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A New Hybrid Strategy for the Optimization of Chemical Processing System

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By structural comparison of process optimization strategies based on Simultaneous Modular Approach , they can be classified into two groups : the Sequential Module Based Approach and the Two-Tier Approach. The Sequential Module Based Approach needs rigorous models and a set of accurate solutions are guranteed. However, it requires large amount of computation time. In the Two-Tier Approach composed of rigorous and simplified models, optimization calculation uses simplified models, therefore comparatively smaller amount of computation time is required but the obtained solutions may not be accurate. These optimization problems were somewhat improved by the alternate application of the two strategies. In this study, improved optimization strategy is suggested, in which Jacobian Matrix is modified to accomodate the strong points of above mentioned strategies. The results of case study show that this approach is superior to the other strategies.

1. Introduction

For the design and improvement of chemical processes, simulation and optimization are indespensible tools. Though process simulation has been used widely since a long time ago, the actual application of process optimization which has far much complex structure was almost impossible because of huge amount of computation. But from the end of 1970's process optimization has entered upon a new phase with the developments in Nonlinear Programming Techniques and optimization strategies [1,2,3,4,5]. More than 100 STE(Simulation Time Equivalence) was required for chemical process optimization till the early of 1970's but only 1-5 STE is sufficient from 1980's as the results of developments in optimization techniques(NLP) and optimization strategies[6,7,8,9,10]. The purpose of this study is to develop more improved strategy of process optimization and to prove its performance with benchmark problems. The strategy of process optimization is developed in two directions : Sequential Module Based Approach and Two-Tier Approach. These two directions have their own merits and demerits. Nowadays, new optimization strategies combining the strong points of both directions by the alternate application of these two directions.

In this study improved optimization strategy named MJS(Modified Jacobian Strategy) is developed, in which Jacobian Matrix is modified to integrate the strong points of above-mentioned strategies. To check the performance of the developed strategy it should be compared with other optimization strategies. For convenience, the developed strategy is compared with Sequential Module Based Approach which is the most popular subject of comparison.

2. Process Optimization Strategy

In general, because the process optimization problem is given in the form of profit maximization or minimization of operating cost, preprocessing is necessary for the application of the optimization technique which is called the process optimization strategy. In other words, process optimization strategy is a procedure to reform an abstract optimization problem to a definite one to which process optimization technique is applicable. Undoubtly, the process optimization strategy is closely connected with the selected optimization technique.

Process optimization strategies are classified into three groups : Sequential Modular Approach, Equation Based Approach and Simultaneous Modular Approach. The third approach which comes from the combination of the first two approaches and it is acknowledged to be most reasonable. In this study, the Simultaneous Modular Approach is selected. But, there are many branches in the Simultaneous Modular Approach as shown is Fig. 1. The differences among those are explained with Table 1 and Fig. 1.

In Figure 2, if we get point d' from c' indicating the complete convergence of process simulation before a optimization step is proceeded it is called a Feasible Path Strategy, and d" from c" indicating little

Table 1. Comparison between Sequential Modular Infeasible Path Approach and Two-Tier Approach.

	Sequential Module Based Approach	Two-Tier Approach
Construction of Jacobian matrix	Tear stream connectivity equations and design specification equations vs. Decision variables and tearing variables	Reduced model equations and design specification equations vs. Decision variables and state variables
Characteristics	An optimal solution is guaranteed Large amount of computation time	A suboptimal solution may be obtained Small amount of computation time
Modifications	Jacobian matrix approximation or Introduction of reduced model for Jacobian matrix calculation when the solution is not near	Restart with Sequential Modular Approach after the solutions based on the reduced model are obtained

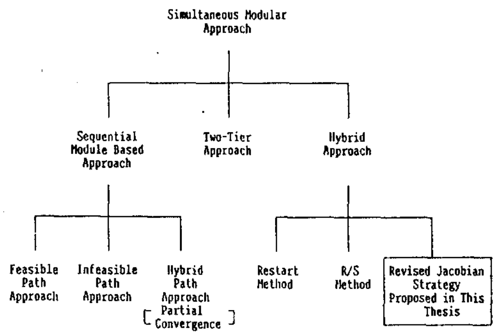

Fig. 1 Classification of Strategies Based on Simultaneous Modular Approach

convergence of process simulation that is called the Infeasible Path Strategy. Also, d from c which is an intermediate case of previous two cases it is called the Partial Convergence Strategy[11,13,14]. So as to compensate demerits appeared in Table 1, the R/S Method[12] and the Restart Method[10] are developed by the alternate application of Sequential Module Based Approach and the Two-Tier Approach.

3. Improved Strategy of Process Optimization

In this study, a hybrid approach which integrates the strong points of Sequential Module Based Approach and Two-Tier Approach is selected and more improved strategy is proposed.

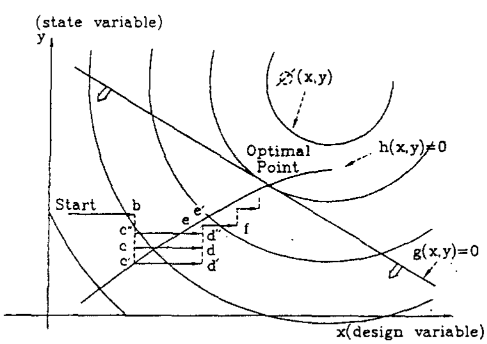

Fig. 2 Strategy of Process Optimization

3.1. Modified Jacobian Strategy

Since the simplified model has been used in process simulation or optimization it is well known that the simplified model provide very good results in process simulation. The difference comes from the fact that optimization problems require accurate gradients, but simulation problems require the same values at base points when two kinds of models (Rigorous and Simplified model) are used and the parameters of simplified models are decided to do that.

So as to solve such as below problems

$$\min_{x} \quad \varnothing(x, y)$$

$$\text{s.t.} \quad h(x, y) = y - W(x, y) = 0$$

$$g(x, y) \leq 0$$

where x : decision variable vector

y : tear variable vector

W : calculated tear stream variable

The Hessian Metrix H should be constructed first. Then, to construct H, Jacobian Matrix which is shown in Fig. 3 is needed next. If we make H with the Jacibian Matrix of Fig. 3-a then it is Sequential Module Based Approach, and if H is combined with the Jacobian Matrix of Fig. 3-b then it is a Two-Tier Approach. The merits and demerits of these two approaches were compared previously.

In the Jacobian Matrix equality constraints vs. state variable parts are related to the convergence of the whole process. On the other hand, the equality constraints vs. independent variable parts and partial differentials of objective functions vs. independent variables are strongly related to the solution of a optimization problem. Objective function is always rigorous and inequality constraints represent lower and upper bounds of variables (inequality constraints representing design specifications which are converted to equality constraints by using slack variables and included in h(x,y) = 0). Objective function and inequality constraints are all the same in the above-mentioned two strategies.

The use of the Two-Tier Approach in process simulation has been adventageous but a rigorous model is necessary for accurate gradients which results in accurate solution of process optimization problem

$$\begin{bmatrix} \frac{\partial h_r}{\partial y} & \frac{\partial h_r}{\partial x} \\ \frac{\partial g}{\partial y} & \frac{\partial g}{\partial x} \end{bmatrix}$$

(a) Jacobian Matrix by Rigorous Model

$$\begin{bmatrix} \frac{\partial h_s}{\partial y} & \frac{\partial h_s}{\partial x} \\ \frac{\partial g}{\partial y} & \frac{\partial g}{\partial x} \end{bmatrix}$$

(b) Jacobian Matrix by Simplified Model

$$\begin{bmatrix} \frac{\partial h_s}{\partial y} & \frac{\partial h_r}{\partial x} \\ \frac{\partial g}{\partial y} & \frac{\partial g}{\partial x} \end{bmatrix}$$

(c) Modified Jacobian Matrix

Fig. 3 Three Types of Jacobian Matrix
(a) Jacobian Matrix by Rigorous Model
(b) Jacobian Matrix by Simplified Model
(c) Modified Jacobian Matrix
where s : simplified, r : rigorous

[19]. With all these facts, it is concluded that the reduced model is good enough for the Jacobian of equality constraints vs. state variables. However, the rigorous model is necessary for the Jacobian of equality constraints vs. design variables in order to obtain an accurate solution with less amount of computation. This particular Jacobian Matrix is named Modified Jacobian Matrix which is shown in Fig. 3-c.

In the Modified Jacobian Matrix, $\partial h_s/\partial y$ reduces computation time and $\partial h_r/\partial x$ guarantees the accuracy of the obtained solution. Here h represents total process modeling equation by using a reduced model. Boston, et al.[16], Jiraphongphan[15], Trevino Rozano [10], etc. developed reduced models for the various unit of chemical processes. If appeared in the form of Modified Jacobian Matrix, the fraction of tear variables in the whole variables increases that is to say if the complexity of a process increases, relative performence of Modified Jacobian Matrix increases. This strategy using Modified Jacobian Matrix is the name for MJS(Modified Jacobian Matrix).

3.2. The validity of Modified Jacobian Strategy

As mentioned previously it is not simple to have accurate solutions and to reduce the amount of computation. In this study accurate solution means the solution which is obtained by using a rigorous model. The accuracy of the obtained solution depends on the kind of model used in the optimization problem. For the chemical process, let α be properties calculated by the rigorous model $P(x,y,\alpha,\gamma)$ such as K-values or enthalpies, where

- x : design variables (ex. reactor pressure)
- y : state (dependent) variables (ex. stream component flow rates)
- γ : values from process database.

(P1) $\quad \text{Min} \quad \varnothing(x,y,\alpha)$

$$\text{s.t.} \quad g(x,y,\alpha) \le 0$$
$$h(x,y,\alpha) = 0$$
$$\alpha - P(x,y,\alpha,\gamma) = 0$$

where $h(x,y,\alpha) = 0$ (process modeling equations) and $\alpha - P(x,y,\alpha,\gamma) = 0$ represents total process. KKT (Karush-Kuhn-Tucker) conditions for this problem are

$$\begin{bmatrix} \nabla_x \varnothing \\ \nabla_y \varnothing \\ \nabla_\alpha \varnothing \end{bmatrix} + \begin{bmatrix} \nabla_x g & \nabla_x h & -\nabla_x P \\ \nabla_y g & \nabla_y h & -\nabla_y P \\ \nabla_\alpha g & \nabla_\alpha h & I - \nabla_\alpha P \end{bmatrix} \begin{bmatrix} U \\ V \\ t \end{bmatrix} = 0 \quad (1)$$

$$g(x,y,\alpha) \le 0$$
$$h(x,y,\alpha) = 0$$
$$\alpha - P(x,y,\alpha,\gamma) = 0$$
$$U \ge 0$$
$$U\, g(x,y,\alpha) = 0$$

where U, V, t are multifliers.

In this optimization problem, to apply Inside-out concept reduced model $K(x,y,\alpha,\beta)$ is introduced and used with rigorous model $P(x,y,\alpha,\gamma)$, where β is determined to satisfy $\alpha = P(x,y,\alpha,\gamma) = K(x,y,\alpha,\beta)$ at base points (for the detail information of the Inside-out concept[16] will be helpful). Therefore, rigorous models are replaced by reduced models $K(x,y,\alpha,\beta)$, KKT conditions are

$$\begin{bmatrix} \nabla_x \varnothing \\ \nabla_y \varnothing \\ \nabla_\alpha \varnothing \end{bmatrix} + \begin{bmatrix} \nabla_x g & \nabla_x h & -\nabla_x K \\ \nabla_y g & \nabla_y h & -\nabla_y K \\ \nabla_\alpha g & \nabla_\alpha h & I - \nabla_\alpha K \end{bmatrix} \begin{bmatrix} U \\ V \\ t \end{bmatrix} = 0 \quad (2)$$

$$g(x,y,\alpha) \le 0$$
$$h(x,y,\alpha) = 0$$
$$\alpha - K(x,y,\alpha,\beta) = 0$$
$$U\, g(x,y,\alpha) = 0$$

(1) is the condition of optimal solution based on rigorous models and (2) is one based on reduced models (that is, by using Two-Tier Approach). Because $\varnothing$, g, h are same for both (1) and (2), they get same solution

$$\begin{cases} \nabla_x K = \nabla_x P \\ \nabla_y K = \nabla_y P \\ \nabla_\alpha K = \nabla_\alpha P \end{cases}$$ should be satisfied.

However, there is no such reduced model, if there is any, it is the rigorous model itself. Therefore optimization strategies using reduced models always have the possibility of getting suboptimal point. (if α values are calculated from a process optimization problem, it can be express as follows

$$\text{(P2)} \quad \text{Min} \quad \varnothing(x,y)$$
$$\text{s.t.} \quad g(x,y) \leq 0$$
$$h(x,y) = y - W(x,y) = 0$$

where x: decision variable vector

y: tear variable vector

W: calculated tear stream variable vector

When a process optimization problem is treated with the Sequential Module Based Approach or the Two-Tier Approach, the tear stream connecting equation stands for all of the equality constraints (process modeling equations). Objective function is a negative function of x,y. So the value of objective function value may not be accurate if the reduced model is used. KKT conditions is applied in three cases : rigorous models, reduced models, rigorous model for design variables and reduce model for state variables which are used in (p2) as followed,

First case

$$\begin{bmatrix} \nabla_x\varnothing_r \\ \\ \nabla_y\varnothing_r \end{bmatrix} + \begin{bmatrix} \nabla_x g & \nabla_x h_r \\ \\ \nabla_y g & \nabla_y h_r \end{bmatrix} \begin{bmatrix} U \\ \\ V \end{bmatrix} = 0 \qquad (3)$$

Second case

$$\begin{bmatrix} \nabla_x\varnothing_s \\ \\ \nabla_y\varnothing_s \end{bmatrix} + \begin{bmatrix} \nabla_x g & \nabla_x h_s \\ \\ \nabla_y g & \nabla_y h_s \end{bmatrix} \begin{bmatrix} U \\ \\ V \end{bmatrix} = 0 \qquad (4)$$

Third case

$$\begin{bmatrix} \nabla_x\varnothing_r \\ \\ \nabla_y\varnothing_s \end{bmatrix} + \begin{bmatrix} \nabla_x g & \nabla_x h_r \\ \\ \nabla_y g & \nabla_y h_s \end{bmatrix} \begin{bmatrix} U \\ \\ V \end{bmatrix} = 0 \qquad (5)$$

Equation (4) and (5) do not exactly coincide with (3). It is well known that in the chemical processes $\nabla_x\varnothing$ vary drastically with the characteristics of design variables. In the Modified Jacobian Strategy, $\nabla_x\varnothing_r$, $\nabla_x h_r$ are used with $\nabla_y\varnothing$ and $\nabla_y h_s$ are the remained differences. However, the objective function is weak related with the tear stream variables. Hence $\nabla_y\varnothing$ have small value and state variables that are bound to h=0 and tear stream converges, the convergence of optimization is not influenced greatly by $\nabla_y\varnothing$.

Boston, et al.[18], Jiraphongphan[15], and Trevino-Rozano[10] developed reduced models for chemical processes and proved that they provide $\nabla_y h$ accurate enough to converge process simulation. In this study these models are used. Through all these facts it is expected that by getting gradients for design variables based on rigorous models optimal solution is obtained with small amount of computation.

In the chemical process of optimization, the importance of design variables appears in the Successive Quadratic Programming algorithm. After Quadratic approximation of (p2), the elimination of equality constraints $h(\delta x,\delta y)$ results in

$$\text{(P3)} \quad \text{Min} \quad q^T\delta x + 1/2\ \delta x^T H \delta x$$
$$\text{s.t.} \quad g(\delta x) \leq 0$$

Of course, the effects of $\nabla_x\varnothing_r$, $\nabla_y\varnothing_s$, $\nabla_x h_r$, $\nabla_y h_s$ are included in q and H. After getting new x from (p3) with the QP solver, the new y which is calculated from linearized equality constraints. Though all other effects are combined the new values of the design variables are decided first and then those of the tear stream variables are decided. This sequence is very important in process optimization. This property is shown clearly in the results of Trevino-Rozano[10], Biegler[22] and Jiraphongphan[15]'s work of optimizing Flash system.

From all these reasons Modified Jacobian Strategy developed in this study is expected to be accurate and time saving. It is proved with case studies. The structure of Modified Jacobian Strategy is shown in Fig. 4.

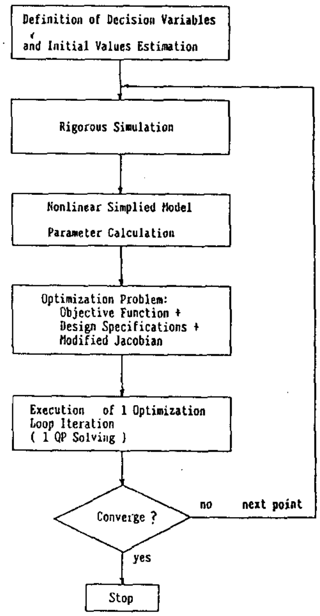

Fig. 4 Algorithm Structure of Proposed Strategy

4. Performance Prediction of Modified Jacobian Strategy(MJS)

The performance of MJS can be predicted as follows. Consequently, the performance of a optimization strategy is decided by the number of rigorous flowsheet iteration.

I. SMIPA(Sequential Modular Infeasible Path Approach) : Representative one of Sequential Module Based Approach

Total number of rigorous flowsheet iteration

$= N_{init} + (N_1 + N_2 + N_3 + N_4) * N_5$

where N_{init} = the number of rigorous flowsheet iteration before starting optimization step

N_1 : the number of rigorous flowsheet iteration between optimization iterations

N_2 : the number of tear variables (component + 1)

N_3 : the number of design variables

N_4 : the number of rigorous flowsheet iteration for line search

N_5 : total number of optimization iteration.

II. MJS (Modified Jacobian Strategy)

Total number of rigorous flowsheet iteration

$= N_{init} + (N_1 + N_3 + N_4) * N_5$

Usually the number of tear variables is larger than that of the design variables, so the performance of MJS is better than SMIPA. For example, for the case of 5 design variables, 5 components system which converge with 10 iterations.

$$\frac{\text{SMIPA}}{\text{MJS}} = \frac{2 + (1 + 6 + 5 + 1) * 10}{2 + (1 + 5 + 1) * 10} = \frac{132}{72}$$

As shown above, MJS is better than SMIPA by 132/72 times. What should be focused is that in this case the number of tear variables is equals to that of design variables. However, usually one is larger than the other.

5 . Case study

For example, Biegler et al.[20] used the process in Fig.5 first and many researchers followed. At the below of Fig. 5, FBD (Function Block Diagram) and the location of the optimizer are represented. The optimization problem of this process is as follows.

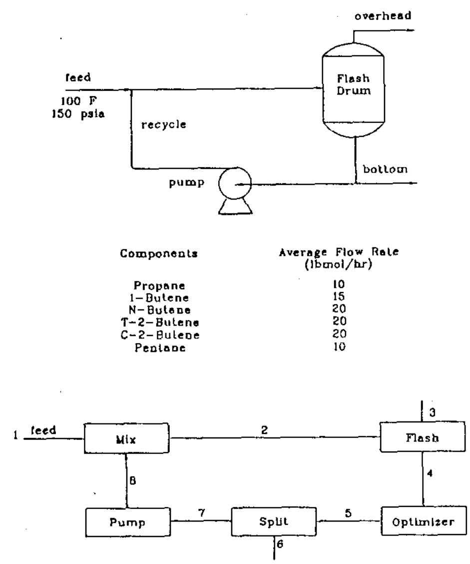

Fig. 5 . A Simple Flash Problem.

The objective function used above has no economic meaning. It is only a discretionary nonlinear function. For instance, Table 2 represents the results of applications of SMIPA and MJS to three cases made by differentiating feed compositions. Table 2 is converted to figures as shown in Fig. 6-a-c. The feed composition of case 1 is shown in Fig. 5 and that of case 2 is 11, 16, 21, 19, 19, 14(lbmol/hr) and that of case 3 is 9.8, 14.8, 19.8, 19.5, 19.5, 14.5(lbmol/hr). Though the differences of feed composition are very small the shapes of the objective function differ by its high nonlinearity.

Table 2 The Results of Three Cases

	Sterategy	Iteration	Pressure (psia)	Obj. Function
Case 1	Sequential Modular Approach	1	18.00	-1.595
		2	20.69	-0.8042
		3	21.69	-0.7018
		4	22.21	-0.6824
		5	22.29	-0.6808
		6	22.28	-0.6810
		7	22.28	-0.6809
	Modified Jacobian Approach	1	18.00	-1.595
		2	20.67	-0.8705
		3	21.56	-0.7092
		4	22.24	-0.6820
		5	22.39	-0.6797
		6	22.36	-0.6799
		7	22.36	-0.6799
Case 2	Sequential Modular Approach	1	18.00	15.742
		2	11.68	19.167
		3	13.83	19.364
		4	12.65	19.620
		5	12.44	19.602
		6	12.46	19.605
		7	12.49	19.608
		8	12.48	19.607
		9	12.46	19.605
		10	12.44	12.603
	Modified Jacobian Approach	1	18.00	15.742
		2	11.66	19.159
		3	13.84	19.362
		4	12.66	19.621
		5	12.43	19.600
		6	12.46	19.604
		7	12.47	12.606
Case 3	Sequential Modular Approach	1	20.00	-2.338
		2	21.93	-1.878
		3	23.62	-1.704
		4	24.62	-1.668
		5	25.01	-1.664
		6	24.95	-1.664
		7	24.99	-1.664
		8	24.97	-1.664
		9	24.95	-1.664
		10	24.95	-1.664
		11	24.95	-1.664
	Modified Jacobian Approach	1	20.00	-2.338
		2	21.93	-1.879
		3	23.38	-1.719
		4	24.61	-1.669
		5	25.14	-1.664
		6	25.01	-1.664
		7	25.13	-1.664
		8	24.98	-1.664
		9	25.04	-1.664
		10	25.07	-1.664
		11	25.01	-1.664
		12	25.08	-1.664
		13	25.03	-1.664
		14	25.03	-1.664
		15	25.05	-1.664
		16	25.05	-1.664

From Table 2 and Fig. 6 it is proved that MJS developed in this study obtains accurate solutions and nearly same path of convergence with SMIPA. In Fig. 7 representing the shape of objective function according to design variable that of case 3 is appeared to be plat though those of case 1,2 are not plat. This is thought to be the reason why the result of case 3 by MJS was a little bad compared to the

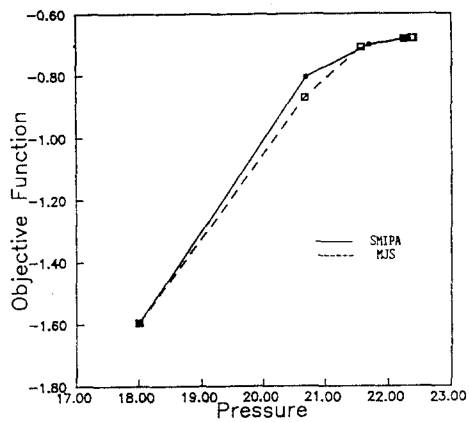

Fig. 6a The Comparison of Convergences Between Sequential Module Based Approach and Modified Jacibian Strategy -- Case 1

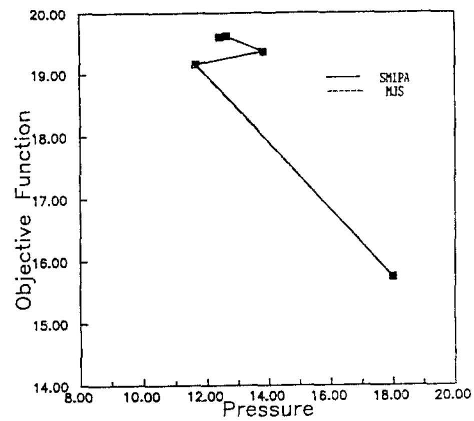

Fig. 6b The Comparison of Convergences Between Sequential Module Based Approach and Modified Jacibian Strategy -- Case 2

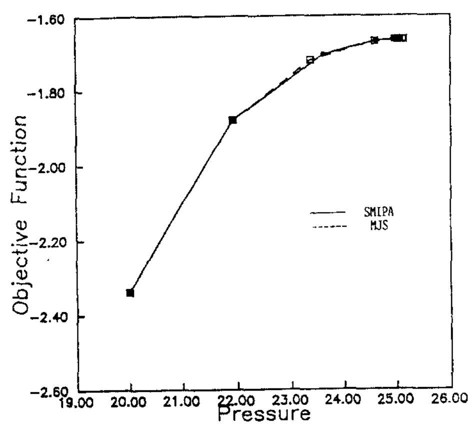

Fig. 6c The Comparison of Convergences Between Sequential Module Based Approach and Modified Jacibian Strategy -- Case 3

results of case 1,2. Hence, in this case the convergency of SMIPA was insufficient too.

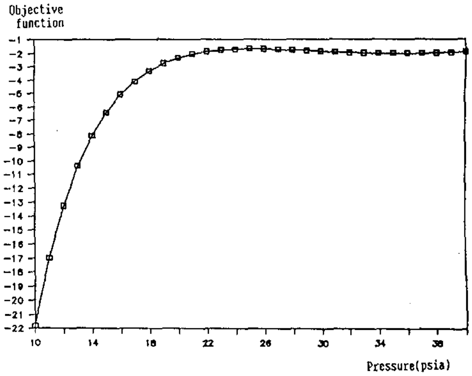

Fig. 7 Variation of Objective Function -- Case 3

Table 3 shows the results of comparisons of performances between SMIPA and MJS for the above-mentioned three cases. Table 4 shows the results of comparison between SMIPA and R/S Method by Ganesh[12] and Restart Method by Trevino (Complete Rigorous Model means SMIPA). Through relative comparison with SMIPA, that is through the comparisons between Table 3, they are different from those of Table 4. It is because of the different methods of thermodynamic properties and equilibrium calculation were used. Table 4 is the result of an ideal method and Table 3 is the result of the RKS method. However, because feeds and operating conditions are same, the results of relative comparison are not influenced by the differences.

Table 3 Comparison between SMIPA and MJS

case	Optimization Strategy	Number of Optimization Iteration	Number of Flowsheet Iteration	Value of Decision variable(psia)	Value of Objective Function
1	SMIPA	7	73	22.28	-0.6809
	MJS	7	31	22.36	-0.6799
2	SMIPA	10	103	12.44	12.603
	MJS	7	31	12.47	12.606
3	SMIPA	11	113	24.95	-1.664
	MJS	16	67	25.05	-1.664

Table 4 The results reported by Ganesh et. al.(73)

Procedure	CPU (sec)	Decision Variable	Objective function
Complete rigorous model	232	18.96	3.66289
Complete simplified model	29	23.79	4.87575
R/S algorithm	184	18.99	3.66308
Restart method	193	19.02	3.66337

6. Conclusion

So to satisfy the accuracy of the detailed solution and reduction of the amount of computation, MJS (Modified Jacobian Strategy) integrating the characteristics of Sequentail Module Based Approach and Two-Tier Approach is developed. MJS is proved to be accurate and efficient by the case studies in spite of using a reduced model by part.

Another characteristic of MJS is that if a problem is defined relative performance to other strategies can be expected and the expectation is proved to be accurate by case studies. Therefore, according to the given optimization problem the applicability of MJS can be evaluated previously. In some cases, it is possible with little modification to lead the given optimization problem to be solved very efficiently by using MJS.

Acknowledgement

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NOMENCLATURE

g : inequality constraint
h : equality constraint
K : simplified model
Ninit : number of initial rigorous flowsheet iteration
N1 : number of rigorous flowsheet iteration for each optimization iteration
N2 : number of tear variables (number of components+1)
N3 : number of decision variables
N4 : number of rigorous flowsheet iteration for line search
N5 : number of total optimization iteration
P : Rigorous model
U,V,t : multipliers
W : calculated tear stream variable
x : decision variable vector
y : tear variable(state variable) vector
α : values calculated by independent routine
β : parameters of simplified model
γ : variables based on data base
$\varnothing$: objective function

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