Functions for Reactors

Various questions can be posed concerning reactors that lead directly to the formulation of an objective function. typical objective fountains in terms of the adjustable variables are:

1. Maximize conversion (yield) per volume with respect to time.

2. Maximize production per batch.

3. Minimize production time for a fixed yield.

4. Minimize total production costs/average production costs with respect to time/fraction conversion.

5. Maximize yield/number of moles of component/concentration with respect to time and/or operating conditions.

6. Design the optimal temperature sequence with respect to time/reactor length to obtain (a) a given fraction conversion, (b) a maximum rate of reaction, or (c) the minimum residence time.

7. Adjust the temperature profile to specifications (via sum of squares) with respect to the independent variables.

8. Minimize volume of the reactor(s) with respect to certain concentration(s).

9. Change the temperature from T_0 to T_f in minimum time subject to heat transfer rate constraints

10. Maximize profit with respect to volume.

11. Maximize profit with respect to fraction conversion to get optimal recycle.

12. Optimize profit/volume/yield with respect to boundary/initial conditions in time.

13. Minimize consumption o f energy with respect to operating conditions.

In some cases a variable can be independent and in another case the same variable can be dependent, but the usual independent variables are pressure, temperature, and flow rate or concentration of a feed.

All of the various optimization techniques described can be applied to one or more types of reactor models. The reactor model forms a set of constraints so that most optimization problems involving reactors must accommodate steady-state algebraic equations or dynamic differential equations as well as inequality constraints. The following are the most commonly used optimization techniques reported in the literature review.

1. Differential calculus after converting the constrained problem to an unconstrained one
2. Linear and nonlinear programming
3. Maximum/minimum principle
4. Dynamic programming