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Optimization of Distillation Column Operation by Simulated Annealing

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Abstract: In this paper, an exergy analysis approach is proposed for optimal design of distillation column by using simulated annealing algorithm. First, the simulation of a distillation column was performed by using the shortcut results and irreversibility in each tray was obtained. The area beneath the exergy loss profile was used as Irreversibility Index in the whole column. Then, First Optimization Algorithm (simulated annealing, SA) was implemented to Grassroots (Number of tray (N) vs. Reflux Ratio (RR)) and Retrofit (Nof vs. Feed splitting) cases, respectively. Next, SA was used to find the maximum recovery in a simple column by seven different variables (Feed Temperature, Feed Pressure, Reflux Rate, Number of theoretical stage, Feed Trays (Feed Splitting, three variables)) simultaneously. During the search for maximum recovery, it was tried to find a better Irreversibility Index. In the second part, SA optimization algorithm was used for a complex column with one pump-around and feed splitter to find a better condition, which means to find the best location for pump-around and feed trays in Distillation column. The main objective in SA was to maximize the recovery of the desired component and to find a better minimum Irreversibility Index. This method was implemented in de-ethanizer; in the first optimization without using pump-around with seven degrees of freedom, Recovery growth was 5.1% and reduction in irreversibility index was 3%. At the best Irreversibility Index, growth of recovery was about 3.7% and irreversibility index reduction was 25%. In the second optimization with pump-around or eight different variables, in the best condition, Recovery Growth was 6.2% but had a very high Irreversibility Index. At the best irreversibility index, recovery reduction was 17% but reduction in irreversibility index was about 21% comparing with initial point. As a result, it is shown that, regarding recovery and Irreversibility, pump-around shouldn't be used in a column. Without using pumparound, a better condition, considering both factors, can be achieved.

Keywords: Exergy Analysis, Irreversibility Index, Process Simulation, Process Optimization, Simulated Annealing.

1. Introduction

One of the most important and oldest methods in chemical process industries for separating mixtures is distillation. Although distillation is a very popular method for separating mixtures, unfortunately, it needs great capital investment and causes energy cost. Besides, as it has a great amount of energy exchanging in condensers and re-boilers of distillation columns (like conventional columns) most of the time, it

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suffers from great energy inefficiency. There has been an endless effort for improving distillation column according to energy and capital investment cost over the years. It seems that energy efficiency considerations are going to have more impact that is significant in the future research.

One of the most important tools for synthesizing and developing energy-efficient distillation column is thermodynamic analysis. Thermodynamic analysis can be used to define targets. As the process moves toward those targets, one can indicate that the process improves thermodynamically. Reducing thermodynamic losses in a distillation column, or on the other hand, getting distillation condition to approach a reversible operation can be a very good thermodynamic target (Dhole & Linnhoff, 1993). A distillation column can be analyzed regarding reversibility, using exergy loss profile. Exergy loss profiles are a curve that indicates irreversibility in each distillation column stage (Dhole & Linnhoff, 1993; Zemp, de Faria, & Oliveira Maia, 1997). It can be considered as a very good target for improving the process and removing those irreversibilities (Chang & Li, 2005; R Rivero, Garcia, & Urguiza, 2004). R Rivero et al. (2004) used this concept and tried to find good modification in distillation column.

Later, Faria & Zemp (2005) used exergy loss profile and enthalpy-temperature profiles for calculating thermodynamic efficiency in distillation column. Irreversibility at each stage of a distillation column is produced as a result of entropy production rate. G. De Koeijer & Rivero (2003) used this concept (theory of irreversible thermodynamics,(de Koeijer & Kjelstrup, 2010)) on both adiabatic and diabatic experimental water/ethanol rectifying columns. Ricardo Rivero (2001) carried out a detailed exergy analysis of a tertiary amyl methyl ether (TAME) unit of a crude oil refinery.

Column optimization is implemented in distillation column considering different optimization targets, such as feed preheating and/or precooling (Dhole & Linnhoff, 1993), feed (Agrawal & Herron, splitting 1997;Bandyopadhyay, 2002, 2007; Wankat & Kessler, 1993), feed trays, reflux ratio and also, adding side condensers/re-boilers. Another important target for optimization in a distillation column is Exergy Loss profile. Mustapha, Sabria, and Fatima (2007) considered this target and tried to study exergy loss profile for improving performance of distillation column. Their results showed that the irreversibility distributes in column in a non-uniform manner and they happen particularly in the condenser, re-boiler and feed tray.

Le Goff, Cachot, and Rivero (1996) in their study on the exergy analysis of distillation processes, due to high exergy losses in distillation operation, proposed a new type of distillation (diabatic column) in which, instead of using the condenser and re-boiler on top and bottom of distillation column, heat exchanging through each stage of the distillation column was used. Le Goff et al. (1996) compared diabatic and adiabatic distillation columns and showed that using diabatic column caused great reduction of entropy production in the column.

There are several works on diabatic column (Ricardo Rivero, 2001; Røsjorde & Kjelstrup, 2005; Sauar, Rivero, Kjelstrup, & Lien, 1997; Schaller, Hoffmann, Siragusa, Salamon, & Andresen, 2001) They showed that a diabatic column was better than diabatic column regarding economic (capital investment reduction) and energy (reduction in energy consumption for heating and cooling, maximizing exergetic effectiveness) aspects. Recently, Khoa, Shuhaimi, Hashim, and Panjeshahi (2010) used a three dimensional diagram to verify the effect of reflux ratio and number of theoretical stage for optimization of a column.

According to the above discussion, there are many works related to exergy analysis in distillation column. However, there are some gaps, too. In most of those methods exergetic efficiency method was used while irreversibility of each tray was not considered. Some others like (Dhole & Linnhoff, 1993; Zemp et al., 1997) that considered irreversibility in each stage, optimized their column with one or two degrees of freedom (preheating and/or precooling or feed splitting (feed stage location) etc, and did not mention or consider recovery precisely. Other works proposed in diabatic columns (Le Goff, Cachot, & Rivero, 1996) cannot be easily applicable in industry.

The purpose of this article is to find the best condition of distillation column with seven degrees of freedom (Feed Temperature, Feed Pressure, Reflux Ratio, Number of theoretical stage, Feed trays (three variables)), and in the next step, to consider pump-around with those seven variables. However, before this step, Grassroot and Retrofit Design are considered, respectively. Separation of components is the main target of distillation column. Therefore, main target in optimization is maximizing recovery of desired component and the second target is to find a better area beneath exergy loss profile (Irreversibility Index) in distillation column.









2. Calculation Procedure

The procedure to optimize single column is well known (Figure 1). In this article, first, estimated reflux ratio, and theoretical stages are determined by Shortcut Method (Fenske-Underwood-Gilliland). Then, column is solved rigorously using Bubble Point method and after finding temperature, enthalpies, and entropies in each stage, Goy-Stodolla relation is used to find irreversibility in each stage and exergy loss profile. Simulation code is written in three steps (Figure 2):

> Shortcut Method:

The purpose of this method is to find a good initial point for starting simulated annealing algorithm. Because the feed components are often non-polar in gas separation processes, this algorithm works well and gives us a good initial point. The purpose of using shortcut method is to find the number of theoretical stage and reflux ratio that can recover most of the desired components in distillate or bottom. Although rigorous method exists, shortcut method is widely used in preliminary design, sequences column, or finding initial points for rigorous method.

> Rigorous Method:

According to Seader and Henley (2006), a rigorous method is finding tearing variables in each stage of distillation column. By assuming specified pressure at each stage, it needs two specifications. Two famous specs used in a column are reflux ratio and distillate rate (both of them are initialized from shortcut method). Then, rigorous method uses them to solve MESH equations and gives us temperatures, flow rates, enthalpies, entropies, and distribution of components in each tray.

There are many methods to solve MESH equations. One of the most famous ones is Inside-Out method. However, simulation code used in gas separation processes and most of the components have narrow range of vaporliquid equilibrium ratios (K-Value). Thus using BP Method is recommended. This procedure was suggested by Friday and Smith (1964) and developed in detail by Wang and Henke (1966). Rigorous procedure using BP method is shown in Figure 3. It is referred to as Bubble Point Method, because in each iteration, a new set of stage temperatures is computed from bubblepoint equations.



Figure 3. Algorithm for Wang-Henke BP method for distillation



Exergy Loss Analysis:

Exergy analysis is based on the Second Law of Thermodynamics and is a measure of the quality and efficient use of energy; in addition, it is also an efficient tool for process optimization (Araújo, Brito, & Vasconcelos, 2007; Khoa, Shuhaimi, Hashim, & Panjeshahi, 2010: Khoa, Shuhaimi, & Nam, 2012: Ricardo Rivero. 2001: Suphanit. Bischert. & Narataruksa, 2007). According to the first law of thermodynamics, energy can neither be destroyed nor be created. However, the quality of the energy always decreases as long as an energetic process continues. The essence of the energy crisis is the degeneration of energy quality instead of the decrease of energy quantity. Accompanied with a lot of heat and mass transfer. distillation process is nonreversible unless there are an infinite number of theoretical trays and heat exchangers. Therefore, exergy loss is unavoidable for distillation process and is distributed in the condenser, reboiler and trays. More theoretical trays and smaller temperature difference can reduce the exergy loss in theory. However, the capital cost will increase greatly. Exergy analysis can provide much valuable information when already existing processes need optimization.

By adjusting the operating parameters and optimizing the heat exchanger network can reduce the amount of exergy loss. Szargut, Morris, and Steward (1987) defined exergy as the following: "Exergy is the amount of work obtainable when some matter is brought to a state thermodynamic equilibrium with the common components of the natural surroundings by means of reversible processes, involving interaction only with the above mentioned components of nature". A simplified definition of exergy might be the maximum amount of useful work that can be obtained from a system as its present state to a state in equilibrium with its surroundings. Kaibel, Blass, and Koehler (1990) investigated the thermodynamic analysis techniques for distillation columns and pointed out that exergy analysis is an important tool for improving the thermodynamic performance and efficiency of the column. Exergy is identical in form to the thermodynamic function known as Gibbs free energy. The exergy content of a stream is defined by Rivero et al. (2004) as: Ex=H-TOS (1)

where H and S represent specific enthalpy and the specific entropy of a stream, and T0 is the temperature of the surroundings (taken as the temperature of the atmosphere, river and ocean). For a distillation column, the minimum amount of work required for the separation is equal to the difference between the exergy of the product streams and that of the feed stream.

$$\Delta ex = \sum_{out} m_k ex_k - \sum_{in} m_j ex_j$$
(2)

where m is the mass flow of the feeds and the products of distillation column. The distillation column needs to provide high-grade heat (QR,TR) at the bottom and remove this heat (QC,TC) in the low-grade form from the top. Distillation process leads to the degradation of energy, similar to a heat engine. Work from the utility system is used to separate the pure components from a mixture. The calculation of the exergy loss of the utility system is based on a model of a reversible heat engine, known as the Carnot Cycle. If a distillation column is compared to a reversible heat engine and assuming that the hot and cold utility temperature is constant, the network consumption of the utility system in distillation process is given by

$$w = Q_R \left(1 - \frac{T_0}{T_R} \right) - Q_C \left(1 - \frac{T_0}{T_C} \right)$$
(3)

For an entirely reversible distillation, the work from the utility system must be equal to the minimum work required for separation. However, due to the differences of temperature and composition of the streams mixing at the different positions in the column, exergy loss presents in any real process. The work consumed by the utility must always be greater than the minimum work required for separation. Then, the overall exergy loss of distillation column can be calculated from the exergy balance

$$I^{\circ} = T_0 \left[\sum m_e^{\circ} S_e - \sum m_i^{\circ} S_i - \sum \frac{Q_r^{\circ}}{T_r} \right]$$
(4)

As temperature, pressure, and composition are known in each tray, by assuming each tray as a control region, one can easily calculate Irreversibility in each tray. Irreversibility Index that is evaluated for a distillation column is the area beneath the exergy loss profile.

2.1. Pump-Around Circuit

As mentioned above, a pump-around circuit is an instrument that withdraws liquid from a tray, cools it, and then sends it back to the upper tray. The original purpose for adding a pump-around was to reduce vapor and liquid traffic at the top section of the column. Without pump-around circuits, all condensation heat must be removed from the condenser, which results in a large vapor flow rate at top trays. It is well known that heat shifting reduces separation efficiency and decreases the number of effective ideal trays.





Figure 4. Pump-Around Circuit

A method for calculating the maximum pump-around heat removal is proposed by Sharma, Jindal, Mandawala, and Jana (1999). Heat balance is used to calculate heat removal in the upper part of the column. The upper part may start from an arbitrary tray and end with the condenser. Next, the upper part is extended tray by tray, and heat surplus is calculated for each tray. Heat surplus data that is calculated is used to construct a column grand composite curve (CGCC). In this article, CGCC is constructed and then, it is tried to find the best location for pump-around based on it to reduce Irreversibility Index in distillation column.

3. Case Study: De-Ethanizer

As the purpose of this article is that it can be used in gas separation processes, as the case study, a de-ethanizer is chosen. Feed information is shown in Table 1. Here, MATLAB and Aspen HYSYS (2006) are used for simulating de-ethanizer column.

Table 1. Feed Data(Seader & Henley, 2006)			
Names	Data		
C2 Composition	0.25		
C3 Composition	0.25		
i-C4 Composition	0.25		
n-C4 Composition	0.25		
T _{Feed} (°C)	50		
P _{Feed} (Kpa)	2500		
Molar Flow (<i>Kgmol/h</i>)	50		

Table 1 Food Data (Se & Hamley 2006)

Application starts with a shortcut method. The result of a shortcut method is used as an initial point for rigorous calculation (BP-Method). Temperature, Enthalpy, Flow rate, and Liquid Composition profile are obtained from shortcut results in Figure 5 and Figure 6 As Figure 7 indicates, the most important irreversibilities happen in condenser, re-boiler and Feed Tray. First, Irreversibility Index is evaluated as a tool to compare different conditions in the optimization. The result of the procedure is shown in Table 2.



Figure 5. Distillation Column Profiles





Figure 6. Distillation Column Profiles



Names	Data
Number Of Stage	12
Feed Tray Number	6
Reflux Rate (Kgmol/h)	44.4
Condenser duty (KJ/h)	4.6833e5
Reboiler duty (KJ/h)	-8.2117e5
Irreversibility index	1.07e5
Recovery of ethane	0.9466

Table 2. Initial point of simulated annealing algorithm from shortcut method





3.1. Grassroot design - Effect of Reflux Rate and Number of Trays

Optimizing a distillation column using a number of trays and reflux rate is one of the most famous approaches used in lots of researches. As a new exergy analysis variable (Irreversibility Index) is introduced in this article and SA algorithm is used for optimization, it is better to consider it again. As Figure 8 indicates, the effect of N and RR on Recovery and Irreversibility Index can easily be understood. (The curve is made by simple For Loops). It is titled Grassroot optimization because these variables are two important variables for Grassroot design of a column. In Table 3 there are 2 categories. Points 1 and 2 are obtained from a simple For Loops without any Optimization algorithm and with a very long run-time. Points 3 and 4 are obtained from SA algorithm. At Point 3, recovery increases about 6% and Irreversibility Index increases about 31% too. At Point 4, as recovery increases 1%, Irreversibility Index reduces about 8%.



a) Irreversibility Index by variation of N and RR



(b) Recovery by variation in N and RR Figure 8. Grass root design by change in N and RR

Names	Recovery	Irr. Index	Ν	RefluxRate (Kgmol=h)
Point 1 best recovery	0.99	1.24e5	23	54
Point 2 best Irreversibility Index	0.93	5.19e4	33	24
Point 3 best recovery from SA	0.996	1.41e5	21	59.36
Point 4 best Irreversibility Index from SA	0.954	9.93e4	13	41.86
shortcut result	0.94	1.07e5	12	44.4



3.2. Retrofit design - Effect of Feed Splitting and Reflux Rate

There are some situations in which an engineer would like to retrofit a distillation column. It means that he must modify that column to work properly. Changing the number of trays is not going to happen easily because of the construction limit. Therefore, the best suggestion for a retrofit design is changing the Reflux Rate (that is much easier than changing the Number of trays), besides using feed splitting, and entering those feeds in different trays. On the other hand, it must be tried to find the best reflux rate and feed trays' location to improve recovery and Irreversibility Index. As shown in Figs.9 and 10, it is obvious that using Feed Splitting is not good for increasing recovery (as SA mentions, too) but in Triple Feed trays (At Point 5), recovery is the same as the initial point, but Irreversibility Index reduces about 7.5%. (Results are shown in Table 4)

As shown in Figure 10a, double feed cannot be shown with reflux rate easily, therefore, the first tray is assumed 3 and the second tray is shown. Results show that often as feed trays are distant from each other, recovery reduces. For Example, if first feed tray is number 5, the best next tray choice for achieving the best recovery is 4 or 6. Irreversibility Index (Figure 10b) does not change greatly with feed splitting and the most important variable is reflux rate. However, as the difference between feed travs' numbers Irreversibility increases. Index decreases.



(b) Recovery vs. Reflux Rate vs. Feed Tray (Without Feed Splitting)



(a) Irreversibility Index vs. Reflux Rate vs. Feed Tray (Without Feed Splitting)

Figure 9. Recovery and Irreversibility Index without Feed Splitting





(a) Irreversibility Index vs. Reflux Rate vs. Feed Tray (Double Feed), First Tray is number 3



(b) Recovery vs. Reflux Rate vs. Feed Tray (Double Feed), First Tray is number 3

Figure 10. Recovery and Irreversibility Index with Double Feed

Table 4. Distillation column optimizing with Feed Splitting and KK					
Names	Recovery	Irreversibility index	Feed trays	Reflux Rate (<i>Kgmol=h</i>)	
Point 1 best recovery One Feed	0.97	1.59e5	[5]	64	
Point 2 best Irreversibility Index One Feed	0.7 4	4.61e4	[11]	24	
Point 3 best recovery Double Feed	0.969	1.59e5	[5,6]	64	
Point 4 best Irreversibility Index Double Feed	0.7418	4.88e4	[10,11]	24	
Point 5 best recovery Triple Feed	0.939	9.36e4	[4,5,6]	39	
Point 6 best Irreversibility Index Triple Feed	0.768	5.05e4	[9,10,11]	24	
Point 7 best recovery from SA	0.973	1.79e5	[5]	71.25	
Point 8 best Irreversibility Index from SA	0.94	1.07e5	[6]	44.4	
Shortcut result	0.94	1.07e5	[6]	44.4	

Fable 4. Distillation column optimizing with Feed Splitting and RR



3.3. Effect of Pump-Around

After solving distillation column rigorously and finding temperatures, entropies, enthalpies, vapor and liquid rates in each tray, now it is time to consider pump-around in the case study. Assumption in this section is that it is permitted to use one pump-around in distillation column. In pump-around, liquid is extracted from a tray (15% of the tray liquid), and cooled until its temperature reaches the temperature 10% lower than tray temperature that is going to be sent back. As Sharma et al. (1999) Method defines, there are 24 different positions for pump-around (12 trays including condenser and re-boiler). In Figure 12, effect of different positions of pump-around on recovery and Irreversibility Index is shown.



Figure 11. Comparing Exergy Loss profile with and without pump-around



Figure 12. Irreversibility Index vs. Recovery in 24 different position of pump-around

Names	Pump-Around position	Recovery	Irreversibility index	
Best Irreversibility index	[6 5]	0.7609	1.119e5	
Best recovery	[11 5]	0.8829	1.16e5	
Without pump-around	[]	0.94	1.07e5	

able 5. Distillation column with one pump-around using shortcut results



In Figure 11 Exergy Loss profile for three different conditions (without pump-around, pump-around the with at greatest irreversibility index and, with pump-around at the lowest irreversibility index) is shown. Greatest Irreversibility Index happens when liquid is extracted from tray number 11, and is sent back to tray number 2 and, lowest Irreversibility Index happens when liquid is extracted from tray 6 and enters tray 5.

Two different approaches are important here: finding the maximum ethane recovery and finding the minimum Irreversibility Index. Therefore, there are two different types of results in this section (Table 5). The first array in the pump-around position is the tray where liquid is extracted, and the second array is the tray to which liquid is going to be sent back. In the best condition, Irreversibility Index increases 4.5% comparing to the column without pump-around and in the best condition, recovery decrease 7% comparing to the column

without pump-around. The results define that using pump-around is not reasonable based on irreversibility or recovery overview.

3.4. Optimization: Part 1 (OPT1)

In the first part of optimization, there are seven degrees of freedom, Number of Theoretical Stage, Reflux Ratio, Feed Trays (Feed Splitting, three variables). Feed Temperature and Feed Pressure. On the other hand, single, double and feed considered in triple are column optimization, but there is not any pump-around in this section. The results (obtained from SA) are shown in Figure 13. Comparing the results with those of the previous section is shown in Table 6. In OPT1 in the best Irreversibility Index, recovery increases about 3.7% and Irreversibility Index reduces about 25%. Exergy Loss profile at two conditions (best recovery and best Irreversibility Index) is shown in Figure 15a.



Figure 13. Irreversibility Index vs. Recovery in OPT1

Names	Recovery	Irreversibility Index
OPT1 ,Best Irreversibility Index	0.9755	8.01e4
OPT1 ,Best Recovery	0.988	1.04e5
Best Irreversibility Index from Table 5	0.7609	1.119e5
Best Recovery from Table 5	0.8829	1.16e5
Initial point of simulated annealing	0.94	1.07e5

Fable 6. Results from OPT	comparing with	previous parts
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3.5. Optimization: Part 2 (OPT2)

Index

In this part, the main purpose is to find the best variables to find maximum recovery. During finding the best recovery, we minimized the Irreversibility Index in the column by using feed splitting (single, double and triple feed) and using one pump-around. The definition of using pump-around in this article is to extract liquid from bottom trays and cool it till 10% below the destination tray temperature. The results are shown in Table 7. Irreversibility

index and recovery profile are shown in Figure 14.

Exergy Loss profile is shown at two conditions in Figure 15b, best Irreversibility Index and best recovery in the column. As it is shown, using pump-around is increasing Irreversibility Index greatly if recovery is desired. And in the best Irreversibility index condition, Irreversibility index reduces 21% but recovery reduces about 17%.



Figure 14. Irreversibility Index vs. Recovery in OPT2



Figure 15. Exergy Loss Profiles in OPT

Table 7. Results from Optimization Part 2 comparing with previous parts						
Names	OPT2 Best IRindex	OPT2 Best Recov	OPT1 Best IRindex	OPT1 Best Recov	Initial point	
Recovery	0.77	0.99	0.975	0.988	0.94	
Irreversibility	8.44e4	1.79e6	8.01e4	1.04e5	1.07e5	



4. Conclusion

In general, Irreversibility in distillation column travs depends on feed conditions, recovery of desired component in distillate, Number of theoretical stage, feed trays and reflux rate. As the real purpose of using a distillation column is to separate components in the feed, increasing recovery of desired component is the first and main goal in the optimization. Another method to improve processes isreducing the irreversibilities in that process. Hence, the second goal is reducing irreversibility in distillation column.

The method in this article has improved previous works in two different ways: first, as distillation column is solved rigorously, Irreversibility Index in each tray can be evaluated. Second, degrees of freedom are seven including Feed Trays (Feed Splitting, three variables), Feed Temperature, Feed Pressure, Reflux Rate, and Number of theoretical stage in optimization and besides one pump-around separately and altogether with those seven degrees freedom.

In the First approach, it was tried to optimize de-ethanizer by using a number of trays and reflux rate (Grassroot Design). It was shown that as the number of trays and reflux rate increases, in the best recovery condition, recovery increases 5.9% and Irreversibility Index increases about 31% comparing with initial point of SA. According to SA results, the best reduction in Irreversibility Index is 7.5% and recovery increases about 1% in that point.

Then, in the second approach, Retrofit design (Optimization using feed splitting and reflux rate), SA mentions that for maximizing recovery, feed splitting is rejected and instead, it is better to use one feed. Only when feed is splitted to three, in one point, recovery doesn't change, but Irreversibility Index reduces about 7.5%.

In the optimizing column with seven variables, in the best recovery condition, recovery increases 5.1% (98.8% recovery) comparing to SA initial point and irreversibility index reduces about 3%. At the best irreversibility index, recovery increases about 3.7% (97.5% recovery) comparing to SA initial point and irreversibility index reduces about 25.2%. Next, pump-around is considered in the optimization, too. In the best recovery condition, 6.2%(99% recoverv increases recoverv) comparing to SA initial point and irreversibility index increases greatly. At the best irreversibility index, recovery reduction is 16.5% (77% recovery) comparing to SA initial point, but reduction in irreversibility index is 21%.

As the results show, using pump-around, if recovery is desired, is not reasonable from Irreversibility Index point of view. But without using pump-around, we can obtain a very good recovery and reducing Irreversibility Index at the same time.

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